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Aberration Corrected Photoemission Electron Microscopy with Photonics Applications

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Aberration Corrected Photoemission Electron
Microscopy with Photonics Applications

by

Joseph P. S. Fitzgerald

A dissertation submitted in partial fulfillment of the
requirements for the degree of

Doctor of Philosophy
in
Applied Physics

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Abstract

Photoemission electron microscopy (PEEM) uses photoelectrons excited from material surfaces by incident photons to probe the interaction of light with surfaces with nanometer-scale resolution. The point resolution of PEEM images is strongly limited by spherical and chromatic aberration. Image aberrations primarily originate from the acceleration of photoelectrons and imaging with the objective lens and vary strongly in magnitude with specimen emission characteristics. Spherical and chromatic aberration can be corrected with an electrostatic mirror, and here I develop a triode mirror with hyperbolic geometry that has two adjacent, field-adjustable regions. I present analytic and numerical models of the mirror and show that the optical properties agree to within a few percent. When this mirror is coupled with an electron lens, it can provide a large dynamic range of correction and the coefficients of spherical and chromatic aberration can be varied independently. I report on efforts to realize a triode mirror corrector, including design, characterization, and alignment in our microscope at Portland State University (PSU). PEEM may be used to investigate optically active nanostructures, and we show that photoelectron emission yields can be identified with diffraction, surface plasmons, and dielectric waveguiding. Furthermore, we find that photoelectron micrographs of nanostructured metal and dielectric structures correlate with electromagnetic field calculations. We conclude that photoemission is highly spatially sensitive to the electromagnetic field intensity, allowing the direct visualization of the interaction of light with material surfaces at nanometer scales and over a wide range of incident light frequencies.

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I Introduction

Photoemission electron microscopy (PEEM) has long been an invaluable tool in investigating physics at the surfaces of materials. PEEM has played an intrinsic and diverse role in high resolution microscopy, from pioneering work in early electron microscopy [1] to understanding biological proteins [2, 3], magnetic domains [4–7], and recent studies of plasmonic structures [8–48]. PEEM has had such wide-ranging impact due to a simple and versatile apparatus, relatively intuitive image interpretation, and an extensive breadth of accessible phenomena, with different photon energies highlighting different material processes and structures.

In photoemission, an electron can be excited with a single UV or higher energy photon or with multiple (n) lower energy photons, where the number of photons satisfies the energy requirement $n \times (hc/\lambda) > W$, and W is the photoemission threshold energy at the surface [49, 50]. The quantum efficiency of photoemission with photons above the photoemission threshold is $\sim 10^{-4}$ [51]. At longer wavelengths, the probability decreases with the power of n , necessitating high electromagnetic field intensities for visible and infrared excitation photons. Photoelectrons are excited with little excess energy, and primarily unscattered photoelectrons are emitted to the vacuum [52], limiting the emission depth to less than a nanometer in most cases [53]. Spatially varying photoemission rates are indicative of the underlying surface structures and processes, revealing surface topology, material and threshold differences, electron densities, electromagnetic interactions, as well as other contrasts, with the dominant process often varying strongly with incident photon energy [8, 54–56]. With such a wide variety of influences, the spatial and spectral distributions of photoelectrons can reveal significant information about the surface environment.

Photoemission electron microscopy is concerned with the spatial distribution of the photoelectron emission yield. In PEEM, photoelectrons are accelerated away from the surface, collimating the electrons into a beam with a cross-sectional distribution preserving relative emission site locations. The beam is then focused with electron lenses, which magnifies the emission pattern, and photoelectrons register on a phosphor screen or other device to generate an image of the photoemission yield. Since electrons are used to create the image, the fundamental resolution is unaffected by the diffraction limit of the light used to illuminate the sample [54]. Instead, the electron de Broglie wavelength, the nature of the emission process, and the quality of the electron optical system set the resolution limit for PEEM. Electron lenses, which focus electrons with electric or magnetic fields, provide high magnification images but also introduce significant image aberrations that limit the maximum width of the aperture angle and the range of photoelectron energies that can be used to produce a focused image. As a result, resolution is typically worse than 20 nm. Addressing aberration with multipole lenses or a mirror could significantly improve resolution to as little as 1-3 nm [57, 58].

Using light to excite electrons, PEEM is at the intersection of light optics and electron microscopy. An intuitive application of aberration-corrected PEEM is nanoscale photonics. Here the advantages of PEEM can be used to great potential, naturally combining sensitivity to surface electromagnetic fields with the resolution of an electron microscope for visualization of light as it interacts with surfaces of photonic structures. To achieve this goal one must overcome the inherent challenges of single- and multi-photon photoemission electron microscopy: low electron emission rates and the imperfect focusing of electron lenses. This can be done by utilizing high intensity light sources and by introducing aberration correction to improve the quality of the electron images, gaining brightness, contrast, and resolution. In realizing these

targets, we increase the scope of PEEM applications by developing a tool well suited to the investigation of light at material surfaces at the smallest scales, with broad applicability to weak and strong field phenomena alike.

In the next two parts, I describe two parallel efforts to advance the optical performance of PEEM and to apply PEEM to the study of photonics. First, Part II Aberration correction investigates the resolution limit of PEEM with improved correction of spherical and chromatic aberrations. This begins with a discussion of how image aberrations arise in the acceleration and focusing of photoelectrons and the impact on micrograph point resolution. Then several models of aberration correction with a mirror are reviewed, followed by the full analytic derivation of the optical properties of a hyperbolic geometry with two variable potentials. When this triode mirror model is combined with an electron lens, aberration correction can be adjusted to match image aberrations, which vary with sample emission characteristics. Subsequently, I describe the optimization and characterization of a design of the triode mirror and lens corrector specifically tailored to our PEEM, replacing the previous diode-based corrector, as well as initial alignment efforts. Second, Part III Photonics explores the relationship between photoelectron emission and optical excitations in the surface near-field. This begins with an outline of the photoemission process and a basic theory relating the surface electromagnetic field intensity and the photoelectron yield. Then I relate the theory to experiments, starting with metals and high-optical-intensity, plasmon-enhanced photoemission and progressing to the optically weaker phenomena of diffraction and dielectric waveguides. Throughout, the incident light wavelength, intensity, and polarization play critical roles as the primary variables of investigation of the photoemission response.

II Aberration correction

1 Electron optics and image resolution

The smallest feature that can be resolved by a traditional optical microscope is determined by the wavelength and aperture angle of the imaging beam

$$R_d = 0.61\lambda / \sin \alpha_{\max}, \quad (1.1)$$

where R_d is the spatial resolution, λ is the wavelength of the imaging beam, and $\alpha_{\max}$ is the aperture angle of the lens [59]. In electron microscopy, the wavelength is determined by the de Broglie relation for electrons $\lambda = h/p$, where h is Planck's constant and p is the electron momentum. In terms of the electron kinetic energy $E = eV_a$ the wavelength is

$$\lambda = hc / \sqrt{E^2 + 2E \cdot m_e c^2}, \quad (1.2)$$

where e and m_e are the charge and rest mass of an electron, and c is the speed of light. The energy of electrons used in PEEM is primarily set by the potential difference between the sample held at the $V_a = -V_C$ and a grounded anode a distance ℓ_a away, as illustrated in Fig. 1.1. For the 20 kV potential difference used in our instrument, the wavelength of electrons is 0.0086 nm. The accelerating field and anode aperture collimates emitted electrons into a beam with angular width

$$\alpha_{\max} = \sqrt{V_e/V_a}, \quad (1.3)$$

Figure 1.1: (a) Trajectories of electrons emitted from a point on the axis showing the curved paths in the accelerating region and the diverging action of the aperture lens. Radial distances have been exaggerated. Adapted from Rempfer and Griffith [57].

where eV_e is the emission energy, eV_a is the accelerating energy, and the small angle approximation is used [57]. In UV and multiphoton PEEM, the electrons are emitted with less energy than the photoemission threshold. For example, 1 eV photoelectrons accelerated to 20 keV, as in our PEEM, have an aperture angle of 7 mrad or 0.4° . Taking the electron wavelength and aperture angle into account, the resolution of a photoelectron micrograph composed of electrons emitted at 1 eV and accelerated to 20 kV is 0.75 nm when considering electron diffraction alone.

However, PEEM is far from realizing the resolution inherent to the electron beam. Electron lenses, which focus electrons with electric or magnetic fields, introduce image aberrations that reduce the quality of images. In an electron beam with a range of emission angles, the point resolution is determined not only by the diffraction limit, Eq. 1.1, but also by spherical aberration,

$$R_s = C_s \alpha_{\max}^3, \quad (1.4)$$

where C_s is the coefficient of spherical aberration. Using simple trigonometry and the

small angle approximation, the coefficient can be defined by its effect on the image distance,

$$z'_0 - z' = C_s \alpha^2, \quad (1.5)$$

where z' is the image distance of an electron trajectory originating from an object with angle α to the optical axis, and $z'_0 = \lim_{\alpha \rightarrow 0} z'$ is the paraxial image distance. A range of emission energies eV_e similarly produces a point resolution governed by chromatic aberration,

$$R_c = C_c (\Delta E / \langle E \rangle) \alpha_{\max}, \quad (1.6)$$

where $\langle E \rangle = e(\langle V_e \rangle + V_a)$ is the mean electron energy, $\Delta E = E - \langle E \rangle$ is the difference in energy from the mean, and C_c is the coefficient of chromatic aberration. This coefficient too can be defined along the optical axis,

$$z'_0 - \langle z'_0 \rangle = C_c (\Delta E / \langle E \rangle), \quad (1.7)$$

where $\langle z'_0 \rangle$ is the paraxial image distance of the mean electron energy. Imaging errors due to lens aberrations combine with diffraction, limiting the point resolution to approximately

$$R^2 = R_d^2 + (R_s/4)^2 + (R_c/2)^2. \quad (1.8)$$

The factors of $1/4$ and $1/2$ reflect that the aberration is evaluated not at the Gaussian plane, where Eqs. (1.4)–(1.7) are defined, but at the circles of least confusion optimized for spherical and chromatic aberration separately [60]. The axial locations of the spherical and chromatic circles of least confusion are generally not coincident, so the prefactors will typically be different than those given here. Nonetheless, Eq. 1.8 provides a simple and reasonably accurate estimate of resolution that compares favorably with more complicated methods [61].

Equations 1.5 and 1.7 represent the lowest order relationship of focus plane deviations with changes in ray image angle and energy. Higher order coefficients are possible with deviations proportional to α^{2n-1} or $\alpha^{2n-1}(\Delta E/E)^m$, where $m, n \in \text{natural numbers}$. When including these coefficients it is common to denote C_s as C_3 ; then higher order spherical aberration coefficients are C_5 (for the α^5 term), C_7 (α^7 term), etc., and higher order chromatic coefficients are C_{3c} (for the $\alpha^3 \Delta E/E$ term), C_{cc} (for the $\alpha(\Delta E/E)^2$ term), etc. These terms become increasingly important at wider aperture angles, with wider energy spectra, or at very high spatial resolution. Higher order terms are explicitly compensated in aberration corrected TEMs, which can resolve single atoms in a lattice spaced less than 0.1 nm apart [62, 63], but are neglected in this discussion. With a normal distribution of emission energies spread out over $\Delta E = 1$ eV, typical aberration coefficients in the range $C_s \approx C_c \approx 0.4$ m [64], and at an optimally limited aperture angle of 0.7 mrad, this formula predicts a best resolution of 10 nm, an order of magnitude greater than the diffraction limit. Including higher order aberration terms, beam coherence, and microscope instability, which will be much greater with the reduced aperture, raises this limit to 15 nm [61], as experimentally reported by Griffith and Rempfer [65]. Clearly aberration has an effect on imaging in PEEM, so it is desirable to minimize or eliminate the magnitude of spherical and chromatic aberration in order to improve resolution. Correcting aberration also allows imaging with a larger aperture acceptance angle, which is of particular importance to multiphoton PEEM where the photoelectron yield can be quite limiting and the spectrum of emission energies can be relatively large.

With the exception of Eqs. (1.2) and (1.3), the formulae in this discussion apply equally well to electron and light microscopy. In light microscopy, methods of aberration correction were developed long ago by combining glasses with different shapes and refractive indices. Correcting the aberrations of glass lenses has developed such

that diffraction is the main limitation, and Eq. 1.1 can be used to directly estimate image resolution. However, refraction in electron optics is qualitatively different; electron trajectories change direction continuously whereas light rays do so discretely at lens surfaces. In light optics, the aberration coefficient of multiple refractions is the sum of the aberration of each individual refraction,

$$C_{\text{tot}} = \sum_j^n a_j C_j, \quad (1.9)$$

where the weighting coefficients a_j depend on changes in magnification and effective refractive index [60, 66]. For a continuous refraction, the aberration coefficients of a lens in electron optics are best expressed as integrals over the axial potential $V = V(z)$. Munro [67] gives computationally useful expressions for electrostatic lenses,

$$C_s = \frac{1}{16r_i'^4 V_C^{1/2}} \int_o^i \left\{ \left[\frac{5}{4} \left(\frac{V''}{V} \right)^2 + \frac{5}{24} \left(\frac{V'}{V} \right)^2 \right] r^2 + \frac{14}{3} \left(\frac{V'}{V} \right)^3 r' r - \frac{3}{2} \left(\frac{V'}{V} \right)^2 r'^2 r^2 V^{1/2} \right\} dz, \quad (1.10)$$

$$C_c = \frac{V_C^{1/2}}{r_i'^2} \int_o^i \left\{ \left(\frac{V'}{2V} \right) r' + \left(\frac{V''}{4V} \right) r \right\} \frac{r}{V^{1/2}} dz, \quad (1.11)$$

where z is the axial position, taken as the sole independent variable, integrated from the location of the object o to the image i ; $r = r(z)$ is the electron trajectory radial position; eV_C and r_i are the electron energy and radial position at the image; and the zero potential is chosen such that $V > 0$ for all z . Through integration by parts, the

integrands can be recast as [68]

$$C_s = \frac{1}{32V_C^{1/2}} \int_o^i \left\{ \left[\frac{V''}{V} + \frac{V'}{V} \frac{r'}{r} - \frac{5}{4} \left(\frac{V'}{V} \right)^2 \right]^2 + \frac{3}{2} \left[\frac{V''}{V} + \frac{V'}{V} \frac{r'}{r} - \left(\frac{V'}{V} \right)^2 \right] \right. \\ \left. + 2 \left(\frac{V'}{V} \right)^2 \left(\frac{r'}{r} + \frac{5}{6} \frac{V'}{V} \right)^2 + \frac{1}{36} \left(\frac{V'}{V} \right)^4 \right\} V^{1/2} r^4 dz, \quad (1.12)$$

$$C_c = \frac{3V_C^{1/2}}{8} \int_o^i \left(\frac{V'}{V} \right)^2 \frac{r^2}{V^{1/2}} dz. \quad (1.13)$$

For a derivation of these formulas, I refer the reader to any number of good textbooks [69–72], which also present formulae for magnetic lenses. The integrands in the previous formulas are a sum of squared terms, and subsequently the coefficients are positive definite. Thus, aberration in electron lenses is unavoidable: all standard electron lenses have positive spherical and chromatic aberrations. This result was originally derived for magnetic lenses by Scherzer [73]. The Scherzer theorem can be bypassed by breaking rotational symmetry (multipole lenses, cf. [74–78]), placing charge on the optical axis (mesh or foil lenses, cf. [74, 79–81]), reflecting electron trajectories so that $r(z)$ is no longer a one-to-one function (mirrors, cf. [64, 74, 82–84]), or using time-varying fields (cf. [74, 85, 86]). All of these approaches have seen recent development, though only multipole and mirror correctors have achieved notable success. Specifically, hexapole and quadrupole-octupole lenses have proven successful for correcting spherical aberration [76, 77], and more recently a system of quadrupole lenses has been employed to correct chromatic aberration [78] (though without improved resolution [87]). These systems use a sophisticated computer system to control the numerous electrode potentials and adapt aberration correction.

While spherical aberration affects all electron microscopies, PEEM, low energy electron microscopy (LEEM), and other emission or low energy electron microscopies must also deal with a relatively large range of electron energies and cannot neglect

chromatic aberration. Electrostatic mirrors can be designed with both spherical and chromatic aberration coefficients of the opposite sign to electron lenses, opening the possibility for their use as aberration correctors [73]. To obtain correction, the electron beam is incident and reflected along the same axis, necessitating a magnet to separate the two beams. Despite early troubles, as presented by Ramberg [88] and others, Rempfer [64] constructed an analytic description of electron trajectories in a diode (two-electrode) mirror with a hyperbolic field distribution and subsequently showed that such a mirror can be employed to achieve spherical and chromatic aberration correction. Indeed, electron mirrors have proven experimentally successful at correcting spherical and chromatic aberration simultaneously [82, 89–92].

The theoretical foundations of these systems are mirrors with two or four electrodes [64, 93], and success at correcting aberration is determined by the number of independent parameters and accurate determination of instrument aberration. A diode mirror is designed to simultaneously correct spherical and chromatic aberration through appropriate choices of its length, spacing from other elements, and operating potential. Choices made during the design stage confine the parameter space to a narrow path traversed by a single potential. Furthermore, the lone degree of freedom link spherical and chromatic aberration correction—they cannot be varied independently. As a result, the correction offered by the diode mirror becomes locked into one optimal potential. This situation is undesirable since aberration may not be well known in the first place, and it is also may change with operating conditions, e.g., sample positioning, surface topology, and particularly photoelectron energy distribution. A three electrode (triode) mirror could potentially address this issue by introducing a second adjustable potential. Subsequently, the triode mirror can simultaneously and independently correct spherical and chromatic aberration, although not without also changing focal length of the mirror significantly. If focal length is held constant, dy-

dynamic adjustment may be limited to a small range around an extremum in either spherical or chromatic aberration [94]. Thus, to achieve the full range of adaptive aberration correction a lens must be used in conjunction with a mirror to maintain constant focus on the beam separating magnet. This is no real problem since in practice a lens is nearly always paired with a mirror to control image distance to the beam-separating magnet and to set magnification. An interactive triode mirror and lens corrector involves three variable electrode potentials. Alternatively, these elements can be built into a single, four-electrode (tetraode) mirror. This device has been studied numerically [90, 93, 95] and successfully incorporated into a LEEM for record resolution [91, 92], though PEEM resolution was not particularly improved. It was found that three adjustable potentials made possible simultaneous, independent, and dynamic manipulation of all three optical properties, z_0 , C_s , and C_c .

However, without an analytic form of the electron trajectories and subsequently derived optical properties to inform design, it is difficult to develop physical intuition for the correcting behavior and the device cannot be readily optimized for other instruments. Without physical insight, the mirror will be difficult to operate; and without optimization capability, it may be difficult to adapt the aberration corrector to other instruments. Therefore I propose to a similar mirror-based corrector incorporating three adjustable electrode potentials, to give fully adaptable correction of spherical and chromatic aberration, but rooted in an analytic description that lends itself to optimization so that it can be used to improve upon an existing microscope. A firm analytic foundation can be found in the mirror described by Rempfer [64], which serves as a starting point here. In the following chapters, I begin with a description of electron optical aberration in PEEM, particularly that of the cathode and objective lens. I then discuss the correction scheme currently implemented in our PEEM. Subsequently, I introduce a compound, three-variable electrostatic mirror based on

two hyperbolic fields and demonstrate its potential for providing adaptive aberration correction. Then I discuss the design, testing, and implementation of the mirror corrector, which requires high-precision control of the PEEM, with work currently in progress.

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2 Resolution before aberration correction

Several types of aberration potentially degrade image resolution [66], of which defocus, astigmatism, coma, and distortion can be corrected in electron microscopes. In UV and multiphoton PEEM, the next most severe aberrations are chromatic and spherical aberration of the accelerating field and the spherical aberration of the objective lens [57]. The aberrations of the accelerating field result from variations in image location with photoelectron emission angle, $\Delta_s z' = (z' - z'_0)_{\text{const } E}$, and emission energy, $\Delta_c z'_0 = z'_0 - \langle z'_0 \rangle_E$. From Rempfer and Griffith [57], the virtual image is located a distance

$$z'_a = 2\ell_a \left(1 - \sqrt{V_e/V_a}\right) \cos \alpha_e \quad (2.1)$$

behind the anode plane (Fig. 1.1 and 2.1), where α_e is the photoelectron emission angle from a flat specimen surface relative to normal. Equation (1.3) gives the maximum angle when the beam is not limited by an aperture stop. At emission angles $\alpha_e \leq \pi/2$, the trajectory angle after acceleration α_a varies with both emission energy and emission angle,

$$\alpha_a = \sqrt{V_e/V_a} \sin \alpha_e. \quad (2.2)$$

The paraxial image location is

$$z'_{a,0} = 2\ell_a \left(1 - \sqrt{V_e/V_a}\right). \quad (2.3)$$

The leading order difference between the image distance and its paraxial limit gives the spherical aberration coefficient

$$C_{s,a} = \ell \sqrt{V_a/V_e} \quad (2.4)$$

Figure 2.1: Detail showing a trajectory and a tangent ray defining the position of the virtual specimen before and after deflection by the anode aperture at the distances $z'_a \approx 2\ell_a$ and $z' \approx 4\ell_a/3$ from the anode. The aperture deflection forms an image with magnification $2/3$ relative to the accelerating field image. The initial, intermediate, and final tangents make angles α_e , α_a , and α' with the axis, respectively. Adapted from Rempfer and Griffith [57].

at a particular emission energy eV_e . The chromatic aberration coefficient is evaluated directly from Eq. 1.7. Plots of $z'_{a,0}$, α_a , and C_s are given in Fig. 2.2. The aperture angle, aberration coefficients, and point resolution can be calculated from these formulas and the axial aberration coefficient definitions. Mean values are obtained by averaging over the photoelectron energy distribution. For example, with UV emission from Cu at 257 nm, the photoelectron beam mean aperture angle is 5 mrad, the mean spherical and chromatic aberration coefficients of 810 mm and 800 mm, respectively, and the estimated point resolution of 28 nm. Similar calculations for the photoelectron spectra in Fig. 2.3 are summarized in Table 2.1. The anode aperture deflects electron trajectories further from the optical axis, forming a demagnified image a distance $z'_0 = 4\ell_a/3$ from the anode plane, as illustrated in Fig. 1.1. The lateral magnification of the image is $m_a = 2/3$, such that a ray exiting the aperture makes an angle with the axis of $\alpha' = 3\alpha_a/2$. This deflection does not contribute significantly to the aberration [57].

The virtual image produced by the accelerating field and anode aperture serves

Figure 2.2: (a) The paraxial image distance of photoelectrons accelerated by a $V_a = 20$ kV potential as a function of emission energy V_e in units of cathode-anode spacing ℓ_a . (b) The trajectory angle of photoelectrons emitted at the angle α_e with energy V_e , as indicated by the contour labels, and accelerated to 20 kV. (c) The spherical aberration coefficient of 20 kV photoelectrons.

Figure 2.3: Photoelectron spectra of (a) silver and (b) copper. Photon energies are 0.3 eV, for Cu 1- and 3-PPE, and 1.7-2 eV for others in excess of the material photoemission threshold, which is 4.5 eV for Cu and 4.3 for Ag. Statistical properties of the spectra, (c) the mean emission energy $\langle eV_e \rangle$ and (d) distribution width σ_e , are plotted against the excess energy. Adapted from Refs. [96–98].

Material	$n\mathbf{PPE}$	λ (nm)	$\langle\alpha_a\rangle$ (mrad)	$\langle C_s\rangle$ (m)	$\langle C_c\rangle$ (m)
Ag	1	207	8.0	0.5	0.5
Ag	2	400	7.0	0.6	0.6
Cu	1	257	5.0	0.8	0.8
Cu	2	385	6.5	0.7	0.6
Cu	3	770	3.5	1.3	1.2

(a)

Mat/$n\mathbf{P}$	$\langle R_d\rangle$ (nm)	$\langle R_s/4\rangle$ (nm)	$\langle R_c/2\rangle$ (nm)	$\langle R\rangle$ (nm)
Ag/1	0.7	63	44	79
Ag/2	0.8	48	27	58
Cu/1	1.1	26	10	28
Cu/2	0.9	47	46	68
Cu/3	1.7	13	13	20

(b)

Table 2.1: Aperture angles, aberration coefficients, mean point resolution contributions, and total point resolution of the photoelectron spectra given in Fig. 2.3. The brackets denote the mean emission energy value, $\langle x \rangle = \int x \rho(E) dE$, where ρ is the normalized photoelectron energy distribution.

as the object of the objective lens. The aberration of the objective lens image is

$$\Delta z'_o = (1 + m_o^2) \Delta g_o + 2m_o \Delta f_o + m_o^2 \Delta z, \quad (2.5)$$

where $m_o = \alpha'/\alpha'_o = m_a \alpha_a/\alpha'_o$ is the paraxial magnification of the objective lens, Δg_o and Δf_o are the variations in the focal point distance g_o and focal length f_o with angle and energy, and Δz is the aberration of the accelerating field, i.e., $\Delta z = z'_a - \langle z'_{0,a} \rangle$. Definitions of the focal point distance g and focal length f are illustrated in Fig. 2.4. The focal variations are of the lens at a particular potential V_o/V_C can be measured experimentally, as in Rempfer [60], or computed using suitable software. The properties of the objective lens in our PEEM are shown in Fig. 2.5, as computed using SIMION [100]. The aberration coefficients given in Fig. 2.5 are related to the

Figure 2.4: The focal properties of a lens are illustrated for a ray parallel incidence ray. The gray region denotes the refracting zone of the electron lens where values of the electric or magnetic field are non-zero. The focal properties of the lens are symmetric about the reference plane. The principle surfaces, marked H and H' , are positioned and curved in a way typical of electron lenses (though atypical in light microscopy). f and g are sufficient to describe this curvature, and change with the field strength of the lens. Adapted from Rempfer [60].

previously defined image aberration coefficients by

$$C_s = - \left[(1 + m^{-2}) S_g + 2m^{-1} S_f \right] (1 + m^{-1})^2 f, \quad (2.6)$$

and

$$C_c = \left[(1 + m^{-2}) C_g + 2m^{-1} C_f \right] f. \quad (2.7)$$

The unitless aberration coefficients— S_f and S_g for spherical aberration, C_f and C_g for chromatic aberration—do not depend on magnification. The relationship between the unitless coefficients and the image coefficients is derived from the Newtonian relations

$$(z' - g) / f = m = f / (z - g) \quad (2.8)$$

and the variations in focal point distance and length, given by Rempfer [60]. Re-

Figure 2.5: The objective lens used in our PEEM. (a) A diagram of the objective lens in cross-section, which is of the swept-back design of Rempfer with a central bore diameter of 6.71 mm [99]. The cathode, shown in gold on left, is a distance 3.95 mm from the front of the objective lens. A potential V_o is applied between the grounded outer electrodes (orange) and center electrode (blue). (b) The objective lens focal length and point distance, f and g , as a function of potential V_o . (c) The spherical aberration coefficients; and (d) the chromatic aberration coefficients. The properties scale with the cathode potential V_C , so they are plotted on a scale of V_o/V_C . These properties were computed using SIMION and formulae from Rempfer [60].

ferred back to the virtual specimen space at unit magnification, the resolution limit contribution due to spherical aberration is

$$R_{s,o} = \left(C_{s,a} + C_{s,o} m_a^{-4} \right) \alpha_a^3, \quad (2.9)$$

and that due to chromatic aberration is

$$R_{c,o} = \left(C_{c,a} + C_{c,o} m_a^{-2} \right) (\Delta E / \langle E \rangle) \alpha_a. \quad (2.10)$$

An aperture stop is positioned between the exit aperture and image of the objective lens. The aperture stop is a 30 μm diaphragm located at $z_{ap} \approx 18$ mm from the center of the lens. At this position, the radius of the electron beam is

$$r_{ap,\max} = (z'_o - z_{ap}) \tan \left(\alpha_a m_a^{-1} m_o^{-1} \right), \quad (2.11)$$

where

$$z'_o = g_o + f_o^2 (z_o - g_o)^{-1}, \quad (2.12)$$

$$m_o = f_o (z_o - g_o)^{-1}, \quad (2.13)$$

and $z_o = z' + \overline{OA}$ is the distance between the image of the anode aperture image and the center of the objective lens with $\overline{OA}$ representing the distance between the front of the anode and the center of the lens. The aperture stop limits the beam waist, effectively reducing the range of photoelectron emission angles and energies, as shown in Fig. 2.6. Limiting the beam can significantly improve resolution by decreasing the magnitude of image aberrations, though with some penalty in increased electron diffraction and decreased luminosity. The image resolutions of a 30- μm aperture stop

Figure 2.6: An aperture stop in the rear focal plane of the objective lens limits the photoelectron aperture angle and range of energies. Contours trace the maximum acceptance angle as a function of emission energy. The aperture stop used in our PEEM is 30 μm .

for some realistic photoelectron energy distributions are given in Table 2.2. Notice that using the aperture stop improves point resolution estimates by more than an order of magnitude when the objective lens aberrations are included. This is primarily due to a reduction in spherical aberration, which is particularly curbed for electron beams with large mean emission energies.

In our PEEM, the objective lens is zoom paired with an auxiliary lens, illustrated in Fig. 2.7 and described in Rempfer et al. [99]. The auxiliary lens decouples specimen focus from the position of the image plane. The potentials that maintain this image position for a given total image magnification $m_a m_o m_x$ are plotted in Fig. 2.8. The auxiliary lens impacts the point resolution in an analogous way to the objective, i.e.,

$$R_{s,x} = \left[C_{s,a} + C_{s,o} m_a^{-4} + C_{s,x} (m_a m_o)^{-4} \right] \alpha_a^3, \quad (2.14)$$

$$R_{c,x} = \left[C_{s,a} + C_{s,o} m_a^{-2} + C_{s,x} (m_a m_o)^{-2} \right] (\Delta E / \langle E \rangle) \alpha_a. \quad (2.15)$$

Mat/nP	$\langle \alpha_a \rangle$ (mrad)	$\langle R_d \rangle$ (nm)	$\langle R_{s,a}/4 \rangle$ (nm)	$\langle R_{c,a}/2 \rangle$ (nm)	$\langle R_a \rangle$ (nm)
Ag/1	2.4	2.2	1.9	14	14.
Ag/2	2.4	2.2	2.1	8.9	10.
Cu/1	2.3	2.3	2.6	4.6	6.1
Cu/2	2.2	2.2	2.2	16.	16.
Cu/3	2.1	2.5	3.2	7.3	8.8

(a) Cathode with aperture stop.

Material/nP	$\langle R_{s,a+o}/4 \rangle$ (nm)	$\langle R_{c,a+o}/2 \rangle$ (nm)	$\langle R_{a+o} \rangle$ (nm)
Ag/1	13	17	22
Ag/2	13	11	19
Cu/1	12.	5.3	14.
Cu/2	13.	19.	24.
Cu/3	11.	8.1	15

(b) Cathode and objective with aperture stop.

Material/nP	$\langle R_{s,a+o}/4 \rangle$ (nm)	$\langle R_{c,a+o}/2 \rangle$ (nm)	$\langle R_{a+o} \rangle$ (nm)
Ag/1	560	55	560
Ag/2	380	34	380
Cu/1	160	11	160
Cu/2	380	56	390
Cu/3	72	15	74

(c) Cathode and objective *without* aperture stop.

Table 2.2: Aperture angles, mean point resolution contributions, and total point resolution $\langle R \rangle$ of the photoelectron spectra given in Fig. 2.3. (a) Resolution of the accelerating field alone with aperture stop; compare to Table 2.1; (b) resolution of the accelerating field and objective lens operating at $0.985V_C$ with aperture stop, and (c) *without* aperture stop. The aberration coefficients of the objective lens at $0.985V_C$ are $C_{s,o} = 630$ mm and $C_{c,o} = 55$ mm, and the magnification is $m_o = 3.6\times$. These values vary slightly with potential, as seen in Fig. 2.5, which may be adjusted to improve focus.

Figure 2.7: The Auxiliary Lens shown in cross-section, used as part of a zoom-pair with the objective lens. A potential V_X is applied between the grounded outer electrodes (red) and center electrode (blue). The arrangement with the objective and aperture stop is shown in App. Appendix A.

The terms in brackets are the total aberration coefficients $C_{s,tot}$ and $C_{c,tot}$. Unlike before, however, the prefactor is much smaller since the objective lens provides a net image magnification in the range $m_a m_o \gtrsim 3$. With prefactors on the order of $(m_a m_o)^{-4} \lesssim 0.03$ and $(m_a m_o)^{-2} \lesssim 0.2$ the aberration imparted by the auxiliary lens is significantly less than that of the objective and accelerating field. The total aberration coefficients and point resolution are plotted in Fig. 2.8. The aberration coefficients and resolution are not significantly different than those of the cathode and objective lens alone, Table 2.2. Further magnifications downstream have negligibly small impact on the image resolution, with the exception of large demagnifications. Thus, the point resolution of our PEEM is effectively that of the accelerating field and the objective, e.g. Table 2.2 or Fig. 2.8.

Figure 2.8: (a) Potentials for constant magnification in the objective and auxiliary lens zoom pair. Several magnifications are possible with the arrangement in our PEEM. Sample focus changes along the contour. (b) The total aberration coefficients and (c) point resolutions of the cathode, objective, and auxiliary lenses for the magnification contours from (a) with a copper specimen at 257 nm. The total aberration coefficients and point resolutions refer to unit magnification in specimen space.

3 Aberration correction with a diode mirror

Rempfer [64] gives the first definitive indications that an electrostatic mirror can correct spherical and chromatic aberration in an electron microscope. Aberration correction in our PEEM follows the scheme outlined there and subsequently refined in Refs. [82, 89, 99, 101, 102]. A schematic diagram of our PEEM incorporating a correcting mirror is shown in Fig. 3.1. The design possesses three branches separated by magnetic beam deflectors and transfer lenses. Following an electron from photoemission to detection, these elements are:

- Branch 1 (objective), cathode and objective lenses;
- Magnetic Deflector A and right transfer lenses;
- Magnetic Deflector B/beam separator;
- Branch 2 (mirror), mirror and interface lens; the beam then returns to Magnetic Deflector B/beam separator;
- Left transfer lenses and Magnetic Deflector C;
- Branch 3 (projection), housing three projection lenses.

An innovation perhaps unique to this design, the magnetic beam separator and deflectors have small deflections and left/right deflection pairs to minimize deflection distortions, instead of the alternative magnetic prism design with right angle deflections [90–92]. The deflections are provided by simple electromagnets, making alignment significantly simpler than the prism design. Though some image stretching occurs in the plane of the deflections, there are no measurable deflection aberrations. A scale drawing of the working instrument is given in App. Appendix A.

Figure 3.1: Diagram of an aberration-corrected PEEM with a Rempfer-type mirror. A detailed scale drawing of our PEEM is given in App. Appendix A. See text for description. Adapted from Rempfer et al. [82].

3.1 Analytic model of a hyperbolic diode mirror

The diode mirror design by Rempfer [64] is based upon a cylindrically symmetric hyperbolic field created between two infinite-radius, contour-conforming electrodes, as in Fig. 3.2. Between the electrodes is charge-free space, where the electric potential $V(\mathbf{x})$ is governed by Laplace's equation, $\nabla^2 V = 0$. Setting the slope of the asymptotic electrode to $2^{-1/2}$ gives the exact solution

$$V(r, z) = V_M + k(z^2 - r^2/2), \quad (3.1)$$

where $k = (V_A - V_M)/\ell^2$ and ℓ is the distance from vertex to terminating electrode, held at potentials V_M and V_A , respectively. Due to this compact analytic description and solution to Laplace's equation, hyperbolic mirrors and lenses of this form have long been a favorite design in electron optics, particularly before the widespread availability of numerical methods [64, 103, 104].

Figure 3.2: Theoretical model of the diode hyperbolic electron mirror. The mirror has cylindrical symmetry about the z -axis with $z = 0$ at the cone vertex. The electric potentials V_M and V_A are applied to the mirror and terminating (here grounded) electrodes, respectively. The distance from the vertex to the opening of the aperture is ℓ . A small aperture in the terminating electrode allows electrons to enter and exit the mirror field. Adapted from Rempfer [64].

The equations of motion for an electron in such a hyperbolic potential are

$$\frac{d^2 r}{dt^2} = \frac{e}{m} \frac{\partial V}{\partial r} = -\frac{ek}{m} r, \quad (3.2)$$

$$\frac{d^2 z}{dt^2} = \frac{e}{m} \frac{\partial V}{\partial z} = 2\frac{ek}{m} z, \quad (3.3)$$

where e and m are the charge and mass of an electron, and r and z describe the particle trajectory at a given time t [64, 69]. The general solutions for the position and velocity of the electron are

$$r = r_0 \cos(\theta - \phi) / \cos \phi, \quad (3.4)$$

$$z = z_0 \cosh(2^{1/2}\theta - \psi) / \cosh \psi, \quad (3.5)$$

$$\dot{r} = -\omega r_0 \sin(\theta - \phi) / \cos \phi, \quad (3.6)$$

$$\dot{z} = 2^{1/2}\omega z_0 \sinh(2^{1/2}\theta - \psi) / \cosh \psi; \quad (3.7)$$

where $\theta = \omega t$, $\omega = (ek/m)^{1/2}$,

$$\tan \phi = \dot{r}_0 / \omega r_0, \quad (3.8)$$

$$\tanh \psi = -\dot{z} / 2^{1/2}\omega z_0; \quad (3.9)$$

and the subscript “0” denotes initial values at time $t = 0$. Expressions for the optical properties of a diode mirror can be fully derived from this description of the electron trajectories combined with the deflecting action of the aperture.

As previously discussed, an aberration-correcting electron mirror is operated in a symmetric mode, with ingoing and outgoing electron trajectories tracing approximately the same path along the optical axis and a magnet separating incident and reflected beams. In this case a returning electron retraces the path of the incident electron, with equal amounts of spherical and chromatic aberration accumulating along each arm of the trajectory. Thus, it is only necessary to follow one half of the trajectory, and here I follow the return path starting with the reflection point (r_C, z_C) where the velocity components are zero. Choosing $t = 0$ at this point, the boundary condition parameters are also $\varphi = \psi = 0$, and the trajectory description simplifies to

$$r = r_C \cos \theta, \quad (3.10)$$

$$z = z_C \cosh 2^{1/2} \theta, \quad (3.11)$$

$$\dot{r} = -\omega r_C \sin \theta, \quad (3.12)$$

$$\dot{z} = 2^{1/2} \omega z_C \sinh 2^{1/2} \theta. \quad (3.13)$$

The maximum penetration of electrons into the mirror field coincides with the equipotential equal to the electron accelerating potential V_C . Points (r_C, z_C) on this reflecting equipotential fall on the hyperbolic contour

$$\ell^2(V_C - V_M)/(V_A - V_M) = z_C^2 - r_C^2/2. \quad (3.14)$$

The returning electron reaches the terminating electrode at time $t_A = \theta_A/\omega$ and at

the coordinates (r_A, z_A) , which lie on the hyperbolic contour

$$\ell^2 = z_A^2 - r_A^2/2. \quad (3.15)$$

The slope of the electron trajectory at this point is

$$\tan \alpha_A = -\dot{r}_A/\dot{z}_A = -\frac{r_A \tan \theta_A}{2^{1/2} z_A \tanh 2^{1/2} \theta_A}. \quad (3.16)$$

As the electron exits the hyperbolic field, it is deflected by the exit aperture through angle δ_A . The Davisson-Calbick approximation, gives the aperture focal length [105], $f_A = -4(V_A - V_C)/(2kz_A)$, which leads to a deflection of

$$\tan \delta_A = r_A/f_A = -\frac{r_A z_A k}{2(V_A - V_C)}. \quad (3.17)$$

Subsequently, the electron travels through field-free space, crossing the optical axis at the location

$$z' = z_A + r_A/\tan(\alpha_A + \delta_A). \quad (3.18)$$

In the absence of aberration, the distance from the axis crossing to the mirror vertex is the paraxial object/image distance

$$z_0 = \ell(1 + 1/q_0), \quad (3.19)$$

where

$$q_0 = \frac{\tan \theta_A^{(0)}}{2^{1/2} \tanh 2^{1/2} \theta_A^{(0)}} - \frac{V_A - V_M}{2(V_A - V_C)}, \quad (3.20)$$

and

$$2^{1/2} \tanh \theta_A^{(0)} = \left(\frac{V_A - V_C}{V_A - V_M} \right)^{1/2}. \quad (3.21)$$

The time constant $\theta_A^{(0)}$ is the paraxial approximation of θ_A , found by taking the limits $r_C \rightarrow 0$ and $r_A \rightarrow 0$ in the contour Eqs. (3.10-3.15). The spherical aberration coefficient is found from the variation of image distance with approach angle $\alpha' = \alpha_A + \delta_A$, using a modified version of Eq. (1.5),

$$C_s = -2 \left(z^{(1)} - z_0 \right) / \alpha^2, \quad (3.22)$$

where $z^{(1)}$ is the first order correction to z_0 , and the doubling is due to the path being traversed twice (in and out). Similarly, the coefficient of chromatic aberration is found from a modified version of Eq. (1.7),

$$C_c = 2V_C \frac{\partial z_0}{\partial V_C}, \quad (3.23)$$

where V_C is the accelerating potential of the electron, and thus related to its energy $-eV_C$. These three optical properties, z_0 , C_s , and C_c , fully characterize the diode mirror, determining the aberration correction it provides and how to interface with it. A parametric plot of the three properties is shown in Fig. 3.3, where the mirror potential difference $V_A - V_M$ is the independent variable.

3.2 Aberration correction applied to our PEEM

The mirror properties scale with the physical length of the mirror, so to some extent the aberration correction provided by the mirror can be arbitrarily scaled. However, the aberration coefficient ratio C_c/C_s is a unique function of mirror potential, as

Figure 3.3: Parametric plot of the optical properties of the diode hyperbolic mirror as a function of the potential difference $V_M - V_A$. Since the properties scale with mirror length, they are plotted in units of mirror length. Adapted from Rempfer [64].

Figure 3.4: Parametric plot of the diode mirror aberration coefficient ratio versus the object/image location as a function of the potential difference $V_A - V_M$. Adapted from Rempfer [64].

shown in Fig. 3.4. This ratio must be matched to that of the instrument, deciding the operating potential of the diode mirror as well as the distance from mirror vertex to the beam axis-crossing point, z_0/ℓ . This is accomplished in our PEEM with a mirror length of $\ell = 25.4$ mm and a lens-mirror spacing of ~ 44 mm, as seen in App. Appendix A. The transfer lenses between magnets and the projection lenses contribute negligibly to spherical and chromatic aberration. Thus, the total aberration of the objective branch can be compared to that of the mirror. The appropriate comparison is made not in the virtual specimen space of Eqs. (2.14) and (2.15), Table 2.2, or Fig. 2.8, but rather in transfer space, where

$$C'_{s,aox} = (m_a m_o m_x)^4 C_{s,tot} \approx 1300 \text{ m}, \quad (3.24)$$

$$C'_{c,aox} = (m_a m_o m_x)^2 C_{c,tot} \approx 18 \text{ m}. \quad (3.25)$$

The aberration coefficient ratio at this stage, $C'_{c,aox}/C'_{s,aox} = 1/70$ is incompatible with the mirror ratio range shown in Fig. 3.4. In fact, the mirror is most compatible with the specimen space coefficients, $C_{c,aox}/C_{s,aox} = 1/3$, or perhaps an even larger ratio close to unity. Reducing image magnification before correcting aberration with the mirror can accomplish this since the ratio scales with m^{-2} . Consequently, instead of acting as a simple transfer lens, the lens interfacing the mirror with the beam separator (magnet B) should be run at magnification $m_I^{-1} \gtrsim 5$. As such, the aberration intrinsic to the interface lens becomes appreciable, and the condition for an aberration free image is

$$C_{sM} + 2C_{sI} + m_2^4 C'_{s,aox} = 0, \quad (3.26)$$

$$C_{cM} + 2C_{cI} + m_2^2 C'_{c,aox} = 0 \quad (3.27)$$

where C_{sI} and C_{cI} are the interface lens aberration coefficients with reference to the mirror side.

Given a particular objective branch lens aberration, the correction the mirror offers can be adjusted through the magnification of the interface lens m_I , the length of the mirror ℓ , and the operating potential difference $V_A - V_M$. This is a sufficiently independent set of variables to address the three optical properties z_0 , C_{sM} , and C_{cM} . Two of these variables are locked in once the microscope is assembled, the length of the mirror and the magnification of the lens, which is primarily determined by positioning. This leaves only one variable available for dynamic refinements, the potential difference $V_A - V_M$. To be clear, changes in the mirror voltage must also be accompanied by a change in lens magnification, but these variables are not independent. Subsequently, the system becomes overdetermined, i.e., it is impossible to improve aberration correction with a single variable. Unfortunately, this situation leads to less than optimal aberration correction for all specimens, as illustrated in Fig. (3.5). To expand the correctable range of aberration coefficient and furthermore introduce independent control C_s and C_c I introduce a third electrode to the mirror design, as discussed in the next chapter.

Figure 3.5: The aberration coefficients of the mirror branch (dark gray) and the objective branch with magnifications 4–7 $\times$ compared in transfer space for Cu illuminated with 257 nm light. The mirror and lens overcorrect the objective branch chromatic aberration in this case, i.e., not only eliminate aberration but adding some of the opposite sign. Because the diode cannot be easily adjusted, not all specimens can have optimal aberration correction.

4 Dynamic aberration correction with a triode mirror

As a result of the previous chapter's discussion, I propose that a mirror-based aberration corrector with independently and dynamically variable spherical and chromatic aberration correction may be possible with a hyperbolic mirror foundation. To provide fully independent control of the correcting spherical and chromatic aberration coefficients requires three variable potentials. In our design this is done with two in the mirror and a third in the adjoining interface lens. In addition, the ideal corrector design incorporates closed form analytic expressions of the electron trajectories and their corresponding optical parameters, the image position and the aberration coefficients. Ultimately, an analytic expression will not be able to capture all of the nuances of real electron optical devices, and the final form of the corrector will be described by a numerical model. However, even approximate or idealized analytic expressions can lend significant physical intuition and guide design optimization. The new aberration corrector must also be able to work within our PEEM since it would be completely impractical to build a new microscope column to house the corrector. This puts space limitations of the arrangement of elements within the aberration correcting system. Three approaches to this problem immediately come to mind, which balance the number of lenses with the number of electrodes in the mirror.

A distinguishing characteristic of the diode mirror solution is the separation between the microscope and the mirror via an interfacing lens. The lens accommodates small changes in the spacing between the mirror and the beam separator and provides the high image magnification change necessary for the mirror correction to operate properly. An interface lens provides more intuitive operation by partitioning demagnification and alignment from aberration correction. A minimal accommodation for

a third variable is a secondary lens coupled with the interface lens. Together, the two lenses act as a zoom pair, and with different lens aberration coefficients, they should be able to provide some range of independent spherical and chromatic aberration adjustment. Unfortunately, after surveying several available electron lenses [60], no lens satisfies the space requirements and leads to a sufficient dynamic range of aberration correction. Thus, a two-lens and diode mirror corrector is not a capable candidate, and the space between the mirror and the interface lens must accommodate additional electrodes.

The simplest approach is to extend the original diode mirror design to include a single additional electrode. It is otherwise paired with the same interface lens, and the lens potential V_I is allowed to vary to accommodate changes in z_0 and magnification. The properties of such a triode mirror can be calculated analytically, applying the general solutions to the hyperbolic potential, Eqs. (3.4-3.7) if the additional electrode faces also follow hyperbolic contours. Once the properties of the triode mirror are analytically derived, the aberration correcting capabilities and dynamism of the combined triode mirror and lens system can be assessed. Alternatively, two adjustable potentials can be incorporated into a single tetrode mirror. Incorporation of all the electrodes into a single mirror reduces the possibility of optical axis misalignment. As found in the literature [93], a tetrode mirror is capable of correcting and dynamically adjusting spherical and chromatic aberration, although no analytic description of a tetrode mirror has been provided. In addition, it is still necessary to pair the tetrode mirror with a lens for alignment adjustments, as seen in one current implementation [91].

Figure 4.1: Theoretical model of the triode hyperbolic electron mirror. The mirror has cylindrical symmetry about the z -axis with $z = 0$ at the cone vertex. The voltages V_M , V_A , and V_G are on the mirror, center, and grounded/terminating electrodes. The distance from the vertex to the center electrode aperture is ℓ , and from the vertex to the grounded electrode aperture is $\mathcal{L}$. Small apertures in the center and terminating electrodes allow electrons to enter and exit both regions of the mirror field. Reprinted from Fitzgerald, Word, and Könenkamp [94].

4.1 Analytic model of hyperbolic triode mirror

In this section, I begin with a theoretical characterization of a triode hyperbolic mirror, as previously presented by Fitzgerald, Word, and Könenkamp [94, 106]. The analytic description builds on the work by Rempfer [64], matching an electron trajectory through two infinite hyperboloid regions joined by an aperture, as shown in Fig. 4.1. The new hyperbolic region exists between the diode mirror anode at $z = \ell$ and a new grounded outer electrode located at $z = \mathcal{L}$. The potential of the two regions is

$$V(r, z) = \begin{cases} k_1 (z^2 - r^2/2), & 0 < z < \ell; \\ -k_2 \mathcal{L}^2 + k_2 (z^2 - r^2/2), & \ell < z < \mathcal{L}; \end{cases} \quad (4.1)$$

where the constants k_1 and k_2 are determined from the potential differences of the inner and outer region, i.e.,

$$k_1 = (V_A - V_M)/\ell^2, \text{ and } k_2 = -V_A/(\mathcal{L}^2 - \ell^2), \quad (4.2)$$

analogous to the diode constant k , Eq. 3.1.

An electron trajectory in the region adjoining the asymptotic electrode can be treated as in the diode mirror description, Eqs. (3.10-3.17). The position and velocity at the boundary between the first and second regions are

$$r_1 = r_C \cos \theta_1; \quad (4.3)$$

$$z_1 = z_C \cosh 2^{1/2} \theta_1; \quad (4.4)$$

$$\dot{r}_1 = -[\sin(\alpha_A + \delta_A) / \sin \alpha_A] \omega_1 r_C \sin \theta_1; \quad (4.5)$$

$$\dot{z}_1 = [\cos(\alpha_A + \delta_A) / \cos \alpha_A] 2^{1/2} \omega_1 z_C \sinh 2^{1/2} \theta_1, \quad (4.6)$$

where $\omega_1 = (ek_1/m)^{1/2}$ and $\theta_1 = \omega_1 t_1$ is the time constant of the first region only. The angles α_A and δ_A are defined in Eqs. (3.16) and (3.17), respectively. The trajectory coordinates in the second region between potentials V_A and $V_G = 0$ (grounded) are given by the general solution, Eqs. (3.4-3.7), i.e.,

$$r_2 = r_1 \cos(\theta_2 - \phi_2) / \cos \phi_2; \quad (4.7)$$

$$z_2 = z_1 \cosh(2^{1/2} \theta_2 - \psi_2) / \cosh \psi_2; \quad (4.8)$$

$$\dot{r}_2 = -\omega_2 r_1 \sin(\theta_2 - \phi_2) / \cos \phi_2; \quad (4.9)$$

$$\dot{z}_2 = 2^{1/2} \omega_2 z_1 \sinh(2^{1/2} \theta_2 - \psi_2) / \cosh \psi_2, \quad (4.10)$$

where $\omega_2 = (ek_2/m)^{1/2}$, $\theta_2 = \omega_2(t_2 - t_1)$ is the time constant of the second region, and $t_2 - t_1$ is the time required for an electron to transit from the electron at potential V_A to the grounded electrode. The coordinates (r_1, z_1) and $(\dot{r}_1, \dot{z}_1)$ are the initial conditions for the second region trajectories, leading to nonzero values of parameters

φ_2 and ψ_2 ,

$$\tan \phi_2 = -[\omega_1 \sin \alpha_A / \omega_2 \sin(\alpha_A + \delta_A)] \tan \theta_1, \quad (4.11)$$

$$\tanh \phi_2 = -[\omega_1 \cos \alpha_A / \omega_2 \cos(\alpha_A + \delta_A)] \tanh 2^{1/2} \theta_1. \quad (4.12)$$

Reaching the aperture in the grounded electrode, an electron trajectory makes the angle $\tan \alpha_2 = -\dot{r}_2 / \dot{z}_2$ with the optical axis. Upon passing through the aperture, an electron is deflected by

$$\tan \delta_G = r_2 z_2 k_2 / 2V_C. \quad (4.13)$$

Finally an electron enters field-free space, crossing the optical axis at

$$z' = z_2 + r_2 / \tan(\alpha_2 + \delta_G). \quad (4.14)$$

From Eq. (4.14) the optical properties of the triode mirror, the image/object distance (z_0) and the coefficients of spherical and chromatic aberration (C_s and C_c), can be computed. This procedure is analogous to the diode description, using the formulas and method outlined in Eqs. (3.19-3.23), albeit with significantly more complicated expressions. For example, the paraxial image/object location

$$z_0 = \mathcal{L}(1 + 1/q_1), \quad (4.15)$$

where

$$q_1 = (k_2 \mathcal{L} / 2V_C) + \tan(\theta_2^{(0)} - \phi_2^{(0)}) / 2^{1/2} \tanh(2^{1/2} \theta_2^{(0)} - \psi_2^{(0)}), \quad (4.16)$$

appears superficially similar to the diode expression Eq. (3.20). However, where the diode expression required the definition of one additional parameter, the triode

expression requires five more:

$$\begin{aligned}
\cosh \left(2^{1/2} \theta_2^{(0)} - \psi_2^{(0)} \right) &= (\mathcal{L}/\ell) \cosh \psi_2^{(0)}, \\
\tan \phi_2^{(0)} &= - (k_1/k_2)^{1/2} [(\alpha_A + \delta_A)/\alpha_A]^{(0)} \tan \theta_1^{(0)}, \\
\tanh \psi_2^{(0)} &= - (k_1/k_2)^{1/2} \tanh 2^{1/2} \theta_1^{(0)}, \\
[(\alpha_A + \delta_A)/\alpha_A]^{(0)} &= 1 + (\ell^2/2) [(k_2 - k_1)/(V_C - V_A)] 2^{1/2} \tanh 2^{1/2} \theta_1^{(0)}, \\
\tanh 2^{1/2} \theta_1^{(0)} &= [(V_A - V_C)/(V_A - V_M)]^{1/2}.
\end{aligned}$$

The coefficients of spherical and chromatic aberration can be calculated from Eqs. (3.22) and (3.23), i.e.,

$$C_s = 2 \frac{z^{(1)} - z_0}{(\alpha^{(1)})^2} = 2 \lim_{\varepsilon \rightarrow 0} \left(\frac{1}{2} \frac{\partial^2 z^{(1)}}{\partial \varepsilon^2} \right) \left(\frac{\partial \alpha^{(1)}}{\partial \varepsilon} \right)^{-2}, \quad (4.17)$$

and

$$C_c = (z_0 - \mathcal{L})^2 \left(\sqrt{2} V_C \frac{\partial q_1}{\partial V_C} + \frac{\mathcal{L}^2 (V_A/V_C)}{(\mathcal{L}^2 - \ell^2)} \right). \quad (4.18)$$

$\varepsilon = r/\mathcal{L}$ is a small, unitless expansion parameter related to the maximum trajectory radial distance r_C . The (1) denotes the first-order approximation for $|\alpha| > 0$, i.e., α is assumed to be very small but non-zero; $z^{(1)}$ and $\alpha^{(1)}$ are the first-order corrections to the paraxial position and angle of the electron trajectory where it crosses the optical axis. Complete closed-form expressions are sufficiently complicated that they will not be presented here, but App. Appendix B gives explicit calculation computer codes. The results are presented in Figs. (4.2)–(4.4).

At many points in the property space the surface described by the dynamic parameters is nearly flat in two out of the three properties. In these locally flat regions the third property can be adjusted almost independently. Each dynamic surface, e.g., Fig. 4.2 or one of the surfaces in Fig. 4.4, has one point surrounded by an optimally

Figure 4.2: Parametric plots of the optical properties of the (a) diode and (b) triode hyperbolic mirrors as a function of the potential differences $V_M - V_A$ (diode and triode) and $V_A - V_G$ (triode only). The triode mirror geometric ratio is $\ell/\mathcal{L} = 0.66$. Contour lines in the surface represent constant z_0 (light gray) and constant C_s (black). Reprinted from Fitzgerald, Word, and Könenkamp [94].

Figure 4.3: Parametric plot of the (a) diode and (b) triode aberration coefficient ratio versus the z_0 as a function of the potential difference differences $V_M - V_A$ (diode and triode) and $V_A - V_G$ (triode only), where $\ell/\mathcal{L} = 0.66$. Contour lines in the surface represent constant z_0 (light gray) and constant V_A (black). Reprinted from Fitzgerald, Word, and Könenkamp [94].

Figure 4.4: The parametric surface of the triode optical properties can be adjusted with the geometric ratio $\ell/\mathcal{L}$. The ratios $\ell/\mathcal{L} = 0.3$ (dark gray) and 0.8 (light gray) are plotted here. Reprinted from Fitzgerald, Word, and Könenkamp [94].

flat region. Around that point one property can be dynamically adjusted while the other two remain fairly constant by changing V_A and V_M . The ratio $\ell/\mathcal{L}$ can be tuned to match the flat region of the dynamic surface with the desired ratio of chromatic to spherical aberration. The ability to fine tune aberration correction is the most attractive feature the triode mirror offers over the diode mirror.

A recipe for the design of a triode mirror to compensate aberration follows:

1. Only one property can be dynamically adjusted independently. This recipe considers C_c as the dynamic property, and consider C_s and z_0 as (ideally) constant.
2. Minimize the change in C_s and z_0 compared to the change in C_c in a region around the desired ratio of aberration coefficients and on a surface of constant $\ell/\mathcal{L}$.

- (a) The property functions in parameter space are nonlinear with many local extrema, so there may be many good optimization methods. One method is to minimize the angle θ between the voltage gradients of C_s and z_0 , where

$\sin \theta \propto -(\partial z_0 / \partial V_M) (\partial C_s / \partial V_A) + (\partial z_0 / \partial V_A) (\partial C_s / \partial V_M)$. This identifies points where constant contours of C_s and z_0 are the most parallel. These points can then be narrowed down by their aberration ratio and the curvature of the surface at that point.

- (b) It may be necessary to consider the physical dimensions of the mirror during the minimization to limit the ranges of $C_s/\mathcal{L}$ and $C_c/\mathcal{L}$.
  - (c) This minimization gives a best parameter configuration $(V_M/V_C, V_A/V_C, \ell/\mathcal{L})$ around which changes in voltage leave the object/image distance and the spherical aberration relatively constant. This fixes $\ell/\mathcal{L}$ and $z_0/\mathcal{L}$, and establishes a relationship between V_M and V_A for which the z_0 does not change.
  - (d) A survey shows that the function $V_M = f(V_A)$ that maintains constant z_0 is often linear throughout the tuning range and that the mirror is not highly sensitive to changes in $\ell/\mathcal{L}$, as shown in Fig. 4.4.
3. Next specify the length of the mirror $\mathcal{L}$ so that its value of C_s matches that of the lens system. This will also set z_0 .
  4. Design the hyperbolic triode mirror with geometry $\ell/\mathcal{L}$ to length $\mathcal{L}$. The mirror should be positioned in the microscope such that paraxial object/image distance z_0 is tuned for the next element, similar to the location of the diode mirror.
  5. Run the mirror electrodes at the potentials V_M and V_A , as set by Step 2. This will provide aberration correction at the set aberration ratio. Change the potentials V_M and V_A according to a relationship that maintains z_0 to adjust the chromatic aberration compensation as needed. Assuming small changes in potential, this will have minimal effect on the spherical aberration compensation.

Figure 4.5: Aberration coefficients of a triode mirror for fixed $\ell/\mathcal{L}$ and object/image distance $z_0/\mathcal{L}$. (a) The relationship between spherical and chromatic aberration once the object/image distance is fixed. Each curve is labeled by its value of $z_0/\mathcal{L}$. (b) The parametric dependence on (V_A, V_M) for $z_0/\mathcal{L} = 1.05$, where the arrows point in the direction of increasing value. Also displayed are the dynamic adaptive aberration ranges for 1% variation in the other coefficient of aberration.

While this recipe describes dynamic chromatic aberration correction, slight procedural modifications would produce dynamic spherical aberration compensation or dynamic alignment control (touch up in z_0). Excluding extreme parameter values, Fig. 4.5 shows that a range of $0.2 < C_c/C_s < 4$ is very realistic, which is almost three times the range of the diode mirror. A survey of aberration ratios between 0.2 and 4 showed that a nominal 10% tuning range is possible for tuning in either C_c or C_s for less than 1% variation in the other property and constant z_0 . By design, a triode mirror cannot dynamically adjust the correction values of *both* spherical and chromatic aberration without changing the focal length of the mirror. In essence, there are three properties (z_0 , C_s , or C_c) and only two variables (V_A and V_M); it is this underspecification which limits the adaptability of the triode mirror. With the introduction of a third dynamic

Figure 4.6: Model of the triode mirror used for numerical simulation. The electric potential distribution was determined by SIMION, with widely-spaced equipotentials between electrodes ($0.05V_C$ spacing), finer spacing ($0.005V_C$) near the apertures, and a dark equipotential highlighting the reflecting surface (at V_C). Reprinted from Fitzgerald, Word, and Könenkamp [94].

variable, i.e. the interface lens, an aberration-correcting system should be able to match any combination of the three properties over a wide range.

4.2 Comparison to realistic model

A realistic electron mirror can not have infinite radial extent nor infinitely thin apertures, as implied in the Davisson-Calbick formula, two major assumptions of the analytic model. The deviations from these approximations in a realistic mirror can be understood qualitatively and the scale of their impact can be calculated. The electron optical properties of a realistic geometry, shown in Fig. 4.6, are calculated using SIMION [100].

In a mirror without infinite radial extent, such as the one shown in Fig. 4.6, the potential distribution is only approximately hyperbolic near the optical axis. Define D as the diameter of the mirror. The near-axis difference between the analytic and realistic potential distributions increases roughly as (ℓ/D) and (d/D) , where ℓ

is the distance between the mirror and center electrodes, and d is the maximum diameter of the electron beam. Additional elements, such as the cylindrical ring on the mirror electrode in Fig. 4.6, can mitigate the difference. Deviations from the hyperbolic distribution impact the spherical aberration strongly. As (ℓ/D) increases, the curvature of the potential distribution near the axis weakens. For $(\ell/D) \lesssim 0.5$ and $(d/D) \lesssim 0.03$ the maximum deviations in C_s are about 15%, though less than 5% is typical over the range of potentials of interest (the 10%-variation-in- C_c region). Geometries with $(\ell/D) \gtrsim 0.75$ are no longer accurately modeled by the analytic model, while geometries with $(\ell/D) \lesssim 0.25$ show deviations of less than 5% from the analytic model over a broad range of electrode potentials.

The analytic model uses the Davisson-Calbick formula for the aperture focal lengths. This model is a limiting case of an infinitely thin aperture which gives a sharp change in potential gradient across the aperture. For relatively weak lenses, the approximation works very well. For strong lenses or large trajectory angles, the focal length of the aperture is shorter than predicted by the formula [107], which results in a longer object/image distance z_0 . In the triode mirror the strengths of the aperture lenses change with the electrode potentials, so chromatic aberration is also affected by the Davisson-Calbick approximation. Ideal apertures do not contribute to spherical aberration, and the effects of real apertures on spherical aberration can be safely ignored [107]. The object/image distances in consideration are typically $0.5 < z_0/\mathcal{L} < 1.5$, so the overall focal length of the mirror is $0.25 < f/\mathcal{L} < 0.75$. Apertures with focal length $|f_{ap}/\mathcal{L}| > 2$ are relatively weak lenses that agree reasonably with the Davisson-Calbick formula, and any differences are minor perturbations to the overall mirror behavior. The grounded electrode aperture focuses weakly for

all mirror electrode potentials if

$$(V_A/V_C) < \left(1 - \ell^2/\mathcal{L}^2\right). \quad (4.19)$$

The center electrode aperture focuses weakly when

$$(V_M/V_C) < 1/\left(1 - \ell^2/\mathcal{L}^2\right), \text{ and} \quad (4.20)$$

$$\frac{(\ell^2/\mathcal{L}^2) + (V_M/V_C)}{(\ell^2/\mathcal{L}^2) + (1 - \ell^2/\mathcal{L}^2)^{-1}} < \frac{V_A}{V_C} < \frac{V_M}{V_C} \left(1 - \ell^2/\mathcal{L}^2\right). \quad (4.21)$$

For example, if $\ell/\mathcal{L} = 1/3$ $\{2/3\}$ then $(V_M/V_C) < 9/8$ $\{9/5\}$ and 0.84 $\{0.29\} < (V_A/V_C) < 1$. Since a greater range of electrode potentials enhances the flexibility of the mirror, smaller $\ell/\mathcal{L}$ appears to be best. In practice, a greater range of V_A can be accommodated by characterizing specific models with an extensive simulation.

A numerical model with realistic geometries provides more concrete validation of the analytic model, as in the analytic Fig. 4.6. The mirror lengths are $\mathcal{L} = 42.3$ mm and $\ell = 0.48\mathcal{L}$, the apertures have diameters $d = 1.52$ mm, and the thicknesses of the center and outer electrodes are 1.5 mm and 2.54 mm, respectively. Both faces of the center electrode different contours of the hyperbolic field. The mirror, center, and grounded electrodes extend radially 19 mm, 19 mm, and 25.4 mm, respectively, from the optical axis. The outer edge of the mirror electrode has been shaped to compensate for the finite radial extent with a ring 3.15 mm wide. A grounded cylinder of diameter 50.8 mm coaxial with the optical axis surrounds the entire model.

The potential distribution was determined by solving Laplace's equation with SIMION using an over-relaxation, finite difference technique to a convergence of one part in 20000 on a cylindrically symmetric mesh composed of $N = N_z \times N_r = 12532 \times 4001$ points spaced $6.35 \mu\text{m}$ apart ($L_z \times L_r = 79.6 \times 25.4 \text{ mm}^2$) in SIMION. A point

source of twenty electrons with randomly distributed angles between 3 and 5 mrad was accelerated to $eV_C = 20$ keV. Electron trajectories were numerically integrated through the model to determine z' and α' in symmetric mode, from which z_0 , C_s , and C_c were computed by fitting to Eqs. (4.15), (4.17), and (4.18). Electrode potentials were sampled over the range -23.770 kV $< V_M < -22.08$ kV and -14 kV $< V_A < 0$ kV. Scan intervals were dynamically varied 1 V $< \Delta V_M < 10$ V and 7 V $< \Delta V_A < 400$ V, for a total of 26,375 configurations of V_M and V_A (non-focusing configurations were not recorded).

Fig. 4.7 shows the results of the simulation. The differences between the analytic and simulated optical properties, z_0 , C_s , and C_c , are shown as contours plotted against the mirror potentials. Highlighted in black is the region centered around aberration corrections of $C_{sSys0}/\mathcal{L} = 8.05 \times 10^4$ and $C_{cSys0}/\mathcal{L} = 721$ and enclosing differences $(\Delta C_{sm}/C_{sSys0})^2 + (\Delta C_{cm}/C_{cSys0})^2 < 0.3^2$ from that central point. Over the highlighted region, all three properties show agreement to within 5%. The object/image distance has an offset from the analytic model of 1.26 mm (3%), but changes by less than 0.4 mm (1%). The spherical and chromatic aberration coefficients exhibit a wider range of variation, but also differ by less than 5% from the analytic model. Thus, while the analytic model may be too inaccurate to use for implementation, it is extremely useful for optimizing the configuration.

4.3 Triode mirror and lens with fixed object distance

The optimization of the mirror-lens system is complicated, so it is instructional to first consider a non-interacting model. This restricts the triode mirror to maintain a constant focus, as previously discussed, and the lens to maintain a constant magnification. The non-interactive corrector is a three-dimensional optimization problem, where the mirror-lens spacing Z , the geometry of the triode mirror $\ell/\mathcal{L}$, and the mir-

Figure 4.7: Comparison of the optical properties of the triode mirror between analytic and simulated models. The 30% aberration variation region is highlighted (black), over which region the difference changes by less than (a) 1%, (b) 5%, (c) 10%. Contours are relative to: (a) the mirror length $\mathcal{L}$, (b) and (c) spherical and chromatic aberration coefficients at the center of the 30% variation region ($C_s/\mathcal{L} = -30$, $C_c/\mathcal{L} = -14$). Reprinted from Fitzgerald, Word, and Könenkamp [106].

Figure 4.8: Properties of the triode mirror with $\ell = 0.48\mathcal{L}$ and $\mathcal{L} = 42.3$ mm. Two constant focal length contours are plotted, with $z_0 = 1.1\mathcal{L}$ (solid) and $z_0 = 1.4\mathcal{L}$ (dashed). Three points along each constant- z_0 contour illustrate a range of aberration correction values. The solid, black point corrects the aberrations $-C_{sSys}$ and $-C_{cSys}$, where C_{sSys} and C_{cSys} are the spherical and chromatic aberrations of a cathode and objective lens. (a) The optical properties C_s , C_c , and z_0 , plotted relative to the triode mirror length $\mathcal{L}$. The gray regions are projections in $C_s \times C_c$ and $z_0 \times C_c$ of the 3D surface in mirror property space spanned by the potential range (shown in b) for any z_0 . The white lines trace contours of constant potential. (b) The mirror and center electrode potentials, V_M and V_A , plotted relative to the accelerating potential V_C . Reprinted from Fitzgerald, Word, and Könenkamp [106].

ror potential V_M are the independent variables and the mirror length $\mathcal{L}$ and center electrode potential V_A are the dependent variables.

An objective-type lens is used for its low spherical and chromatic aberration coefficients, C_{si} and C_{ci} , at relatively high focusing power. This is important since this lens images the electron beam twice. In this first treatment the lens-specific properties are determined from experimental data in Rempfer [60]. Subsequently the angular magnification, m_i , and the aberration coefficients (in mm) are parameterized as functions of the incident image distance, z'_i (in mm),

$$m_i = -0.07474 + 0.0001108z'_i + 66.19(z'_i)^{-0.9637}, \quad (4.22a)$$

$$C_{si} [\text{mm}] = -18.13 + 4.773z'_i + 0.01598(z'_i)^{3.388}, \quad (4.22b)$$

$$C_{ci} [\text{mm}] = 4.347 + 1.442z'_i + 0.01289(z'_i)^{2.035}. \quad (4.22c)$$

The incident beam object distance is 72.9 mm, as in Fig. 4.9b. Since the distance from the mirror electrode vertex to the lens center Z also remains constant, the lens image and mirror object/image distances are related by $z'_i = Z - z_0$. Hence, the lens properties become functions of the mirror potentials.

For each constant z_0 curve, the triode mirror has a fixed relationship between V_A and V_M (Fig. 4.8). Along a particular curve, e.g., $z_0 = 1.1\mathcal{L}$, the amount of spherical aberration correction has a maximum value. Around this point, chromatic aberration correction can dynamically change without significantly affecting spherical aberration correction. Thus the triode mirror aberration correction system has an adaptive quality that allows for small corrections, at least in chromatic aberration. For a different curve, e.g., $z_0 = 1.4\mathcal{L}$, the triode mirror has dynamically adjustable spherical aberration at nearly constant chromatic aberration. So for each z_0 there is one best combination of V_A and V_M around which aberration tuning is optimized.

Figure 4.9: The mirror has cylindrical symmetry about the z -axis with $z = r = 0$ at the cone vertex. The mirror electrode, at potential V_M , is a cone with opening angle $\Delta r / \Delta z = \sqrt{2}$. The center electrode, at potential V_A , follows the hyperbolic contour $z^2 - \frac{1}{2}r^2 = \ell^2$; and the outer electrode, at potential $V_G = 0$, follows $z^2 - \frac{1}{2}r^2 = \mathcal{L}^2$. Small apertures in the center and outer electrodes allow electrons to enter and exit the mirror field. The distance from the mirror vertex to the opening of the first aperture is ℓ , and the distance from the mirror vertex to the opening of the second aperture is $\mathcal{L}$. An einzel lens, at potential V_L , accompanies the mirror a distance Z away. Z is measured from $z = 0$ to the center of the einzel lens. (a) Schematic diagram of the triode hyperbolic electron mirror with an einzel lens. (b) Simulation model of a mirror-lens combination showing the symmetric incident and exit beams. Reprinted from Fitzgerald, Word, and Könenkamp [106].

Matching the aberration of the mirror, C_s and C_c to that of the microscope, C_{sTot} and C_{cTot} , at this value of $\ell/\mathcal{L}$ and z_0 fixes Z and $\mathcal{L}$. For a given choice of these physical parameters— Z , $\ell/\mathcal{L}$, and $\mathcal{L}$ —the mirror potentials describe a surface in the three-dimensional property space $C_s \times C_c \times z_0$, as shown in Fig. 4.8, which is accessible once the aberration correction system is installed. Examining the projections of this surface onto $C_s \times C_c$ and $z_0 \times C_c$ it becomes clear that there is one best z_0 for spherical aberration tuning and another for chromatic aberration tuning.

Allowing z_0 to change would greatly enhance the dynamic range of correction, potentially yielding simultaneous and independent correction of spherical and chromatic aberration. However, for a fixed mirror to lens spacing, a dynamic z_0 also changes the magnification of the lens, which, in turn, changes the amount and ratio of the aberration to be corrected. The interacting mirror and lens system must be studied more carefully to determine whether it allows for independent variability of spherical and chromatic aberration correction and how the dynamic range or independent correction can be optimized.

4.4 *Interacting triode mirror-lens corrector*

The one-to-one relationship between the coefficients of spherical and chromatic aberration in the previous section is due to an overspecification of the system of equations: two variables— V_M and V_A —are used to specify the two aberration coefficients and align the focus of the microscope, i.e., three properties. If the triode mirror were no longer constrained to constant focus, the resulting interacting mirror-lens system would be able to independently compensate spherical and chromatic aberration. In this way the focus and coefficients of aberration would be specified by three variable potentials, V_M , V_A , and V_I , where V_I is the interface lens potential, and an exact specification of the system of equations is possible over the range in which the three

Figure 4.10: Properties of a triode mirror, with $\ell = 0.48\mathcal{L}$, used interactively with a lens in symmetric mode. The dark gray region highlights the property range that can be accessed by changing the potentials while maintaining a focus. This region encloses aberration correction changes of up 30% from the central point. The four perimeter points (black/white) indicate the maximum variation of each coefficient. (a) The triode optical properties, zoomed in from Fig. 4.8a. (b) The triode mirror and lens potentials. Compare to Fig. 4.8b. Reprinted from Fitzgerald, Word, and Könenkamp [106].

variables are linearly independent and physically meaningful. This system is quite similar to the non-interactive corrector described above. The focus equation,

$$z_0 + z'_i = Z, \quad (4.23)$$

implies that z'_i is a function of the mirror object/image distance z_0 for fixed mirror to lens spacing Z . Thus, the lens properties in Eq. (4.22) are functions of the mirror potentials, and the two equations for the cancellation of spherical and chromatic aberration, Eqs. (3.26) and (3.27), depend only on the two variable potentials V_M and V_A .

The optimization of the interactive system has only a few modifications from the previous section. Instead of a single best combination V_M and V_A for each z_0 , the best interactive mirror-lens corrector maximizes the area enclosed by the range of spherical and chromatic aberration that can be corrected. This can be measured by the parametric area $(\Delta C_{sSys}/C_{sSys0}) \times (\Delta C_{cSys}/C_{cSys0})$, where the range of aberration is $\Delta C_{Sys} = C_{Sys0} - C_{Sys,cor}$ and $C_{Sys,corr}$ is the value of aberration corrected as measured in transfer space, i.e., at the beam separator Magnet B. The current discussion uses $C_{sSys0} = 3.40 \times 10^6$ mm and $C_{cSys0} = 3.05 \times 10^4$ mm. Optimization solutions are found by first setting $V_A = \frac{1}{2}(1 - \ell^2/\mathcal{L}^2)V_M$ as the center of the correction area, and second the maximum correction area is limited by $(\Delta C_{sSys}/C_{sSys0})^2 + (\Delta C_{cSys}/C_{cSys0})^2 \leq 1$. This boundary traces out a unit circle in aberration correction coordinates, and the area of this circle can be used as a standard to judge the maximum correction region. The maximum aberration correction that this survey can find is $\pm 100\%$.

The maximum coverage was found to be 69% for the parameters $\ell/\mathcal{L} = 0.47$, $\mathcal{L} = 42.3$ mm, and $Z = 48.9$ mm. C_{sSys0} and C_{cSys0} are fully corrected with the potentials $V_M/V_C = 1.104$, $V_A/V_C = 0.43$, and $V_I/V_C = 1.015$ and can independently

correct any values of spherical and chromatic aberration within 38% of this central value since z_0 is only weakly constrained. The primary limitation of that region is that the range of V_A is maximized. Spherical aberration correction, adjusted primarily by the magnification of the lens, can be freely adjusted to any value within $\pm 100\%$, since the lens potential range is far from bounded. The potential relationships and the aberration and object/image distance of the triode mirror run in this configuration are shown in Fig. 4.10, with the 30% aberration variation region highlighted. Note that a $\mp 5\%$ change to triode mirror spherical aberration produces a $\pm 30\%$ change in spherical aberration correction. The lens magnification change of $\sim 0.5X$ accounts for an effective correction change of $\sim \pm 33.5\% C_{sSy0}$. The remaining 2.5% change is accounted for by the lens. For chromatic aberration, nearly all correction change is provided at constant z_0 , and so it is the mirror potentials that adapt the correction.

In conclusion, I find that a triode mirror and lens can simultaneously correct spherical and chromatic aberration of a PEEM image when the two elements are used interactively. As implemented, the corrections can be independently varied over a range of greater than 100% and 30% for spherical and chromatic aberration, respectively. This allows for increased precision in aberration corrected microscopes, and opens the door to fine-tuning spherical *and* chromatic aberration correction for each imaging session. In addition, the analytic model developed here grants a degree of intuitive understanding that allows optimization of the mirror-lens interacting pair corrector. This model is accurate to within 5%, so the optimized model relates well to a physical correction system. The triode mirror can correct aberration over a relatively large range because lens magnification can transform a wide range of microscope aberrations to the range of the mirror.

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5 Experimental adaptation and preparation

5.1 Corrector design parameters

The range of aberration correction of the triode mirror is matched to the calculated aberration range of our PEEM. The corrector is comprised of a two-region, hyperboloid-shaped mirror, as shown in Figs. 4.1 and 4.6, paired with a unipotential lens, as shown in Fig. 4.9. For comparison, the prior configuration of the PEEM used a diode mirror and lens, as shown in App. Appendix A. The new corrector is designed to work within the same physical space. To minimize changes to the established hardware, the interface lens is kept at the same distance from magnetic beam separator as in the diode design. The triode fits within the remaining ~ 90 mm of the lens tube. Due to limited space, the triode hyperbolic potential regions are $\mathcal{L} \lesssim 55$ mm. The central aberration range was estimated from the correction offered by the past diode mirror and interface lens, with the mirror operating at -21.9 kV. The diode interface lens is a swept-back design (App. ??) with an estimated bore diameter of 6.71 mm (0.264 in). The diode mirror and interface lens were modeled in SIMION to accurately characterize their spherical and chromatic aberration coefficients. I wrote a Lua language program to automate SIMION simulations and a Mathematica program to analyze the simulation results (Apps. Appendix D, Appendix E, and Appendix G). From the diode mirror corrector simulation, I found aberration coefficients of $C_{sSys0} = 3.40 \times 10^6$ mm and $C_{cSys0} = 3.05 \times 10^4$ mm, as measured in transfer space. Finally, the analytic triode mirror theory was geometrically optimized to provide the maximum aberration correction range, resulting in a geometric factor of $\ell/\mathcal{L} = 0.47$ and a total distance $\mathcal{L} = 42.3$ mm, as measured from the cone vertex to grounded electrode aperture.

Figure 5.1: Direct, side-by-side comparison of the triode mirror and diode mirror branch designs. The final version of the triode mirror was installed without the grounded front electrode, as noted. Credit: R.C. Word.

The triode mirror with the optimized geometric parameters was based on the successful diode hyperbolic mirror designed by G. Rempfer. The part specifications and PEEM modifications were drawn by T. Dornan. A direct comparison of the diode and triode correctors as installed is given in Fig. 5.1. The design of the insulating spacers separating the additional mirror electrode at potential V_A required a careful compromise between the demands of leakage currents, beam exposure, secure alignment, breakdown, and additional considerations, and may bear future investigation. The

optimal aberration correction range is only provided when the interface lens is closely positioned to the triode mirror. It was determined that a spacing between of only 1.4 mm between the grounded mirror electrode and the grounded swept-back lens electrode could satisfy the design. However, the close proximity of the two apertures introduces some difficulties in characterization and alignment. In order to alleviate some of the potential problems with alignment, the triode mirror was ultimately installed without the grounded electrode. Instead, a spacer ring holds the remaining parts in place, and the outer electrode of the interface lens provides the grounding of the mirror field. It is expected that the modified geometry will compare favorably to a triode mirror lengthened by the distance between the grounded aperture of the mirror and the lens, ~ 4.72 mm. The lengthening of $\mathcal{L} \rightarrow \mathcal{L}'$ changes the geometry ratio from $\ell/\mathcal{L} = 0.47$ to $\ell/\mathcal{L}' = 0.42$. With the following simulation, I show that this change does not significantly alter the aberration correction properties.

5.2 Numerical simulation via SIMION

In the theoretical study of the mirror corrector, it was found that the analytic and numerical models differed by enough that only a numerical model could characterize the optical properties with sufficient precision. The precision of the power supplies in our PEEM is about 1–2 V, so the characterization has an electric potential resolution an order of magnitude larger or better, at 10^{-6} – $10^{-7} \times V_C$. The useful mirror electrode potential ranges from $V_M/V_C \gtrsim 1.02$ to $V_M/V_C \lesssim 1.22$, and the useful additional electrode potential varies $0 < V_A/V_C \lesssim 0.75$. At the desired resolution, the simulation space occupies up to $(4 \times 10^5) \times (1.5 \times 10^6) = 6 \times 10^{11} \equiv N_{V,\max}$ mirror potential configurations. Because of the close proximity of the mirror and lens, the two cannot be treated independently in a numerical characterization since the aperture fields of the two elements influence each other. When the grounded mirror electrode is

removed, the interaction becomes stronger. Thus the lens voltage is a third dimension in the corrector configuration space $V_M \times V_A \times V_I$. The useful lens range is $0.9 \lesssim V_I/V_C \lesssim 1.15$ for a 6.7 mm center bore diameter swept-back lens, leading to an upper limit to the corrector configuration space of $N_{V,\max}^{(\text{tot})} = (4 \times 10^5) \times N_{V,\max} = 2 \times 10^{17}$ at a resolution of $5 \times 10^{-7} \times V_C$. If only 5×10^{-6} is required—one volt in 20 kV precision—then the configuration space is 2×10^{14} potential combinations.

To determine each characterization in SIMION requires numerically tracing trajectories through the electric potential distribution of the corrector. The potential of a numerical model was refined in SIMION to a relative gradient precision of 5×10^{-7} on an array with grid unit size of $6.25 \mu\text{m}$. This was done for models both with and without the grounded front electrode, as shown in Fig. 5.2. The electric potential between V_A and 0 differs by a few percent from a hyperbolic distribution in both models, and the difference between them is consistent with lengthening the triode mirror as expected. Examining the figure, it seems likely the deviation from a hyperbolic potential in this region is a large contributor to the difference between the analytic and numerical models of the triode mirror. Electron trajectories were numerically integrated through the potential, and information about those trajectories was collected with a Lua user program (App. Appendix H). The final implementation of this analysis includes several refinements over the initial code, similar to that used to analyze the diode mirror (App. Appendix G). First, three beam energies are used: the central energy of 20 keV, with the others differing by +1 eV and −1 eV. The use of three beam energies increases the confidence in the chromatic aberration calculation, which is now a linear fit instead of a two-point slope calculation. Second, the computation only obtains a symmetric mode image distance for the central beam energy. It was found that tuning object position for symmetric mode in the other cases introduces chromatic aberration into the point source object since different beam energies

(a) Original model.

(b) Installed model *without* triode grounded electrode.

Figure 5.2: Electric potential distributions of triode correctors (a) *with* the original front electrode design and (b) *without* the electrode, as determined by SIMION. The electrodes are shown in brown, and potential contours are shown in blue, green, and red. The electrodes are at potentials $V_M = -22.5$ kV, $V_A = -8$ kV, and $V_L = -20.5$ kV. The contours are color coded: blue contours range from -0.1 V to -100 V by powers of ten; green contours change by 2 kV from -2 kV to -22 kV; and the red contour shows the electron beam acceleration potential of -20 kV.

Figure 5.3: Relationship between triode mirror V_M and V_A that produces real images. All surveyed configurations that produced real images are plotted (black points) and fit to a quadratic polynomial $V_{A,\text{est}}(V_M)$ (black line). All points lie within $|V_A - V_{A,\text{est}}| < 2$ kV, as highlighted the limits in red, and almost all points lie within 1.5 kV, particularly at lower V_M .

have different object points. The desired model is one in which the object has no aberration and the image has all the aberration, instead of some in the image and some in the object, as before. Removing the additional object distance tuning also increased the speed of the computation and decreased the uncertainty of the final result, since there is explicitly no aberration in the object source.

It was also observed that only narrow ranges of potentials give real images with aberration correction. The interface lens is limited to between -20.0 and -21.5 kV for a 20 keV electron beam. The mirror potentials vary together, such that configurations satisfying $|V_A - [-21.94 - 7.23(V_M + 20) - 0.319(V_M + 20)^2]| \lesssim 1.5$ kV give real images, for V_M and V_A in kV. This relationship was determined from an initial survey, and it is illustrated in Fig. 5.3. This reduces the maximum configuration space by two orders of magnitude to $N_{V_M} \times N_{V_A} \times N_{V_I} = (4 \times 10^5) \times (1.5 \times 10^5) \times (1.5 \times 10^5) = 9 \times 10^{15}$. The code is further optimized to scan through potential configurations

more quickly when the previous configuration does not produce a real image, further decreasing the configuration space by a factor of ~ 2 . Next, the object distance is fixed to the value assessed from the scaled drawings (Apps. Appendix A and ??), and symmetric mode is determined by tuning the lens potential instead of the object position. The tuning is limited to 5–20 attempts, depending on the convergence of the first few attempts. Over the range in interest, this potential is close to linear; however, over wider ranges this method breaks down somewhat. With most of the $V_M \times V_A$ configurations not producing a real image, on average there are only ~ 10 V_L configurations attempted. This reduces the number of configurations significantly to

$$N_{V,\text{tot}} = N_{V_M} \times N_{V_A} \times N_{V_L} = (4 \times 10^5) \times (1 \times 10^5) \times 10 = 2 \times 10^{12}.$$

This is the estimated number of viable electric potential configurations of the triode mirror corrector to a voltage tolerance $5 \times 10^{-7} \times V_C$, or about 0.01 V in 20 kV. It is still too large to probe the complete configuration space in a reasonable amount of time, so instead the precision of V_M and V_A were limited to $10^{-3}V_C$ in the SIMION survey. Approximately 1.4×10^5 voltage configurations were simulated with over 5×10^6 electron trajectories, of which only 1.5×10^3 configurations give real images. The new Lua code dumps basic trajectory data into a file, and Mathematica is used to calculate the optical properties (App. Appendix I). For a given V_M , V_A and V_L could be extrapolated to an accuracy of $10^{-7}V_C$ with a 4–8 term polynomial. In the final result, only V_M is limited to $\sim N_{V_M}/400$ intervals in the final characterization, leading to an effective configuration space of $N_{V,\text{tot}} \sim 5 \times 10^9$.

This characterization of the mirror branch was found to give the desired spherical and chromatic aberration correction to within one percent, giving sufficient accuracy to test the effects of changes in aberration correction on the resolution of our PEEM.

Figure 5.4: Discrete values of aberration correction provided by the triode mirror corrector. Changes in spherical and chromatic aberration coefficients of the mirror branch as measured in transfer space are presented relative to the aberration correction the diode mirror correction, $\delta C = (C_{\text{triode}} - C_{\text{diode}})/C_{\text{diode}}$. Since coefficients vary with magnification according to a power law, values are varied logarithmically over a wide range. Correction is strongly limited in the direction of more spherical and less chromatic aberration (lower right corner), but is otherwise unbounded. The upper left corner was not predicted to be of significant interest, so has less dense coverage.

Tables of the mirror branch voltages and aberration coefficients in transfer space are given in App. Appendix J. These tables can be used to control the power supplies providing V_M , V_A , and V_I . The changes in aberration coefficient correction relative to the diode mirror of those tables are plotted in Fig. 5.4. Clearly, aberration can be corrected over a wide range. Other swept-back lenses can be used by adjusting the potential V_I such that the thick-lens paraxial image distance between the lens and mirror is preserved. The effect on the aberration coefficients is approximately 10% in C_s and 5% in C_c for each 0.5 mm change in bore diameter.

The optical characterization presented in Ch. 2 also allows precise control of the objective branch, as well as an estimate of the aberration produced in configuration space. The main uncertainty in this estimate is from the cathode, which here has

Figure 5.5: The aberration coefficients of the mirror branch (dark gray) and the objective branch with magnifications 4–7 $\times$ compared in transfer space for Cu illuminated with 257 nm light. Compared to the diode, the triode corrector can accommodate a wider range of aberration correction values, and provides significant room for resolution optimization. Compare this to the diode corrector, Fig. 3.5.

only been characterized to no better than $\sim 10\%$ precision. The overlap between the objective branch image aberration coefficients and the triode branch correction is presented in Fig. 5.5. From the results of the simulation, the triode mirror has the potential to correct the image aberration of this specimen. For another specimen, the image aberration can be approximately matched up with the ideal mirror branch correction by adjusting the magnification of the objective-auxiliary lens zoom pair. Subsequently, the mirror branch aberration can be varied by the microscope user to find the best image resolution, making UPS characterization perhaps less necessary. Examining Fig. 5.5, it appears that by varying objective branch magnification, the aberration correction space can accommodate almost any realistic combination of spherical and chromatic aberration.

(a)

(b)

(c)

Figure 5.6: Triode mirror parts and assembly. The metal parts are constructed of naval brass and the insulators of rexolite.

5.3 Quality control and beam alignment

Work is underway to install and test the aberration correction of the triode mirror and lens. These two elements will replace the previous aberration correcting diode mirror and interface lens. Individual electrodes and spacers were built by Turk Manufacturing. They were assembled by hand, with various stages of assembly shown in Fig. 5.6. The triode interface lens is shown atop the mirror in Fig. 5.7, as it would be arranged in our PEEM. An as-built external comparison of the two lenses and the diode and triode mirrors is given in Fig. 5.8.

Figure 5.7: Interface lens and spacer atop the triode mirror, arranged as they would be installed in the PEEM. Three high-voltage feed-throughs are shown to the left, just behind.

Figure 5.8: Diode (right) and triode (left) mirror branch assemblies, including the mirrors (back), interface lenses (forward), and appropriate spacers.

Figure 5.9: Electron gun straight bench with triode mirror (left) and interface lens (right). The interface lens is connected to a power supply by the white wire, while the triode mirror is not yet connected. The electron beam is incident from the left and the focused spot is imaged on a phosphor screen just off camera to the right.

The most sensitive part of the construction is the concentricity of the metal apertures, which is made increasingly difficult with the large number of apertures. Alignment of the apertures is tested in an electron gun straight bench, shown in Fig. 5.9. An electron beam is prepared so as to be incident on the test lens with nearly parallel rays. Then the test lens is run at the highest possible potential, up to the acceleration potential of the electron, such that a fine spot is formed by the electron beam on a phosphor screen at the end of the bench. Then, the lens is rotated 180° degrees, and another spot is formed on the screen. The position of the two points is compared, as in Fig. 5.10, and internal alignment of the lens is assessed by the translation between the two spots. Typically, the test lens is used with a projection lens to increase this translation. This test is less indicative of misalignment with the triode mirror because the element is not designed to operate as a lens, as confirmed by simulations Fig. 5.11. As a result, the test reveals only the grossest of misalignments, and further testing must be done in the PEEM when the mirror is operated in reflection mode. The design of the mirror involves several axially thick pieces that ensure alignment with the optical axis, and alignment of the triode mirror was not a significant problem.

Figure 5.10: Visual comparison of electron beam focus points on a phosphor screen created the triode mirror operated as a transmission lens in the electron gun straight bench. These images compare a specific test where both electrodes in the mirror are at high potential. The second point is captured after the mirror was rotated by 180° . A total displacement of 0.1 grid units (about 0.1 mm) is evident. This shift is at about resolution of the experiment, and any further mis-alignment must be checked or compensated for in our PEEM.

Figure 5.11: Numerical studies of the triode mirror as a lens in the straight bench. There are two electrodes, which allow three distinct tests with one electrode at high voltage and the other grounded (denoted A or M) or with both at potential (denoted AM). The studies show that all three tests are sensitive to similar alignment problems, and that they are not particularly sensitive to alignment.

Figure 5.12: Interface lenses from diode (right) and triode (left) installations. Several spacers make up the difference in housing length. With these spacers, the lenses were interchangeable in the diode assembly. Testing the triode lens with the diode assembly allowed us to determine its alignment independent of the triode mirror.

In contrast, the swept-back design used for the interface lens does not give the most reliable part positioning. As a result, the interface lens required several assemblies and trials in the electron gun straight bench. The diode interface lens could not be used directly in the triode assembly because of its extra long housing. The difference is shown in spacers in Fig. 5.12.

Following initial tests for rotational symmetry of the lens and mirror in the straight bench, we continued tests in our PEEM. The electron image is sensitive to the total alignment of the mirror branch, including not only the internal alignment of the lens and mirror elements, but also the alignment of the lens and the mirror externally with each other and the magnetic beam deflector, Magnet B. This assumes that the alignment of the other branches is already acceptable. After several failed attempts, a triode mirror configuration without the front electrode successfully produced the most satisfactory image. The triode mirror with replacement spacers is shown in Fig. 5.13. Subsequently, beam alignment through the system was improved with electrostatic deflectors positioned throughout the PEEM. Finally, reasonable quality images could be produced with triode mirror corrector installed, as shown in Fig.

Figure 5.13: Triode mirror without the grounded electrode, showing the replacement spacer. The second image shows the grounded electrode to the side.

Figure 5.14: First images from the triode PEEM. The specimen is an evaporated gold film on ITO. Images are 5 second exposures with 244 nm light at 200 mW of two adjacent regions, (a) with and (b) without an aperture stop. Image resolution is low ($\sim 900\times$), with the field of view at several microns, so these images are not strongly sensitive to first-order image aberrations. However, they do confirm that the PEEM is basically aligned.

5.14. These images are at resolutions that are sensitive to the optical alignment of the electron beam but not sensitive to spherical and chromatic aberration.. Instead, image quality is significantly reduced by off-axis shifts, magnetic deflectors, and distortion. After correction of these defects, astigmatism and spherical and chromatic aberration become dominant contributions at higher magnifications where CCD pixel size limits are overcome. With astigmatism corrected by a multipole deflector, the bare effects of spherical and chromatic aberration can be seen, and with them, the image correcting properties of the triode mirror corrector can be confirmed.

III Photonics

6 Photoemission and photonics

The photoelectric effect, the emission of an electron from an atom upon absorption of an energetic photon, is among the most elementary quantum-mechanical phenomena. Hertz [108] originally discovered the effect in 1887, when he noticed that the incidence of light on an electrode at high electric potential facilitated sparking across the gap. Furthermore, he determined that intercepting the light with glass removed this effect, while a quartz slide did not, leading him to conclude ultraviolet radiation was the relevant portion of the spectrum. Further investigation by Hallwachs [109], Stoletow [110], and others showed that the photocurrent is proportional to the incident light intensity above threshold some threshold. Finally, after almost two decades of experiments, Einstein [111] successfully explained the phenomenon in terms of the interaction of discrete packets of light with electrons, ushering in the modern era of quantum physics.

In the simplest picture, a light quantum gives all its energy to a single electron. Neglecting thermal effects, maximum energy of an electron emitted directly from the surface is given by

$$E_{max} = hc/\lambda - W, \quad (6.1)$$

where h is Planck's constant, c is the vacuum speed of light, λ is the wavelength of the incident light, and W is the photoemission threshold energy, the minimum photon energy at which photoemission occurs. The photoemission threshold is closely related to the work function, a measure of the electron binding energy that is the difference between the Fermi energy and the vacuum energy. Above W , the photoelectron

current j_e is expected to increase linearly with the incident light intensity I ,

$$j_e = \eta I, \quad (6.2)$$

where c is the efficiency [49, 50]. Photoemission is a low-probability process, typically yielding less than one electron per ten thousand incident photons [51]. At photon energies less than the threshold W photoemission proceeds by an even lower probability, nonlinear processes, e.g., two-photon photoemission (2PPE), where multiple photons collude to excite a single electron. In general there is an n th order power law relationship for multiphoton photoemission (n PPE),

$$j_e = \eta_n I^n \text{ for } hf > W_n, \quad (6.3)$$

where η_n and W_n are the n -photon efficiency and threshold [8, 112]. The multiphoton values of the threshold and efficiency are typically comparable to ultraviolet (UV) photon values by $\eta_n \approx \eta^{1/n}$ and $W_n \approx W/n$, and likewise show a general correlation with material surface composition. An energy level representation of one- and two-photon photoemission is shown in Fig. 6.1.

The energy of photoelectrons is the experimental quantity used to determine the paths of photoexcitation, either through spectroscopic measurement or by comparing incident photon energy to known binding energies. Some representative spectra from Ag and Cu are presented in Fig. 2.3. As one would guess from the simple picture presented above, photoelectron emission energy distributions depend primarily upon the energy in excess of a material's photoemission threshold energy. However, the non-Gaussian spectral distributions and the differences between single- and multi-photon photoemission distributions (especially for Cu 1- vs. 3-PPE) serve to highlight the

Figure 6.1: Energy level diagram representation of the photoelectric effect, adapted from [113]. An electron is excited from an energy level below the Fermi level by a photon of energy hf or two photons of energy $hf/2$ to above the vacuum level. Intermediate energy levels can be bulk, surface, virtual, or quasiparticle states.

complexity of the process, a point driven home by the independence of the mean emission energy $\langle eV_e \rangle$ and distribution width σ_e on excess energy. Due to the complexity, photoemission in materials is usually discussed in terms of a three-step model: electrons are first optically excited, then travel to the solid surface (with or without scattering), and subsequently are emitted to the vacuum [49]. The spectral distribution of photoelectrons exhibits sensitivity to optical excitation processes and electron scattering processes. Because these processes vary within the material, spectra also change with sample position. In near-threshold studies, the mean electron energy and total yield shift in particular [96–98]. It is this contrast that PEEM utilizes, examining spatial variations in surface photoemission rates to reveal changes in photoexcitation pathways.

The photoemission threshold, efficiency, and photoelectron energy spectrum vary not only with the static electron environment and excess energy, determined primarily by the material and excitation energy, but also with dynamic processes and other experimental conditions, such as incident light intensity. These variations highlight a

more intimate dependence on topological structure and energy redistribution channels and underscore that a single electron emitted from an atom that absorbs a photon is, strictly speaking, not a single-electron process. Hence, the properties of the emitted photoelectron [114], exhibit sensitivity to the effects of temperature and phonons [115], interband transitions, surface roughness [116], Tamm and Shockley surface states [117], collective oscillations and optical excitations [118].

The manifold paths of photoexcitation can be represented as various elements of a scattering matrix T connecting the initial state i (ψ_i) to the final electron state f (ψ_f). Starting with Fermi's Golden Rule, the transition probability per unit time (up to second order) is

$$T_{if} = \frac{2\pi}{\hbar} \left| \langle f | H_{\text{int}} | i \rangle + \sum_n \frac{\langle f | H_{\text{int}} | n \rangle \langle n | H_{\text{int}} | i \rangle}{\epsilon_i - \epsilon_n} \right|^2 \delta(\epsilon_f - \epsilon_i - \hbar\omega)$$

for an initial energy ϵ_i , final energy ϵ_f , and real or virtual intermediate states n (ψ_n) in response to the Hamiltonian H_{int} [119]. The interaction Hamiltonian H_{int} and wave functions ψ_i , ψ_f , and ψ_n are chosen to fit the system states and interactions with the electromagnetic field. Mahan [120] describes how to go about this with simple metals. The initial electron state is derived from the band structure, and it can be represented as a sum of Bloch function plane waves,

$$\psi(\mathbf{k}, \mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \left\{ 1 + \sum_{G \neq 0} u_{k,G} e^{i\mathbf{G}\cdot\mathbf{r}} \right\} \left\{ 1 + \sum_{G \neq 0} u_{k,G}^2 \right\}^{-1/2}, \quad (6.4)$$

where an electron in the outgoing state $\mathbf{k}$ has plane-wave components in the directions $\mathbf{k} + \mathbf{G}$. Each of these components has an external distribution of electrons which may overlap with a free electron final state, represented by a Green's function evaluated

Figure 6.2: Graphical representation of the photoelectric effect using Feynman diagrams, where γ represents a photon, e^- an electron, and T is the transmission/scattering matrix standing in for the potentially mixed photoexcitation path; adapted from [121]. (a) Single photon photoemission (1PPE), (b) multiphoton photoemission (n PPE), and (c) a diagrammatic representation of two-photon photoemission as the sum of several contributions, each with its own efficiency. The loop contribution is the interaction with surface plasmon polariton quasiparticles.

in the presence of the material surface,

$$G_E(\mathbf{r}, \mathbf{r}') = \int d\mathbf{k}_{\parallel} \int_0^{\infty} dk_z \sum_i \frac{\psi_i(\mathbf{k}, \mathbf{r}) \psi_i(\mathbf{k}, \mathbf{r}')^*}{E_k - E - i\delta}, \quad (6.5)$$

where $E_k = (k_{\parallel}^2/2m) + E_{k_z}$ and the wave functions ψ_i are the initial electron wave functions. The amplitude of the overlap may be adequately described by a scattering T -matrix that connects the initial and final states through potentially several scattering events and intermediate states. Both virtual and real states are rigorously included, with the difference being largely semantic in this formalism. The interaction can be viewed as a perturbative sum of contributions, with individual terms often identified as quasiparticle interactions and represented by Feynman diagrams as in Fig. 6.2. Excitation paths can be direct, that is approximately a singular electron-

photon interaction that conserves photon momentum, or indirect, involving one or several intermediate resonances or scattering events which may not conserve photon momentum [120]. In particular, multiphoton photoemission necessarily involves intermediate states, but these may be real or virtual states, with a range of lifetimes and potentially separately direct or indirect partial or complete pathways [98, 122]. The sum of excitation pathways, which depends on the density of states and the incident radiation, not only sets the total efficiency but also dictates the energy threshold. The sensitivity of photoemission efficiency to several processes invites careful scrutiny of the excited photoelectrons, allowing us understand the electron environment before emission and the processes in which photoelectrons participate [49, 123].

Low photoemission rates are the primary practical limitation in imaging with photoelectrons. Ultraviolet, single-photon quantum efficiencies for metals are on the order of $\eta = 10^{-5}$ electrons per photon [51], so two- and three-photon quantum efficiencies are on the order of $\eta_2 \approx \eta^2 = 10^{-10}$ and $\eta_3 \approx \eta^3 = 10^{-15}$. Higher order processes are prohibitively rare for imaging. The availability of ultrafast, high-intensity lasers coupled with parallel developments in high sensitivity CCD cameras and aberration correction have increased the applicability of nonlinear n P-PEEM, such that the near infrared and visible spectral region can be routinely used. Furthermore, contrast, brightness, and resolution are enhanced by corrected optics as discussed in Part II. These advances combine to make PEEM a potentially powerful tool for the study of all types of electromagnetic field excitations in materials, including guided optical modes, vacuum modes, and surface plasmons. With spatial resolution approaching 5 nm [89], PEEM may advance optical surface studies to scales well beyond standard optical microscopes and currently available super-resolution techniques.

Despite photoemission being an explicitly quantum process, imaging—i.e., the recording of emission yields of photoelectrons—requires such a high density of pho-

tons that there is a nearly exact equivalence between quantum and classical descriptions, as given by the quantum correspondence principle [124]. This theorem states that in the limit of infinite quantum numbers, such as excitation state or particle density, that the difference between quantum and classical descriptions becomes merely semantic, i.e., that measurable quantities can be equally well explained either way. PEEM operates very close to this regime; therefore, no effort is made to distinguish between high photon densities and large field intensities in explaining the link between photoemission and optical phenomena. To better relate to optical literature, the electromagnetic field intensity is preferred in the following work. However, photoemission is a purely quantum effect, one that cannot be explained as a classical threshold process. Thus, PEEM images are more representative of the photon density, and only through the quantum equivalence principle can we conclude that this is also the electromagnetic field intensity.

With some notable exceptions [52, 125–129], the information reported by the low-energy photoelectrons imaged in PEEM primarily originates from within a nanometer of the sample surface [53]. In this zone, optical interactions dominate the electron environment. PEEM allows us to visualize and scrutinize these processes on a scale significantly less than a wavelength of the incident light. The nanoscale observation of electromagnetic field intensity at material surfaces is receiving increased interest, as optical information processing now approaches frequencies in the visible spectral region and device sizes have moved into the sub-micron range [41]. Precise manipulation of the interaction between light and materials promises several applications, ranging from directing antenna radiation without moving parts [130] and micrometer-sized solid-state lasing cavities [131], to the more exotic pursuits of invisibility cloaking [132] and slow light [133].

Visual confirmation of electromagnetic processes in such nano-devices can only

improve characterization and development. Near-field electromagnetic field distributions at surfaces are typically observed by scanning methods, such as photon scanning tunneling microscopy (PSTM) [134], near-field scanning optical microscopy (NSOM) [135], electron energy-loss spectroscopy (EELS) [136, 137], and cathodoluminescence [138]. In contrast, PEEM is a probe-free non-scanning technique in image resolution is independent of the light source [139, 140]. The results are qualitatively similar to those obtained by PSTM [141] and NSOM [142].

Polarization is important to this investigation for two reasons. First, as a fundamental property of the incident light, photoemission should exhibit a strong sensitivity to the incident light polarization if it is at all sensitive to the optical fields. It is a variable along which the correlation between photoelectron and optical responses can be probed. Second, the optical control possible with polarization switching is of interest in a wide range of applications, particularly in ultrafast light-controlled optical switches, plasmonic routers, and path selectors. Even on slower time scales, the possibility of spatial control of optical fields and electron emission will be useful in sensors and actuators and in nanoscale electron sources.

Previous studies have demonstrated that photoemission from metal surfaces is highly sensitive to optical phenomena. In particular, high yielding multiphoton photoelectron sites, “hot spots,” have been found from metallic surfaces and nanostructures [7, 10, 15, 143, 144] 2P- and 3P-PEEM. As illustrated in Fig. 6.3, there are several potential photoexcitation paths in multiphoton photoemission, but observations indicate hot spots are the result of surface plasmons [8, 9, 31, 33, 113, 118]. Plasmons are dynamic excitations that result from the collective oscillation of conduction-band electrons. At surfaces they couple to intense, highly-confined electromagnetic fields in a surface plasmon polariton (SPP) quasiparticle. While plasmon excitations are typically propagating waves, they can be localized in metal films with nanostructured

Figure 6.3: Two-photon excitation pathways in metals, including direct single-particle excitations (black, thin arrows) and surface plasmon excitations (gray, thick arrows). Coherent excitations proceed via a virtual intermediate state (direct) or through a multiply excited surface plasmon. Incoherent excitations involve relaxation time in an intermediate state, where electrons lose connection to the initial excitation, followed by excitation to the vacuum state.

surface, in random geometries, and in clustered metal films [145, 146]. The localization occurs essentially by the confinement of local modes within the nanostructure. Intense localized surface plasmon resonances (LSPRs) increase optical field strengths by several orders of magnitude [147–150] and are thought to be the source for surface-enhanced Raman scattering, enhanced luminescence, lasing, and other phenomena, including enhanced nanoscale photoemission in hot spots.

Surface plasmon polaritons have attracted wide interest for applications in ultrafast electronic and photonic devices, information devices, and for enhanced electron and light microscopy. Plasmon generation can be enhanced and manipulated in antenna structures [151–153]. Devices for controlling plasmon propagation have been demonstrated in the form of beam-splitters [154, 155] focusing lenses [156], and routers and multiplexers [157]. It is believed that the exploration of these basic device functions is needed for the realization of numerous applications ranging from ultra-sensing [158–161] and nano-lasing [162, 163] to cloaking [164, 165] and imaging

[166, 167]. Optical control is desirable for some of these applications and is essential for high-speed transfer of plasmonic signals, energy, or charge. As a next step in this development, it is desirable to motion the confined field region either to fine-tune the spatial overlap between probing field and sample, to carry out spatial scanning procedures or to selectively address separate receivers in routing applications.

While plasmonic phenomena have received significant attention lately, diffraction from particles or edges are also familiar image features in PEEM. These so-called ‘fringe fields’ can be used to obtain information on the diffracting object [13], but are usually ignored as image artifacts. Here I report that photoemission can also be used to image the near field of a photonic wave bound to a dielectric thin film, showing phase contrast in a manner similar to near field scanning optical microscopy [141]. Instead of responding strongly to incident light with collective oscillations as in metals, electrons in optical dielectrics are relatively tightly bound to lattice sites and allow light to pass through with little attenuation, albeit at a slightly reduced average speed. Layered dielectric structures, composed of electrically semiconducting or insulating materials, can guide and confine light in a specific layer through differences in refractive indices. Optical fibers are an exemplary application, where a graded index glass cylinder confines light to the center; signals in optical fiber can propagate several kilometers without significant signal deterioration. Planar, or “slab,” waveguides (see schematic in Fig. 6.4) with spatially ordered holes in the central layer, so-called photonic crystals, can manipulate the properties of guided light [168]. Precision changes in the periodicity or defects can be used to create coupled micro-optical elements, such as micro-filters and micro-cavities, which scale communications processing and mirror arrangements down to micrometer scales [131, 169–171]. The possibility of visualizing optical fields in dielectric media with photoelectrons has not been previously investigated.

Figure 6.4: Dielectric slab model. Two semi-infinite dielectric layers, with refractive indices n_1 and n_3 , bound a central layer with index n_2 and thickness d . The layers extend infinitely in x and y dimensions. Refracted electromagnetic waves can be guided and confined to the central layer if it has the appropriate wave vector. A geometric ray-tracing schematic and an intensity profile of one possible mode are overlaid in yellow and orange.

In the following, I explore the photoelectron response to these optical phenomena: surface plasmons in structured metals, photonic guided modes in optical dielectric structures, and diffraction at grooves, holes, and knife-edge steps. In the process I hope to demonstrate that PEEM can directly and quantitatively visualize optical phenomena in the near-field of solid surfaces. First, I examine localized and extended plasmon modes that arise in randomly [28, 30, 42] and deliberately [37, 41, 172] nanostructured metallic thin films, where diffraction and optical antenna resonances scatter the incident light wave vectors to match the plasmonic modes. Despite numerous experimental investigations of localized plasmon modes, a detailed understanding of the various conversion processes occurring in the photoemission process is still at the beginning. With high spatial resolution, PEEM can conclusively show that photoexcitation is enhanced from both participating metal surfaces and passive semiconducting surfaces in the vicinity, and that the location of emission is strongly responsive to the polarization of incident light. Similar wave vector matching conditions in more de-

liberate diffracting structures [41, 173–175] lead to the emergence of photonic modes in the vicinity of transparent and absorbing semiconductors and of plasmonic modes at metal surfaces. A quantitative evaluation of the obtained images allows a distinction between modes that propagate inside the samples with propagation parameters given by the sample dielectric constant or refractive index, and modes propagating above the sample surface in vacuum and subject to the vacuum dielectric properties. In these extended modes, the surface electromagnetic near-field intensity can be calculated using a finite-element-method solution to Maxwell’s equations or a more conceptually simple formula based on Huygens’ principle and Fresnel diffraction. Using only a simple power-law relationship, I show that there is a close correspondence between photoemission patterns and calculated field intensities, demonstrating that PEEM is suitable for visualizing virtually any surface electromagnetic interaction.

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7 Methods and materials for photonics

Imaging with photoelectrons in an aberration corrected PEEM is described in detail in Part II. Here, I describe the illumination conditions and specimen preparations used to in photonics investigations.

7.1 *Light sources*

In all of our PEEM experiments, light is incident at 60° to the sample surface normal for all investigations, as illustrated in Fig. 7.1. Furthermore, the laser beams were polarized to $>99\%$ linearity by a tunable wave plate and focused to an incident spot of about $100\text{-}\mu\text{m}$ diameter. Both linear and circular polarizations were investigated. Transverse magnetic (TM) polarized light induces a larger photoelectron response than transverse electric (TE) polarized light [176], typically by a factor of 2–5, so images with different linear polarization angles have different mean intensities. This was often compensated by adjusting the exposure time, which varied widely with light source and material from a few seconds to several minutes.

Our PEEM is equipped with three light sources that provide limited ranges of IR, visible, and UV light. First, a mercury arc lamp provides low-intensity incoherent UV light, particularly at 253.7 nm. Second, a continuous-mode, frequency-doubled Ar^+ -ion laser provides UV light at 244 nm and a power of 100–200 mW. We found that a coherent and higher-power light source greatly increased the photoemission contrast in optical phenomena, so the Ar^+ -ion laser is the primary UV source. Third, a Spectra-Physics Mai Tai Ti:sapphire laser, produces $11\text{-}\mu\text{J}$, 80-fs pulsed IR light at 780–900 nm at a frequency of 80 MHz. The output can be up-converted to 410 nm with pulse energies of 2-nJ and a 100-fs duration using a Del Mar Photonics second

Figure 7.1: Schematic representation of sample conditions in PEEM, showing one of the diffracting nanostructures investigated here. The sample is illuminated by light at 60° to surface normal, and emitted photoelectrons are imaged with electron lenses to produce a magnified image of the interaction. Reprinted from Fitzgerald, Word, Saliba, and Könenkamp [173].

harmonic generator. The up-converted pulses have a line-width of 4 nm, full width at half-maximum. As a result of the limited spectrum of the light sources employed, I am only concerned with the optical properties of samples for wavelengths at 244 nm (5.1 eV), 410 nm (3.0 eV), or between 780-900 nm (~ 1.5 eV). In the case of each sample, I will also consider the photoemission threshold of the material and the excess photoemission energy, defined by $E_{max}(n) = n \times (hc/\lambda) - W$, where n is the order of the photoemission process. Actual photoelectron energy spectra (Fig. 2.3) and mean energies exhibit complex characteristics, but can be grossly distinguished by E_{max} .

7.2 Materials

We used two types of PEEM specimens. The first was a single silicon magnification standard (10- μm pitch), commercially prepared by electron beam lithography (Planotec Si Test Specimen, Ted Pella, Inc.). At wavelengths less than 450 nm, silicon is practically opaque with an absorption coefficient greater than $24,000 \text{ cm}^{-1}$ [177].

The photoemission thresholds of silicon and SiO_2 range from 4.3 eV [178] to 5.1 eV [179], with a mean of ~ 4.8 eV, so processes studied here are 1PPE (244 nm) or 2PPE (410 nm), with an excess energies of 0.3 eV and 1.2 eV, respectively. Silicon was not studied at longer wavelengths.

Other experiments employ conductive ITO slides, purchased from SPI Supplies, that consist of 2 mm borosilicate glass substrates sputter-coated with a 200–300 nm thick film of indium-tin-oxide (ITO). The borosilicate glass has a refractive index of 1.53 at 410 nm. The ITO layer is a mixture of indium-oxide (In_2O_3) and tin-oxide (SnO_2), approximately 90% indium oxide by weight with a sheet resistivity of 15–20 $\Omega/\square$ and a photoemission threshold of 4.1–4.25 eV [180–187]. It is opaque to wavelengths less than 300 nm, and 1PPE events with 244 nm light have an excess energy of 0.83 eV. At 410 nm, the refractive index is $2.14 + 0.25i$, corresponding to an absorption coefficient of 8000 cm^{-1} ; and photoelectrons are the result of 2PPE events with an excess energy of 1.8 eV. In the near-infrared, the index of refraction converges to 2.0 and the absorption coefficient drops below 500 cm^{-1} . Photoemission using 780 nm light involve a 3PPE process with excess energy of 0.5 eV, but the photoelectron yield was generally not sufficient for independent study because of low absorption. At wavelengths significantly longer than 900 nm, the optical response of ITO is plasmonic, as can be seen from the dispersion relation is shown in Fig. 7.2.

In experiments involving metallic thin films, conductive ITO-glass slides were used as a substrate. Gold was used for its low surface oxidation rates. In gold, the localized surface plasmon resonance typically lies between 400 and 800 nm depending on geometry. Photoelectrons emitted directly from gold at this wavelength are the result of a 4PPE process, with an excess energy of ~ 1 eV above the threshold of 4.5–5.3 eV [188–190]. A non-plasmonic, optical antenna response is also possible across a wider spectrum of wavelengths, but is highly sensitive to the nanostructure geometry.

Figure 7.2: Dispersion relationship for SPPs propagating at the interface of indium-tin-oxide with vacuum. The visible light used here (3.0 eV) is above the surface plasma frequency in the infrared (0.8–1.0 eV). Calculated from optical constants of Refs. [185] (red line) and [186] (blue dotted line). Reprinted from Fitzgerald, Word, Saliba, and Könenkamp [173].

Photoelectrons are the result of 2PPE and 1PPE processes when excited with 410-nm and 244-nm light, with excess energies of ~ 1 eV and ~ 0.3 eV, respectively.

Metallic thin films used here were composed of polycrystalline gold, single-crystalline gold, or polycrystalline gold and copper in separate layers, and were deposited using two distinct methods. Polycrystalline films were prepared by vacuum evaporation to thicknesses of 50–100 nm with a hexagonal mask for position determination, as shown in Fig. 7.3. In one case, a bi-layer arrangement of gold and copper, each 50 nm thick, was used because the layer of copper between the ITO and gold was found to increase the precision of sample structuring with a focused ion beam. In the other gold deposition procedure, single-crystalline gold platelets were obtained from an aqueous gold-chloride solution with aniline acting as a growth modifier, as described in Refs. [191, 192]. All compounds were analytical pure agents purchased from Sigma Aldrich. 50 mL of ethylene glycol solution containing 0.036 mM $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$ was heated to 95°C for 20 min. Then, 0.1 M aniline solution in ethylene glycol was added

Figure 7.3: (a & b) A thin layer of polycrystalline gold (~ 60 nm) on ITO-glass substrate. The gold deposition was masked with a TEM grid, leaving a pattern of gold hexagons (lighter gray) surrounded by uncoated ITO (darker gray). The highlighted hexagon contains patterns milled by FIB. Both images taken at a beam energy of 10 keV at a working distance of 4.9 mm.

under mild stirring to obtain a 1:1 molar ratio of aniline to gold. After 24 hours, a variety of gold flakes and platelets with diameters 3–15 μm and thicknesses 50–100 nm were obtained. These particles were washed of the solution with several cycles of ethanol and centrifuge separation, dispersed in water, and then cast on ITO-covered glass-substrates, as seen in Fig. 7.4.

7.3 Nanostructures

Diffraction nanostructures were milled using a focused ion beam (FIB) in a FEI DB237 dual-beam system, with the exception of the silicon magnification standard, which was used as purchased. Random and deliberate nanostructures were milled in gold and ITO, and the deliberate structures had varied complexity from simple rectangles and holes, the basic building blocks, to more elaborate patterns giving Y-shaped antennae.

Polycrystalline gold films on ITO were milled with a 100 pA Ga^+ beam current over a 10 $\mu\text{m} \times 10 \mu\text{m}$ area for varying times up to 300 s. The approach exploits the varying response of gold crystal orientations to the gallium beam, creating random gold-ITO nanostructures with various degrees of connectivity and feature size, as seen in Fig. 7.5. The patterns shown here vary only in gallium beam exposure time, differing in increments of 10 seconds, allowing gold surface coverage to be optimized for photoemission during PEEM imaging without controlling for other experimental parameters, such as gold film thickness. The variations in gallium beam response of the polycrystalline film that worked in favor of random nanostructures inhibit sufficiently precise milling control for deliberate nanostructures. This can be somewhat remedied with an intermediate copper layer, as discussed by Word, Fitzgerald, and Könenkamp [172].

Alternatively, deliberate structures can be made from chemically grown single

Figure 7.4: SEM images showing single-crystalline gold nanoflakes that were grown in solution, dispersed in water, and deposited on ITO-glass substrate. Gold crystals form equilateral triangles and hexagons with widths from 0.3–30 μm and thicknesses ranging from 20–100 nm, though some spheroids also form. Thicknesses of very large flakes were as little as 20 nm, as shown in (c), at a viewing angle of 60° relative to normal.

Figure 7.5: (a) Region of interest in specimen. Twenty boxes sized approximately $10\text{ }\mu\text{m} \times 10\text{ }\mu\text{m}$ were created by imaging each box with a gallium ion beam with different exposure times. The boxes are labeled by their FIB imaging times in the figure. The resulting boxes have varying degrees of etching, ranging from very little material removal (top right corner, light gray) to nearly complete removal of the gold and ITO layers (bottom left corner, dark gray). (b) This area was FIB imaged for 30 seconds. The gallium beam imaging creates random metal and semiconductor structures which are quite complicated and narrow. Both images were taken at a beam energy of 10 keV at a working distance of 4.9 mm.

Figure 7.6: Y-shaped antenna nanostructures carved from a single-crystalline nanoflake using a FIB. The SEM images, taken at an angle of 52° , show a time-lapse of the process as milling progresses over several minutes at low beam current (10 pA).

gold crystals. Following Huang et al. [192], nanostructures were milled from single-crystalline gold nanoflakes using 10 pA beam currents, as shown in Fig. 7.6. A series of adjacent or overlapping rectangular milling regions define the edges of the structures by removing gold material. The complex patterns of rectangles forming Y-shapes of various sizes were mapped out in advance by a Mathematica script, which subsequently output a file that the FIB could execute. The selected 20-nm-thick gold platelet was large enough to carve eleven 500-nm Y-shaped antenna structures as well as a few larger and smaller size-structures.

For photonics experiments, several dielectric nanostructures were milled into ITO, with two representatives shown in Fig. 7.7. The nature of the investigation was much

Figure 7.7: SEM images of diffracting structures milled with a FIB into ITO thin film on glass, viewed at an angle of 52° . (a) A deep groove and an adjacent shallow groove. (b) A semicircular array of holes. (c) Four adjacent circular grooves.

Figure 7.8: SEM micrograph of a cluster of crystalline Au platelets in the vicinity of a diffracting groove in the ITO substrate. The groove is 10 μm long, and 650 nm from the closest flake. The SEM image is taken at a tilt of 52°.

more exploratory, and simple rectangles and holes were used. The simplest of these structures is a 320-nm deep, $6.0 \times 0.4\text{-}\mu\text{m}^2$ groove adjoined by a wide, shallow trench 50-nm deep and measuring $2.0 \times 5.0\text{-}\mu\text{m}^2$ oriented perpendicular to the slit. The first groove is deeper than the 290-nm thick ITO film, exposing the glass layer at the bottom, while milling the shallower groove only served to thin the ITO layer to 240 nm. The second structure is a semicircular array of holes 500 nm in diameter with centers spaced 1 μm apart, following a circular arc with radius 5 μm . In the third structure the groove width is 500 nm with a diameter of 15 μm . The groove depth less than the ITO film thickness of 265 nm. A straight groove was also milled into the ITO layer adjacent to single crystalline nanoflakes, as shown in Fig. 7.8.

8 Theory of electromagnetic fields as relevant to photoemission

Spatial and temporal changes in photoemission rates are generally due to variations in the electron states (steady-state initial, intermediate, and final states), the electromagnetic field intensity (photon energy and density), and dynamic electron excitations (resonant or scattering events) [56]. The local density of states can be difficult to calculate or measure; however, in many cases, a simple model that incorporates the approximate photoemission threshold and any large band gaps is sufficient. Typically the incident light intensity is assumed to be spatially uniform since the field of view in PEEM images is usually less than the illumination area. Subsequently, local variations in light intensity or photon energy can be assumed to be dynamic responses of the sample as the result of surface features or electron excitations. These dynamic electron excitations also influence the local electromagnetic field. The local photoelectron yield is related to the local photon density, which corresponds to the intensity of the classical electromagnetic field $I \propto E_{\text{tot}}^2$ [10, 11, 16, 19, 33]. $\mathbf{E}_{\text{tot}}$ is the total surface optical electric field, including the incident light and optical response of the material. At any surface location $\mathbf{x}$, there is a power law relationship between the photoelectron current j_e and the intensity of the total electromagnetic field ,

$$j_e \propto \int E_{\text{tot}}^{2n} dt, \quad (8.1)$$

where integration is over exposure time t , and n is the order of the process, e.g., $n = 2$ for two-photon photoemission. The order n is typically assumed to be the minimum number of photons satisfying the energetic consideration $n(hc/\lambda) > W$, though this is only an approximation. Experimental determination from a plot of j_e vs light intensity $I \propto E^2$ via Eq. (6.3) often gives fractional exponents, revealing

several competing processes, some operating above threshold, i.e., proportional to $E^{2(n+1)}$ [96, 193]. When incident light is polarized, limited cross-polarized response is expected and a complex scalar field is sufficient.

The total scalar field is the superposition of incident and response fields, $E_{\text{tot}} = E_{\text{inc}} + E_{\text{exc}}$. The response field includes localized and propagating optical excitations, and may be separated into these constituents $E_{\text{exc}} = E_1 + E_2 + \dots$. Each component has a unique combination of spatial propagation wave vector (where appropriate), frequency (typically same as incident), excitation efficiency, phase delay relative to the incident wave, and absorption coefficient. For pulsed light sources, when the time between pulses is much greater than the duration of a single pulse, j_e is directly proportional to the integration over one pulse. A steady state approximation $j_e \propto \|E_{\text{tot}}\|^2$ is appropriate when the response field decay time is much less than the pulse duration. For propagating optical excitations, the steady state can be used when surface waves travel across the viewing window ℓ in significantly less time than the pulse duration τ . With a maximum speed of c the vacuum speed of light, this condition is met when $\ell/c \ll \tau$. Optical responses in metals and semiconductors attenuate quickly in the visible and UV, so the viewing window is limited by the absorption length $\ell \sim (2\alpha)^{-1}$. With $\alpha \gg 1000 \text{ cm}^{-1}$, $(2\alpha c)^{-1} \ll 17 \text{ fs}$ and pulse durations of $\tau \gtrsim 100 \text{ fs}$ can be considered steady state. Differences from the steady state approximation for pulses even in the regime of $\sim 50 \text{ fs}$ are generally small enough to ignore since most attenuation constants are greater than $10,000 \text{ cm}^{-1}$ in this spectral range. Working in the single-polarization and steady-state regimes, the time-independent photoelectron current at a position $\mathbf{x}$ is proportional to the $2n$ power of the absolute value of the

Figure 8.1: Cross section diagram of stationary interference pattern generation near a diffracting groove in a waveguide with propagating surface electromagnetic fields in PEEM. Incident wave fronts 1 and 4 (red) excite guided wave fronts 1 and 4 (yellow) through diffraction and scattering. The reverse-direction modes (4) are very weakly coupled. These propagate away from the excitation point and interfere constructively with the next incident wave fronts 2 and 5, enhancing photoemission there. Reprinted from Fitzgerald, Word, Saliba, and Könenkamp [173].

superposition of the incident and response fields at that location,

$$j_e(\mathbf{x}) \propto \|E_{\text{inc}} + E_1 + E_2 + \dots\|^{2n} = \left\| E_{\text{inc}} + \sum_j E_j \right\|^{2n}. \quad (8.2)$$

For a localized oscillation, the photoelectron yield measures the correlation between the incident and response fields. Using a variable delay between two incident pulses, this correlation can be measured (cf. Refs. [8, 9]).

With a propagating optical excitation, the correlation takes on a spatial characteristic, producing a stationary interference pattern, as shown in Figs. 8.1 and 7.1. This pattern is readily imaged in PEEM, so it bears further elaboration. If the excitation amplitudes $B_j = |E_j|$ are much less than the incident amplitude $A = |E_{\text{inc}}| \gg B_j$, then spatial distribution of the electric field intensity is

$$\|E_{\text{tot}}\|^2 \approx A^{2n} \left[1 + A^{-1} \left(B_1 \cos k_I^{(0,1)} y + B_2 \cos k_I^{(0,2)} y + \dots \right) + \mathcal{O}(A^{-2} B_j^2) \right] \quad (8.3)$$

with interference wave vectors

$$k_I^{(0,j)} = k_j - k_0 \sin \theta, \quad (8.4)$$

where $\mathbf{k}_0 = k_0 (\hat{\mathbf{y}} \sin \theta - \hat{\mathbf{z}} \cos \theta)$, θ is the angle of incidence relative to the surface normal $\hat{\mathbf{z}}$, $k_0 = 2\pi/\lambda$ is the incident wave number, and $k_j = \mathbf{k}_j \cdot \hat{\mathbf{y}}$ is the surface-parallel component of the excited wave vector. For a single mode, which is the typical case for surface plasmons, the interference maxima are separated by

$$d_I = 2\pi/k_I, \quad (8.5)$$

and allows the ready determination of the excited wave vector k_1 . This uniquely characterizes the response mechanism, especially if the analysis is repeated for more than one polarization [16, 33, 38, 44–46]. For example, if the effective index $N_1 \equiv k_1/k_0 = 1$ is unitary, then the response wave must be traveling in the vacuum, a good indication of a diffracted surface wave [13] or a surface plasmon polariton with most of the field intensity in the vacuum (as occurs with gold and copper at frequencies above the plasmon frequency).

With more than one mode, the interference pattern is less readily interpreted. Instead, it becomes more convenient to examine the power spectrum of the spatial Fourier transform of the interference profile. Then spectrum has peaks centered on the interference wavenumbers with widths proportional to the absorption coefficient α . The Fourier transform also typically shows higher order interference terms, such as the interference between modes with wavenumbers $k_I^{(j,l)} = |k_j - k_l|$. With particularly good signal to noise ratios, nonlinear interference terms are also identifiable in the Fourier spectrum, e.g., $k_I^{(0,j,l)} = k_j + k_l - 2k_0 \sin \theta$ in 2PPE. As an example, the largest

<i>Single-photon accessible</i>			
Label	1	2	3
Intensity	$A^3 B_1$	$A^3 B_2$	$A^2 B_1 B_2$
Wavenumber k_I	$k_1 - k_0 \sin \theta$	$k_2 - k_0 \sin \theta$	$k_2 - k_1$
<i>Multi-photon only</i>			
Label	4	5	6
Intensity	$A^2 B_1^2$	$A^2 B_2^2$	$A^2 B_1 B_2$
Wavenumber k_I	$2(k_1 - k_0 \sin \theta)$	$2(k_2 - k_0 \sin \theta)$	$k_1 + k_2 - 2k_0 \sin \theta$

Table 8.1: Theoretical interference model signal wavenumbers, obtained from the Fourier transform of Eq. (8.3) with two modes $j = \{1, 2\}$ at photoemission rank $n = 2$. The signals are roughly sorted by intensity assuming $A > B_1 > B_2$ and $k_2 > k_1$. Signals 4-6 are unique to multiphoton photoemission, but are often near the noise threshold. Six weaker signals of $\mathcal{O}(AB_j^3)$ are omitted. Additionally, the coefficients B_j may contain attenuation and offset factors that reduce intensity, especially in signals 3 and 6. Adapted from Fitzgerald, Word, Saliba, and Könenkamp [173].

six interference signals of a two-mode, 2PPE interference pattern are presented in Table 8.1. Identifying all the peaks in the Fourier transforms allows an accurate computation of the excited wavenumbers and absorption coefficients, a calculation that becomes highly redundant as more interference signals can be identified.

Experimentally determined wavenumbers for propagating surface plasmon and photonic waveguide modes can be compared to the asymmetric slab waveguide model (see Fig. 6.4), as presented in [194–196]. The asymmetric slab model considers three semi-infinite layers and uses boundary matching conditions of Maxwell’s equations to determine guided wave numbers. The discrete solutions depend on polarization, film thickness, and material optical parameters. For example, following the notation of Yariv [194], photonic modes are determined by solving

$$\frac{p + q}{h(1 - pq/h^2)} = \tan(ht), \quad (8.6)$$

where

$$h = k_0 \sqrt{n_2^2 - N^2},$$

$$q = k_0 \sqrt{N^2 - n_1^2} \times \begin{cases} 1 & (\text{TE}) \\ n_2^2/n_1^2 & (\text{TM}) \end{cases},$$

$$p = k_0 \sqrt{N^2 - n_3^2} \times \begin{cases} 1 & (\text{TE}) \\ n_2^2/n_3^2 & (\text{TM}) \end{cases},$$

n_j are the layer refractive indices, and $N = k/k_0$ is the guided wave effective index. In photoemission experiments one outer layer is always vacuum, with $n = 1$, and here the other layers are limited to gold, ITO, and glass, with optical properties and thicknesses given in the previous chapter. Effective indices solving this equation for vacuum/ITO/glass layers vary with film thickness, as shown in Fig. 8.2. Potentially several modes can be excited for each polarization, with the excited wave effective indices ranging between the refractive index of the central layer and the outer layers. In photonic waveguides, the lower limit is the larger refractive of the outer layers, while in PEEM plasmonics it is the vacuum index 1. These modes represent distinct standing wave patterns between the outer layer boundaries. With the thin films considered here, only symmetric and antisymmetric modes are relevant. Examples of the field intensities of symmetric modes are shown in Fig. 8.2.

The asymmetric slab model applies equally well to plasmonic propagating waves, though some adjustments on solution methods must be made to accommodate the unique role of the complex part of the refractive index (or dielectric constant) [197]. The three-layer model provides sufficient accuracy in the cases examined here, but many cases can be approximated by two layers. Specifically with gold films thicker than 60–100 nm at the wavelengths probed here, essentially all of the excitation energy is concentrated at the gold-vacuum interface or in the vacuum. In this case,

Figure 8.2: (a) Single-mode solutions to the dielectric asymmetric slab model consisting of vacuum/ITO/glass, as illustrated in Fig. 6.4. For thicker films, multiple modes exist. (b) Guided mode field intensity for an ITO film thickness of 60 nm. The modes shown here are symmetric.

the complex propagation constant β is given by

$$\beta = k_0 \sqrt{\frac{\epsilon_1 \epsilon_2}{\epsilon_1 + \epsilon_2}}, \quad (8.7)$$

where the dielectric constant of the insulating layer (vacuum) is ϵ_1 and complex dielectric constant of the metal (gold) is ϵ_2 [198]. The SPP wavenumber $k_j = \Re(\beta)$ and its characteristic propagation length $L = [2\Im(\beta)]^{-1}$ follow from β . For thinner metal films, the modes bound to the vacuum interface interact with those at the ITO (or glass) interface, and the full three-layer model is more appropriate. Solutions (Fig. 8.3) give symmetric and antisymmetric coupled modes that deviate significantly from the single-mode solutions of the simple vacuum/gold and gold/ITO interfaces for gold thicknesses less than ~ 80 nm. The symmetric mode generally has low spatial confinement with fields that extend far into the boundary dielectric layers (Fig. 8.3). As a result the symmetric mode has high velocity and hence low N . In contrast, the antisymmetric mode is more spatially confined, not limited by thickness, shorter ranged, and more importantly, has generally high N , which is more suitable to waveguide coupling.

Optical field excitations can be coupled to the surface or near-surface region only when the incident light wave vector is appropriately matched. Diffraction at sharp surface features bends rays to range of wave vectors, as illustrated for propagating modes in Fig. 8.4, some of which are resonant with the nanoparticle or surface geometry or material properties and can excite the optical response. For the metals and semiconductors, with absorption coefficients greater than 500 cm^{-1} , diffraction is the most efficient and convenient coupling mechanism. The efficiency of this mechanism depends on the feature geometry and incident wavelength, but generally falls off quickly with increasing deflection angle. When more than one propagating optical

Figure 8.3: (a) Graphical method of solution for the SPP supermodes of a three-layer slab model of vacuum/gold/ITO. In this complex space graph, the propagation constants β plotted here independently satisfy the real and imaginary parts of the equivalent of Eq. 8.6, which are shown as solid and dashed lines, respectively. Complete solutions exist where real and imaginary lines intersect. There are generally two solutions for each gold thickness d , which correspond to the symmetric (s_b) and (a_b) modes. Solutions for five gold film thicknesses shown: (1) 25 nm, (2) 30 nm, (3) 35 nm, (4), 40 nm, and (5) 45 nm. (b) Time-averaged Poynting vector $\langle S_x \rangle$ of the asymmetric field (a_b) and symmetric field (s_b) SPP modes of a 3-layer slab model comprised of ITO, a 40-nm thick gold platelet, and vacuum. Scale normalized such that each SPP wave carries 1 watt per meter along the y-axis, with the x-axis being the propagation direction. Reprinted from Word, Fitzgerald, and Könenkamp [41].

Figure 8.4: Incident light wave vectors can be matched to material and surface optical excitations near diffracting features, such as (a) a narrow slit or (b) a step or edge. The intensity of the diffracted waves is shown below plotted versus scattering angle, and contributes to the coupling efficiency.

mode is excited with coupling coefficients B_1 and B_2 , then the ratio of excited mode amplitudes can be determined from the wavenumber and Fraunhofer diffraction as follows. The geometries considered here are groove, hole, and knife-edge diffraction. Adjacent to a groove, such as in Fig. 7.7, the relative mode coupling strength is

$$B_2/B_1 = \text{sinc}\zeta_2/\text{sinc}\zeta_1, \quad (8.8)$$

where $\zeta_j = k_0 w \sin(\theta - \sin^{-1} k_j/k'_0)$, w is the slit width, and $k'_0 = nk_0$ is the wavenumber in the surface material with refractive index n . For a hole geometry, such as Fig. 7.7, diffraction intensity follows an Airy disc distribution, and the relative intensity is

$$B_2/B_1 = [J_1(\zeta_2)/\zeta_2] / [J_1(\zeta_1)/\zeta_1], \quad (8.9)$$

where $J_1(x)$ is a Bessel function of the first kind, and ζ_j is the same as before with w measuring the hole diameter. Knife-edge diffraction has a more complex relationship and here involved only single modes. Finally, the Fresnel transmission coefficients and phase changes must also be calculated in order to determine the coupling efficiency [199].

With both wavenumbers and coefficients readily calculable from a priori properties, it is possible to compute the electromagnetic field distribution of extended, two-dimensional diffracting structures. The structures can be considered apertures, and guided wave propagate away from the apertures across the surface according to Huygens' principle, which treats every point of a scalar wavefront as a new source wavelet propagating outward in all directions. Since guided waves are bound to the thin film (photonic) or the surface (plasmonic, vacuum-radiative), they can be represented by a two-dimensional wavelet [200],

$$G_j(\mathbf{x}, \mathbf{x}') = \frac{i}{4} e^{-\alpha|\mathbf{x}-\mathbf{x}'|} H_0^{(1)}(k_j|\mathbf{x}-\mathbf{x}'|), \quad (8.10)$$

where $\mathbf{x}$ is the sample location, $\mathbf{x}'$ is the aperture source location, and $H_0^{(1)}(x)$ is a zero-order Hankel function of the first kind. The complex field E_j at any point $\mathbf{x}$ is the superposition of all the wavelets that originated at the boundary of the waveguide $\mathbf{x}'$. Fresnel, and later Kirchhoff, Rayleigh, and Sommerfeld, developed a rigorous method to give $E_j(\mathbf{x})$ by integrating over the boundary values $E_j(\mathbf{x}')$, which is the product of the incident wave phase $e^{i\mathbf{k}_j \cdot \mathbf{x}'}$ and the complex coupling coefficient B_j . With both the wavelet function and the boundary value, it is now possible to calculate the complex scalar field $E_j(\mathbf{x})$ from the two-dimensional Fresnel-Kirchhoff integral [199],

$$E_j(\mathbf{x}) = \oint_{\mathcal{C}} \{E_j(\mathbf{x}') \mathbf{n}' \cdot \nabla' G_j(\mathbf{x}, \mathbf{x}') - G_j(\mathbf{x}, \mathbf{x}') \mathbf{n}' \cdot \nabla' E_j(\mathbf{x}')\} d\ell', \quad (8.11)$$

where $\mathcal{C}$ is a closed curve surrounding the sample points of interest $\mathbf{x}$, $\mathbf{n}'$ is the inward-directed normal vector, and the integration is over the boundary (primed) terms. Suitable approximations exist for partially unbounded regions, such that many situations can be computed. The electromagnetic field distribution of each excited mode can be individually calculated at each sample point $\mathbf{x}$ with Eq. (8.11), and then the intensity distribution is the sum of terms, squared. A map can be created by repeating the computation for several thousand points $\mathbf{x}$. The n th power of the intensity distribution at each point $\mathbf{x}$, as given by Eq. 8.2, is directly comparable to the photoelectron micrograph, where n is the rank of the photoexcitation process.

The Kirchhoff integration approach has the advantages of being relatively intuitive and computationally fast, but it works best for optical excitations with propagation distances longer than a half wavelength. For optical excitations with shorter attenuation lengths or geometries highly sensitive to the near-field effects, it is necessary to solve Maxwell's equations directly. In this case, the calculation can be carried out by the RF-Module of COMSOL 4.3, which solves Maxwell's equations for a triangular mesh to obtain the electric field distribution utilizing a finite-element approach with the full dielectric functions of the materials and the true, three-dimensional spatial dimensions of the device. Whether the field intensity is obtained from Eq. (8.11) or COMSOL, the field can be compared to the photoelectron yield by the power law relationship given in Eqs. (8.1) and (8.2).

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9 Photonics results & discussion

In this chapter, I examine photoelectron images from several different materials and nanostructures. With Eq. 8.1 we can connect photoemission rates to surface fields. Going one step further with Eq. 8.11, we can compute the electromagnetic field distribution at the surface of a material in response to diffracting nanostructures. Looking at PEEM images in this light, we can then view them in terms of the electromagnetic fields and processes they represent.

9.1 *Metal nanostructures*

I begin by examining photoemission patterns from gold nanostructures on ITO, as originally presented in Refs. [28, 30, 37, 42, 172]. This work connects optical excitations at the material surface with the emission of electrons.

First, work done by Word, Dornan, and Könenkamp [28] as I joined the group establishes that specimens illuminated with IR light emit electrons via multiphoton processes. Figure 9.1 shows the UV and IR photoelectron response imaged in PEEM from a random gold nanostructure. The tunable pulsed laser provides photon energies between 1.37 and 1.6 eV. Since the photoemission thresholds for ITO and Au are significantly larger than the IR photon energies, the electrons are emitted via multiphoton processes. Figure 9.2 shows the emission intensity to be proportional to the third power of the laser intensity, indicating a 3PPE process. In the $10 \times 10 \mu\text{m}^2$ area shown in Fig. 9.1 there are ~ 1000 high-intensity photoemission sites, primarily located along the margins of the gold-ITO boundary. Figure 9.2 shows that the photoemission threshold is 4.1 eV, consistent with that of ITO and not that of gold, which is greater than 4.5 eV. Photoelectrons most likely originate from the ITO. A

Figure 9.1: Plasmonic gold random nanostructures. (a) UV-PEEM image using 244 nm light of random gold-ITO nanostructures in one 10×10 micron square (field of view 9×9 microns). (b) 3P-PEEM image using pulsed 790 nm light of the same region, clearly showing plasmonic hot spots.

Figure 9.2: (a) Intensity dependence of the photoemission yield for 800 nm light. Inset: illumination scheme for nanostructured Au films on ITO. (b) Photon-energy dependence of the photoemission yield showing a threshold 3×1.37 eV. Reprinted from Word, Dornan, and Könenkamp [28].

Figure 9.3: Composite micrographs of SEM and multiphoton PEEM images of localized photoemission from ITO in gaps of a plasmonic Au nanostructure at a wavelength of 792 nm. Reprinted from Word, Dornan, and Könenkamp [28], Word, Fitzgerald, and Könenkamp [30].

high magnification image a photoemission hot spot, Fig. 9.3, reinforces this assertion. In this particular example a bridge-type geometry is depicted where the planar ITO film connects two separate Au areas with gaps of ~ 100 nm. The composite micrograph clearly shows that the photoemission originates from the ITO film. Since the ITO has a low absorption coefficient at $\lambda = 780$ nm [187], the photoemission is assumed to be due to energy transfer from the SPP fields of the adjacent, highly absorbing Au film.

The electron emission process is thought to involve the following steps: Infrared light is absorbed in the gold film exciting surface plasmon polaritons—predominantly with the same quantum energy as the exciting photons. The high peak intensities of the femtosecond pulses increase the rate of non-linear excitations to measurable amounts, and plasmons with doubled, tripled, and possibly higher quantum energies are also excited [113]. These coherently excited higher order collective excitations provide the energy needed for single-electron excitations beyond the photoemission threshold barrier, such that electron emission is observed. Alternatively, the high intensity pulses create a high population density of coherent singly-excited surface plasmons. There is enough overlap of the quantum wavefunctions of several quasi-

particles to contribute to the emission of an electron. In either case, the electron emission is observed to originate from ITO in the optical near-field zone of the gold structures. Essentially, the gold films are found to act as optical receivers, inducing electron emission in adjacent ITO regions whose threshold is substantially lower than that of gold. For this near-field emission it is currently not known, if it involves a decay of surface plasmons into photons prior to the observed electron emission, or if the emission energy is also of plasmonic nature.

This photoemission process can be controlled with more selective nanostructures and polarization, as discussed by Könenkamp, Word, Fitzgerald, Nadarajah, and Saliba [37]. Figure 9.4 shows the photoemission from single-crystalline, Y-shaped antennae on ITO in response to an incident light pulse with wavelength 410 nm. At this wavelength both gold and ITO require a two-quanta emission process for the 3.1 eV photons. However, the gold surface—with its higher electron density—dominates in the emission images and, on a linear scale, hardly any emission from the ITO is apparent. The micrographs in Fig. 9.4 show two superimposed electron emission images obtained under illumination with -45° and $+45^\circ$ polarizations. We see that emission sites are distributed quite differently for the two light polarizations. This is apparently due to polarization-dependent in-coupling of the optical power: The in-coupling of light is most efficient at the edge of the Y structure, where the light polarization vector can have a large component perpendicular to the metal surface. This is the case along the left edge of the Y for a polarization of -45° and along the right edge at a polarization of $+45^\circ$. The micrographs indicate a fairly high selectivity for the polarization direction based on the in-coupling process. Under infrared illumination, Fig. 9.5, electron emission originate from the near-field vicinity outside the plasmon excited metal structures instead of from the plasmonically active metal region itself, consistent with our previous interpretation. The eleven structures shown in Fig. 9.5

Figure 9.4: (a) Eleven routers carved from a triangular gold platelet. False color composite image of two PEEM micrographs taken with pulse illumination at 410 nm and -45° and $+45^\circ$ polarizations. Green brightness represents electron emission rate obtained for $+45^\circ$ polarization, red brightness represents electron emission obtained for -45° polarization. (b) Details of a structure from part (a). (c) Emission rate distribution for -45° polarization (left) and $+45^\circ$ polarization (right). Reprinted from Könenkamp, Word, Fitzgerald, Nadarajah, and Saliba [37].

Figure 9.5: (a) Composite PEEM images obtained with DC-illumination at 244 nm (gray scale) and pulse illumination at 780 nm (color). Electron emission for -45° polarization is represented in red, for $+45^\circ$ electron emission is in green. Hot spots at the end points of the Y structure are clearly seen indicating polarization-selective emission from ITO. No emission from the front edge or the surface of the Y-structure is seen. (b) Digital plot of the emission rate for -45° degree polarization. This image is obtained with simultaneous illumination from a Hg lamp (~ 253.7 nm) to provide the contour of the Y structure, and laser pulses at 780 nm for the plasmon excitation. When the emission from the Hg lamp is taken into account, the brightness ratio between the right and left-hand tips of the Y is found to be >10 . Reprinted from Könenkamp, Word, Fitzgerald, Nadarajah, and Saliba [37].

show good reliability in the polarization response. Finally, Word et al. [172] reports similar results with another metallic antennae structure. This report goes one step further by calculating the optical field intensity of the circular antenna structure. The comparison shows good agreement for the lateral distribution and symmetry of the emission pattern across all four polarizations, making the connection between optical excitations and photoemission response even more concrete.

9.2 Dielectric waveguide structures

Photoemission electron microscopy allows the direct visualization of plasmonic near fields through nonlinear multiphoton photoemission. Each of these examples of emission from gold appears to adhere to Eq. (8.2), allowing predictable and precise position control of plasmon-enhanced optical fields and electron emission on a nanometer scale. I next investigate photoemission from dielectric structures, where electrons do not participate in plasmonic quasi-particles; this work was originally presented by Fitzgerald, Word, Saliba, and Könenkamp [173], Fitzgerald, Word, and Könenkamp [175].

Figure 9.6a shows a PEEM micrograph of a diffracting structure in ITO obtained at 244 nm from a frequency doubled Ar⁺-ion laser. The photon energy for this ultraviolet light is 5.1 eV, which is larger than the photoemission threshold energy of ITO, and the PEEM image is therefore obtained in a single-photon photoemission process. Mostly topological contrast is obtained in this imaging mode. The center region B is particularly bright due to surface roughness created by FIB milling.

When illuminated by pulsed light at a wavelength of 410 nm, the character of the PEEM image changes dramatically, as in Fig. 9.6b-c. The vacuum wavelength of 410 nm corresponds to a photon energy of 3.0 eV. As this is less than the threshold, multiphoton photoemission must be assumed. In these images some of the topographical

Figure 9.6: PEEM images of diffracting ITO structure. Laser is obliquely incident from the bottom edge at 60° to surface normal. Regions of interest are indicated by A, B, and C. (a) Single-photon, 244-nm, continuous-wave (CW), TM polarized illumination. (b-c) Two-photon, 410-nm, 100-fs pulsed, (b) TM and (c) TE polarized illumination; shown in false color. Reprinted from Fitzgerald, Word, Saliba, and Könenkamp [173].

features are still recognizable, but many edges now appear highlighted and wave-like interference patterns with wavefronts perpendicular to the illumination direction are now visible. Edges facing the incident light have enhanced emission compared to edges at other orientations, especially in TE polarization. Strong localized emission due to surface inhomogeneities or deposited particles are evident across the sample surface, with varying intensities. These localized features are the signatures of diffraction and near-field radiative modes. Wave-like patterns surround the structure in Fig. 9.6b-c. The patterns exhibit different spacings, decay lengths, and intensity variations in different regions and for different polarizations. With closer inspection, all regions appear to have an offset maximum and beating phenomena. Three different wave fields can be identified; these have been labeled A, B, and C in Fig. 9.6. Region A is in the forward direction of the incident laser beam, i.e., above the slit and outside the trench area. Region B is the trench center region, and region C is in the reverse direction incident to the beam, i.e., below the slit. The average intensity profiles across each region and polarization are shown in Fig. 9.7.

These wave-like patterns are well explained as interference between the guided modes in the ITO layer and the incident light. The interference, illustrated in Fig. 8.1, is similar to those found in plasmonic metal structures, as reported, for example, in [15, 33, 38]. There are, however, significant differences between the plasmonic and the photonic cases: Due to the lower electron densities in the ITO material and the much lower optical absorptivities in ITO as compared to typical metals, the electron emission rates are lower in the photonic case. The observed interference fringes extend over distances of some 10 micrometers, which we can explain with the following formalism. The incident and guided waves have propagation vectors $\mathbf{k}$ and $\mathbf{k}_j$ with in-plane components $k \sin \theta$ and $\pm k N_j$, respectively, where $k = 2\pi/410 \text{ nm}$, $\omega = ck$, $\theta = 60^\circ$, and $\pm N_j$ is the effective refractive index of guided wave $j = 1, 2$ traveling in

Figure 9.7: Two-photon PEEM interference pattern profiles, averaged from the regions marked in insets. (a-b) TM-polarized, (c-d) TE-polarized. Reprinted from Fitzgerald, Word, Saliba, and Könenkamp [173].

Figure 9.8: Fourier transform spectra of Fig. 9.7, where $k = 2\pi/410$ nm. Six interference peaks are highlighted in each spectrum, with signals 4-6 unique to multiphoton interference. The six spectra are (a-c) TM-polarized, (d-f) TE-polarized; from the regions marked in insets. Reprinted from Fitzgerald, Word, Saliba, and Könenkamp [173].

the forward (+) or reverse (−) direction. Interference maxima are separated by distances $d_{j=1,2} = 2\pi/k_I^{(0,j)} = 2\pi/k(N_j \mp \sin \theta)$ and $d_3 = 2\pi/k(N_2 - N_1)$, where $N_2 > N_1$, just as discussed the previous chapter. Furthermore, we may extract additional information by applying a Fourier transform (FT) to the interference pattern, which allows comparison of the image to the theory relating photoemission to the superposition of electric fields at the surface. The one-dimensional FT of the patterns in the three regions are shown in Fig. 9.8. There are a total of at most six different wave numbers k_I in the interference patterns, which are apparent as peaks in the Fourier transform, and summarized in the previous chapter (Table 8.1). These six signals are labeled in the experimental fast Fourier transforms (FFTs), Fig. 9.8. With two N_j for each surface region (A and B) and polarization (TM, TE), a total of eight modes in

Signal	k/k_0	Theory, TM	Exp., TM	Theory, TE	Exp., TE
1	$N_1 - \sin \theta$	0.86	0.86	0.99	0.98
2	$N_2 - \sin \theta$	1.17	1.19	1.20	1.22
3	$N_2 - N_1$	0.30	0.34	0.22	0.22
4*	$N_1 + N_2$	2.03	2.05	2.19	2.22
5*	$2(N_1 - \sin \theta)$	1.73	1.72	1.97	1.95
6*	$2(N_2 - \sin \theta)$	2.34	2.39	2.40	2.44

Table 9.1: Effective indices calculated using asymmetric dielectric slab waveguide model: $N_1 = 1.73$ (TM), 1.85 (TE), $N_2 = 2.03$ (TM), 2.07 (TE). Signals 4-6 are unique to multiphoton photoemission. These are compared to indices measured from the PE interference pattern.

the forward direction is obtained. There are also four modes in the reverse direction (region C). These modes in the reverse direction have different interference spacing but the same effective indices as in region A, as indicated in Table 8.1, providing an additional consistency check.

The Fourier spectra in Fig. 9.8 exhibit broadened resonances due to the short decay length of the surface waves. In the Fourier transforms, attenuation produces a Lorentzian peak shape whose half width at half maximum (HWHM) is the absorption coefficient, α . In both TM and TE region A modes, $\text{HWHM} \approx 0.05k = 7700 \text{ cm}^{-1}$. These values are in very good agreement with transmission measurement on ITO films [180, 185]. This is a confirmation that the observed waves propagate through the ITO layer. The asymmetric slab waveguide model predicts two guided modes for both TM and TE polarizations, and also provides theoretical predictions for the effective indices, which can now be compared with the experimental results. Such a comparison is presented in Fig. 9.9 and Table 9.1. Table 9.1 demonstrates that the theoretical effective indices are consistent with those obtained experimentally. The predictions also nicely show the observed index difference for the two thicknesses available in the structure. The ratio of two mode coefficients, B_1/B_2 , can be measured from the Fourier transform, Fig. 9.8, using the coefficients given in Table 8.1. The ratio can

Figure 9.9: Allowed modes of the vacuum/ITO/glass waveguide model for ITO films of 200 to 320 nm. Experimental results determined from FFT indicated with error bars. Reprinted from Fitzgerald, Word, Saliba, and Könenkamp [173].

also be calculated from the effective indices, independently measured from the Fourier transform. These two methods are found to be in good agreement. In addition, diffraction can explain why the primary propagating wave interference maxima are not coincident with the slit edge. Following an argument similar to [?], light diffracted into the ITO layer at angle β_j is reflected at the ITO-glass boundary. That ray returns to the ITO-vacuum surface a distance $\Delta y_j = 2t[1 - (N_j/n_{\text{ITO}})^2]^{-1/2}$ from the slit, eliminating the angle $\beta_j = \sin^{-1} N_j/n_{\text{ITO}}$ with Eq. (8.8). Δy_j is the distance between the slit edge and the primary maximum. Using the effective indices measured from the Fourier spectrum, the computed distances are 0.6–1 μm in the dominant waveguide modes, as given in Table (9.2), consistent with the observed phase offsets in regions A and B of Fig. 9.6b-c.

The center region modes have some obvious differences from the surrounding region modes. The most striking observation is that the spacing of the interference

	Expression	Thy., TM	Exp., TM	Thy., TE	Exp., TE
Δy_1	$2t (n_{\text{ITO}}^2/N_1^2 - 1)^{-1/2}$	0.77 μm	0.76 μm	1.03 μm	0.93 μm
Δy_2	$2t (n_{\text{ITO}}^2/N_2^2 - 1)^{-1/2}$	2.06 μm	2.06 μm	2.66 μm	2.69 μm

Table 9.2: Distances Δy_i are the distance an equivalent ray would travel from trench edge to reflection at glass boundary and back to ITO surface.

pattern in Region B is smaller than in Region A, indicating a smaller effective refractive index. This is explained by the fact that the guided wave also probes the space outside the geometrical volume of the ITO layer in the trench. As Region B is thinner than Region A, the vacuum refractive index has a larger contribution to the effective index for the guided modes in Region B. As a consequence, a lower effective index, a longer wavelength, and a larger spacing in the interference pattern result. This is in complete agreement with the asymmetric slab waveguide model, as compared in Fig. 9.9. Another difference is the extremely rapid decay of the center modes, which have attenuation coefficients in the range $12\text{--}21 \times 10^3 \text{ cm}^{-1}$, 2-3 times larger than in Region A. This is most likely due to lateral confinement of the trench region. Guided modes are best confined if the refractive index of the confining layer is greater than the surrounding materials. Since the effective indices of Region B are less than in Regions A and C, the confinement in the center trench is “leaky” which results in a stronger damping of the propagating modes [194]. Region B has two additional interesting features which contribute to increased background brightness. At the far edge, reverse modes (counter propagating modes) are coupled in and interfere with the forward propagating waves. The result is that the region is generally brighter than the surrounding bulk surface but without a strong contrast in the interference pattern, as seen in the profiles Fig. 9.7. Secondly, the surface of the trench was FIB milled, unlike Regions A and C. FIB milling modifies surfaces, changing surface roughness and disrupting the surface homogeneity due to gallium impact [201]. The difference

in surface roughness between the center and bulk surface regions is also visible in the 1PPE image, Fig. 9.6a. These changes are generally limited to a shallow surface depth, so FIB milling should have negligible effect on wave-guiding within the ITO layer.

It is worth briefly discussing other features of the two-photon photoemission images. The top edges of the slit and center region are significantly narrower than the interference pattern maxima, indicating tightly confined electromagnetic fields. Diffraction fringe fields extend around hot spot sites in the multiphoton PEEM micrographs and are significantly weaker under TE polarization. The occurrence of these fringes has been discussed in some detail in Chelaru et al. [13]. The width of the fringe maxima varies with particle size and is projected further in the forward direction than in the reverse. These features clearly distinguish the waveguide modes from diffraction phenomena. The fringe fields can be explained using Fraunhofer (far field) diffraction around an opaque aperture-like object, which predicts a minima immediately surrounding the particles and gives a first maximum spacing $\Delta y \approx 3.83\lambda A/\pi \sin 30^\circ$ in the forward direction, where A is the aspect ratio of height to diameter [13]. For $A \leq 1$, this formula predicts a variable spacing $\Delta y \lesssim 1 \mu\text{m}$, consistent with the forward fringes observed in Fig. 9.6.

It is of interest to determine the potential accuracy of PEEM in this optical application, particularly for the experimentally observed optical parameters such as the refractive index, the absorption coefficient and relative phase shifts. The Fourier transform evaluation provides interference pattern spacings with an accuracy of 3%, the effective indices of the guided modes with 5%, and the absorption coefficient with 9%. If the laser wavelength, the angle of incidence, and the film thickness could be determined with significantly better accuracy, then the optical parameters of the waveguide might be determined with high precision in areas as small as a few

Figure 9.10: PEEM micrographs of a waveguide bounded by a circular groove. Light is incident from the bottom edge of the images. The 1PPE image shows the milled groove down to the glass substrate as a lighter shade. The 2PPE images (in false color) show modulations in the surface electromagnetic field due to interference between incident and guided light. Reprinted from Fitzgerald, Word, and Könenkamp [175].

microns. The determination of relative phase shifts can be obtained from a direct image analysis of Fig. 9.7 once the periods are determined from the Fourier analysis. The slit edge can be taken as the reference position for this comparison. A basic analysis using fitted waveforms indicates that the two images provide an accuracy of 24 nm for the relative phase shifts of the two polarization modes depicted. This corresponds to $\lambda/17$. These results for local averages of the optical constants and the dynamic phase shifts in diffractive in-coupling nicely demonstrate the potential for PEEM imaging in planar optics applications.

Bolstered by the success of Eq. (8.2) in one-dimensional photonic waves, I next consider two-dimensional patterns, calculating the electromagnetic field from Eq. (8.11). Figures 9.10 and 9.11 show PEEM micrographs of the semicircular hole assembly and groove encircling a disc-shaped waveguide region, respectively. As before, the 1PPE images show topographic features, similar to an SEM image. Modulations in electron emission due to surface light interference are less pronounced. On the other hand, the 2PPE images show much stronger contrast resulting from the superposition

Figure 9.11: PEEM micrographs of a semicircle of holes. Light is incident from the bottom edge of the images. The 1PPE image shows topographic features, similar to an SEM image, as well as some diffraction. The 2PPE images (in false color) show modulations in the surface electromagnetic field due to interference between incident and guided light. Reprinted from Fitzgerald, Word, and Könenkamp [175].

of guided fields from curved sources and the incident light. Guided waves refracted into the disc structure in Fig. 9.10 converge at multiple foci, with the dominant focus attributable to the forward direction and a weaker, secondary focus from the reverse direction found just below the primary focus. Bright line patterns diverge from the structure in Fig. 9.11 as a result of constructive interference between two or more holes. The presence of multiple waveguide modes leads to the fractured appearance of beating in Fig. 9.10 and the line patterns in Fig. 9.11.

Analysis of Figs. 9.10 and 9.11 yields the guided mode effective indices and relative mode intensities, which can be quantitatively compared to theoretical calculations to complement qualitative comparison of the experimental and theoretical images. The fields of a single, representative hole are shown in Fig. 9.12, which is reconstructed from an average of the fields surrounding a selection of holes in the assembly. Figure 9.13 shows line profiles bisecting the hole in the direction of incident light. The effective indices and relative strengths of the two guided modes can be more readily

Figure 9.12: Experimental and simulated 2PPE interference patterns generated by a single hole. The experimentally derived patterns are composite sums of the 2PPE near each hole in Figure (9.11). Reprinted from Fitzgerald, Word, and Könenkamp [175].

Figure 9.13: 2PPE pattern from a single $0.5\text{-}\mu\text{m}$ hole. (a,b) Line profiles taken in the direction of incident light, with simulated line profile shown in light gray. (c,d) Fourier transform power spectra of the line profiles plotted vs. interference wavenumbers normalized by vacuum wavenumber. Simulated spectra are shown in light gray, experimental data in heavy black. Reprinted from Fitzgerald, Word, and Könenkamp [175].

determined from the Fourier transform power spectra of the line profiles, also shown in Fig. 9.13. Adding the in-plane component of the incident wavenumber to the interference wavenumber gives the guided mode wavenumber, or, in terms of the effective index, $N = k_I/(k + \sin \theta)$. The measured values are $N_{1\text{TE}} = 1.78$, $N_{2\text{TE}} = 2.05$, $N_{1\text{TM}} = 1.68$, and $N_{2\text{TM}} = 2.02$. Using these effective indices, I calculate an ITO film thickness of 265 nm, which is consistent with the 250 ± 40 nm measured in SEM. Fig. 9.10 gives similar effective indices as the holes since the film is roughly the same thickness. The relative intensities can also be determined from the peak intensities of the Fourier transform power spectrum, giving 0.28 (TE) and 0.38 (TM) for the holes. These values conform to within 6% with a Fraunhofer diffraction model based on the Airy disc, Eq. (8.9). In the disc, $(B_2/B_1)_{\text{TM}} = 0.84$ and $(B_2/B_1)_{\text{TE}} = 0.41$, which agree with a slit diffraction model, Eq. (8.8), also to within 6%.

Next, I compute the expected photoelectron yield intensity of our theory, beginning with the coupling coefficient, B_j . Fields diffracted through a hole could be approximately modeled with a real transmission coefficient that is unity for the top edge and 0.66 for TE and 1.0 for TM modes for the bottom edge of a hole. Because of the extended nature of the circular groove, it was necessary to use boundary values that vary with position around the circular groove edge [199]. The results for this calculation are shown in Fig. 9.14. Next, individual field distributions E_j are calculated from a numerical integration of the Kirchhoff formula Eq. (8.11), with the calculated wave mode numbers in the Green's function wavelet. Subsequently the total surface fields are linear superpositions of the incident wave field and the two guided mode fields, as in Eq. (8.3), weighted according to their diffractive coefficients, given by Eqs. 8.8 and 8.9. Constructing the field distribution of multiple holes requires a further superposition of individual hole fields. The relative 2PPE intensities are then computed from the total surface fields using Eq. (8.2). Figure 9.12 shows the theo-

Figure 9.14: (Top) Calculated efficiency of TE and TM incident light for generating TE-like (solid line) and TM-like (dotted line) guided modes in the ITO, with 0° position at the bottom and 180° at the top of the disc. (Bottom) Simulated 2PPE pattern for the disc structure. Reprinted from Fitzgerald, Word, and Könenkamp [175].

Figure 9.15: Simulated 2PPE patterns constructed from a superposition of single hole simulations. Individual hole line profiles and spectra are compared to experiment in Fig. 9.13. Reprinted from Fitzgerald, Word, and Könenkamp [175].

retical photoelectron yield intensities of a single hole, with quantitative comparisons to experimental data given in Fig. 9.13. Theoretical PE yields of the more advanced structures of a disc and semicircle of holes are shown in Figs. 9.14 and 9.15.

Overall the calculations in Figs. 9.13, 9.14, and 9.15 show excellent agreement with the experimental 2PPE electron micrographs in Figs. 9.10 and 9.11. Single hole simulations reproduce the observed asymmetric interference patterns, with bright, widely-spaced interference maxima in the direction of the incident light wave vector, weak, finely-spaced maxima in the opposite direction, and a smooth gradient of maxima intensity and spacing along the sides. Both modeled and experimental images of the hole assembly have similar patterns of speckles, diverging lines of constructive interference maxima in the forward direction, and finer lines of interference maxima parallel to the incident wave vector in the reverse direction. In the disc structure, the model maxima follow the contour of the groove edge as observed. Additionally, the locations and intensities of foci as well as the beating between the two guided modes are accurately reproduced. Differences between model and observed 2PPE images highlight the depth of information in present 2P-PEEM electron micrographs. These are especially apparent in near-field zones, around groove and hole edges, and are

Figure 9.16: (a) Ultraviolet PEEM micrograph of diffraction at the edges of a nanostructured Si wafer. The arrow indicates the direction for the line scan. (b) Photoemission line profile in the direction of the arrow in (a). The experimental data are plotted as black dots, the calculated profile is plotted as a continuous line in red and is based on Eq. (8.5) with a propagation velocity $v = c$ and a decay length of 470 nm. Reprinted from Word, Fitzgerald, and Könenkamp [174].

likely the result of more complicated optical and geometric properties than in the idealized simulation.

9.3 Diffracted waves

Diffraction without guided modes and the interaction between plasmonic and photonic modes provide final examples of the close relationship between photoemission and optical near-fields. The results presented here were originally presented in Word, Fitzgerald, and Könenkamp [41, 174]. Replacing the transparent ITO film with a highly absorbing silicon wafer strongly suppresses wave propagation within the sample material, as the high optical absorption coefficient corresponds to an absorption length of only 3 nm. Yet a diffraction-based interference pattern is still observed in this case as shown in Fig. 9.16. The analysis of the diffraction pattern shows that the diffracted wave propagates in an effective index $N = 1$, indicating that the photoemission image is now due to interference between a diffracted wave propagating through vacuum and the incident light. This wave is apparently part of a wave scattered by a linear feature at the Si surface and propagating in the vacuum above the Si surface. The physical mechanism to generate the photoemission image in this case is

the spatially varying electric field immediately above the samples surface. Apparently the spatially modulated field strength changes the photoemission rate. Figure 9.16 shows that similar to the waveguide case in ITO, the experimental data are good enough to establish phase shifts occurring within the near-field of the diffracting edge feature as well as losses along the propagation. Rotating the illumination vector and comparing two polarizations, Fig. 9.17a shows that the strength of the forward edge scattered wave varies significantly with polarization. By applying Eq. (8.11) to each electromagnetic field component, the Fresnel-Kirchhoff method of calculating the two-dimensional field can more readily accommodate the differences in diffraction strength with polarization. The intensity and photoemission pattern can be computed from the norm of the vectorial field. Fitting the PE micrograph for the coupling coefficients and polarization yields Fig. 9.17b. The fitting indicates that the maximum diffracted wave coupling strength is $\sim 20\%$, and the scattered wave couples more strongly with the forward perpendicular edge than parallel edges, by a factor of $\sim 2.5\times$, or the reverse edge by $\sim 3\times$. These factors are multiplicative to the coupling already built into the Kirchhoff diffraction formula.

A second example of optical diffraction is shown in Fig. 9.18. In this case, incident light diffracts at the edge of an unmodified, single-crystalline 60-nm-thick, gold platelet on an ITO substrate. Analysis of the interference pattern in the forward direction yields a wave traveling at the speed of light. Fig. 9.18c shows the photoemission distribution calculated by the same method as the silicon square. Near the triangle, a groove has been milled into the ITO layer, as seen in Fig. 7.8, and several nanoflakes are located in the vicinity. This cluster is of further interest because PEEM images in Fig. 9.19 capture the interaction between photonic modes, which are diffraction coupled into the ITO layer at the 10- μm groove, and plasmonic excitations in the Au flakes. The presence of many types of optical phenomena makes description and

Figure 9.17: (a-b) PEEM micrographs of diffraction at the edges of a nanostructured Si wafer, rotated relative to Fig. 9.16. Ultraviolet light incident from the bottom edge is TM- (a) or TE- (b) polarized. (c-d) Photoemission patterns calculated using Eq. (8.11) and the optical properties of Si for a diffracted (radiative) wave for (a) TM and (b) TE incident light.

Figure 9.18: (a) 2P-PEEM micrograph of diffraction at the edges of a triangular Au platelet. Visible 410-nm, TM-polarized light is incident from the bottom. (b) Line profile of the photoemission rate taken perpendicular to the bottom edge. Black dots: experimental data, red line: fit based on optical data of Palik [202] with a decay length of 380 nm. Reprinted from Word, Fitzgerald, and Könenkamp [174]. (c) Photoemission patterns calculated using Eq. (8.11) and the optical data of Au.

Figure 9.19: (a) Imaging photoelectrons are emitted as the incident laser interferes with guided photonic waves coupled into a slit or plasmonic waves bound to gold. (b) UV-PEEM of gold flakes on ITO. (c) False color 2P-PEEM taken with 410-nm TM-polarized light and (d) TE-polarized light. Reprinted from Word, Fitzgerald, and Könenkamp [41].

analysis complicated. In the UV, ITO is opaque and the micrograph shows the ITO substrate, FIB-milled groove in the ITO, and gold platelets and particles with mostly topographical detail plus some yield modulation due to diffraction. In 2P-PEEM the images are very different. The most obvious difference is a series of horizontal bands due to interference between the incident laser and the guided photonic modes.

Direct imaging of photonic and plasmonic waves is an important demonstration of the use of PEEM in the study of integrated photonic circuits. The experimental identification of a photonic vacuum mode above a solid surface indicates that PEEM can also be used to probe electric fields outside the electron emitting material. The examples discussed here indicate that a complete visualization of diffraction phenomena including plasmonic and photonic modes and their inter-conversion may be achievable.

IV Conclusions

The work presented here demonstrates that photoemission microscopy is a sensitive, powerful, and versatile tool for exploring near-field optical phenomena. While aberration limits current resolution, in Part II demonstrate that spherical and chromatic aberration can be corrected with an electrostatic mirror. Part III shows evidence of vacuum modes, guided photonic modes, and plasmonic surface modes that can be directly visualized in conceptually simple interference experiments.

The hyperbolic mirror geometry presented here has the virtue of allowing analytic solutions in the calculation of electron trajectories and optical properties. The expressions derived for a single hyperbolic region can be coupled together to give an analytic description of a multi-electrode mirror. Such an analytic solution is a very powerful tool in understanding the behavior of a corrector as a tool. Analytic treatment also allows for efficient design optimization. I gave a description of a triode mirror, with two hyperbolic regions, and a simple einzel lens. This mirror-lens combination is the simplest arrangement that can provide a wide range of dynamic correction in which the spherical and chromatic coefficients of correction can be independently varied. All variations can be controlled with three electrode potentials. The analytic description of this corrector agrees well with results from a numerical model based on a simple version of a realistic device.

Implementation of a triode mirror corrector into our PEEM is underway. This process has required high precision characterization of the new corrector as well as of previously installed elements of the microscope. To better estimate the aberration of the microscope, I have presented an optical characterization of several photoemission specimens after imaging by the accelerating field, objective lens, and auxiliary lens.

This characterization has already been implemented in the PEEM software, leading to a decoupling between specimen focusing and magnification of the objective-auxiliary lens zoom pair. Second, the new hyperbolic triode mirror was designed based on the proven diode hyperbolic mirror already installed in the PEEM, placing several physical constraints on the device. The spacing of the electrodes and the lens was optimized within this framework to nonetheless provide a large range of dynamic and independent aberration correction. A complete characterization of the full triode mirror configuration space demonstrates that this range should be more than enough to correct photoelectron image aberrations. With the characterization presented here, the objective and mirror branches of our PEEM can be controlled with high precision, promising aberration free photoelectron micrographs.

Part III shows evidence of photonic vacuum modes, guided photonic modes in transparent media, and plasmonic surface modes that can be directly visualized in conceptually simple interference experiments. The high spatial resolution of PEEM provided by aberration-corrected electron optics with a diode mirror allows for quantitative analysis of wave speed, propagation length, and relative intensities, differentiating between the various forms of surface electromagnetic phenomena and leading to a better understanding of the physics of nanophotonic structures. By extending the interferometric analysis, I have also analyzed the interactions between surface plasmons and guided photons. In addition, I also offered a method for calculating surface fields and relative photoemission rates of more complicated optical structures based on the wave diffraction theory of Kirchhoff. The calculated field intensity, either from this method or a finite-element simulation, can be simply and convincingly related to the observed photoemission patterns with a simple power-law relationship. These findings complement and significantly augment earlier work that has demonstrated the visualization of plasmon propagation in thin metallic films using a very similar

approach [9, 24, 32, 33, 38, 44–46].

Thus, PEEM combines the ability to observe a wide range of electromagnetic phenomena with sub-wavelength sensitivity and excellent resolution. The high contrast inherent to multiphoton photoemission is particularly well suited to planar nanoscale optical devices where these parameters are of importance [203], as, for example, in high-confinement waveguides [204], high sensitivity biochemical sensing devices [205], quantum coherent devices [206], and ultrafast optical switches [207]. Such intimate knowledge opens near-field optics to quantitative experimental analysis and allows new approaches for the development of photonic and plasmonic metamaterials.

V References & Appendices

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-

Appendix A Scale drawings: diode PEEM

Scale drawing of our PEEM before installation of the triode mirror corrector. This drawing is significantly the same as the working instrument, with the exception of the objective lens and interface lens bore diameters, of which a variety of lenses were used. Credit: R.C. Word.

Appendix B   Code, *Mathematica*: hyperbolic mirror theory

The optical properties in Figs. 3.3, 3.4, 4.2, 4.3, 4.4, 4.8a, 4.8b, and 4.8 were evaluated using Mathematica 8 running the following code.

```

SetOptions[Plot, Frame → True, Axes → False,
  AspectRatio → 1, GridLines → Automatic, PlotStyle → Thick,
  BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ParametricPlot, Frame → True, Axes → False,
  AspectRatio → 1, GridLines → Automatic, PlotStyle → Thick,
  BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ParametricPlot3D, AspectRatio → 1, BoxRatios → {1, 1, 1},
  PlotStyle → Thick, BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ListPlot3D, AspectRatio → 1, BoxRatios → {1, 1, 1},
  PlotStyle → Thick, BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[Plot3D, AspectRatio → 1, BoxRatios → {1, 1, 1},
  PlotStyle → Thick, BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ListPointPlot3D, AspectRatio → 1, BoxRatios → {1, 1, 1},
  PlotStyle → Thick, BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ListSurfacePlot3D, AspectRatio → 1, BoxRatios → {1, 1, 1},
  PlotStyle → Thick, BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ListPlot, Frame → True, Axes → False,
  AspectRatio → 1, GridLines → Automatic, PlotStyle → Thick,
  BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ListLogPlot, Frame → True, Axes → False,
  AspectRatio → 1, GridLines → Automatic, PlotStyle → Thick,
  BaseStyle → {FontFamily → "Arial", FontSize → 7}];
SetOptions[ListLinePlot, Frame → True, Axes → False,
  AspectRatio → 1, GridLines → Automatic, PlotStyle → Thick,
  BaseStyle → {FontFamily → "Arial", FontSize → 7}];

```

Basic Theory

This is a reproduction of Gert's paper (1990), specifically the graphs (fig 4).

■ Theory

The position of an electron at the turn-around (potential there is V_C). The turn-around is a hyperboloid surface. This treats $\rho_C > 0$ as the independent variable.

$$\xi_C = \sqrt{(\nu - 1) \ell^2 - \left(\frac{\rho_C}{2}\right)^2};$$

The position, velocity, and angle of an electron at electrode V_A . t_A is the time of flight from the turn-around.

$$\begin{aligned} \nu &= \frac{V_A - V_C}{V_A - V_m}; \\ k &= \frac{V_A - V_m}{\ell^2}; \\ \omega &= \sqrt{e k / m}; \\ \Theta &= \omega t_A; \end{aligned}$$

$$\begin{aligned}
\xi_a &= \xi_c \cosh[\sqrt{2} \theta]; \\
\rho_a &= \rho_c \cos[2 \theta]; \\
d\rho_a &= -\omega \rho_a \tan[\theta]; \\
d\xi_a &= \sqrt{2} \omega \xi_a \tanh[\sqrt{2} \theta]; \\
\alpha_a &= \text{ArcTan}\left[-\frac{d\rho_a}{d\xi_a}\right];
\end{aligned}$$

The V_A position coordinates are also related by

$$\xi_a = \sqrt{\ell^2 - \left(\frac{\rho_a}{2}\right)^2};$$

The position, velocity, and angle of an electron when it crosses the axis. This includes the lensing effects of the opening in V_A .

$$\rho_x = 0;$$

$$\alpha_x = \alpha_a - \frac{\rho_a \sqrt{1 + \left(\frac{\rho_a}{2\ell}\right)^2}}{2\sqrt{\ell}};$$

$$\xi_x = \xi_a + \frac{\rho_a}{\tan[\alpha_x]};$$

■ Solution, Functions & Plots

■ Solving for $\theta^{(1)}$

Simplifying in terms of some unitless parameters:

$$\alpha = V_a / V_m; \quad v = (V_a - V_c) / (V_a - V_m); \quad rc = \rho_c / \ell; \quad \tau = \sqrt{-\frac{m \ell^2}{e V_m}}; \quad zc = \xi_c / \ell;$$

To first order, $\xi_A = \ell$, which allows solution for t_A . Simplifying this equation into unitless parameters,

$$\text{Solve}\left[\sqrt{1 - v - rc^2} \cosh[\sqrt{2} \theta] == 1, \theta\right]$$

$$\theta_1 = \sqrt{\frac{1}{2}} \text{ArcCosh}\left[\sqrt{\frac{1}{1 - v - rc^2}}\right];$$

■ Solving for $\theta^{(2)}$

Take the first order solution and use it to calculate $r_A = \rho_A / \ell$, $z_A = \xi_A / \ell$:

$$ra_1 = rc \cos[\theta_1];$$

$$za_1 = \sqrt{1 + \frac{ra_1^2}{2}};$$

$$\text{Solve } z_A^{(1)} = \xi_c \cosh \sqrt{2} \theta^{(2)}:$$

$$\text{Solve}\left[\text{za1} == \sqrt{1 - \nu\nu - \text{rc}^2} \cosh\left[\sqrt{2} \theta\right], \theta\right]$$

$$\theta_2 = \sqrt{\frac{1}{2}} \text{ArcCosh}\left[\frac{\sqrt{1 + \frac{\text{rc}^2}{2} \left(\cos\left[\sqrt{\frac{1}{2}} \text{ArcCosh}\left[\sqrt{\frac{1}{1 - \text{rc}^2 - \nu\nu}}\right]\right)\right)^2}}{\sqrt{1 - \nu\nu - \text{rc}^2}}}\right];$$

■ z_0 / ℓ

Only solve for paraxial rays ($\rho_c = 0$):

$$\theta_0 = \sqrt{\frac{1}{2}} \text{ArcCosh}\left[\frac{1}{\sqrt{1 - \nu\nu}}\right];$$

Using equation (15) from the paper, the paraxial object/image distance:

$$\text{zx0} = 1 + 2 \frac{\nu\nu}{\sqrt{2 \nu\nu} \tan[\theta_0] - 1}$$

```
GraphicsRow[{Plot[zx0, {vv, .65, .99}, PlotLabel -> "Basic Hyperbolic Mirror",
  FrameLabel -> {"v = (V_A - V_C) / (V_A - V_M)", "z_0 / {"},
  PlotRange -> {0, 8}, Frame -> True, Axes -> False],
  Plot3D[zx0 /. {vv -> (alpha - chi) / (alpha - 1)}, {chi, .65, .999}, {alpha, 0, 1},
  PlotLabel -> "Basic Hyperbolic Mirror", AxesLabel ->
    {"V_C/V_M", "V_A/V_M", "z_0 / {"}, PlotRange -> {0, 8}]], ImageSize -> 800]
```

■ C_c / ℓ

$$\theta_0 = \sqrt{\frac{1}{2}} \text{ArcCosh}\left[\sqrt{\frac{1}{1 - \nu\nu}}\right];$$

From equation (17), C_c / ℓ

$$\text{Cc0} = -\frac{\nu\nu}{1 - \nu\nu} \left(1 + 2 \frac{\nu\nu}{\sqrt{2 \nu\nu} \tan[\theta_0] - 1} + \frac{3}{4} \frac{1}{\nu\nu^2} \left(\frac{2 \nu\nu}{\sqrt{2 \nu\nu} \tan[\theta_0] - 1} \right)^2 \right)$$

```
GraphicsRow[
  {Plot[-Cc0, {vv, .65, .99}, PlotLabel -> "Basic Hyperbolic Mirror",
    FrameLabel -> {"v = (V_A - V_C) / (V_A - V_M)", "-C_c / {"},
    Frame -> True, Axes -> False, PlotRange -> {0, 160}],
    Plot3D[-Cc0 /. {vv -> (alpha - chi) / (alpha - 1)}, {chi, .65, .99}, {alpha, 0.001, 1},
    PlotLabel -> "Basic Hyperbolic Mirror", AxesLabel ->
      {"V_C/V_M", "V_A/V_M", "-C_c / {"}, PlotRange -> {0, 160}]], ImageSize -> 800]
```

■ Solving for C_s / ℓ

Need to calculate $z_A(\rho_c)$

$$\text{ra2} = \text{rc} \cos[\theta_2];$$

$$\text{za2} = \sqrt{1 + \frac{\text{ra2}^2}{2}};$$

Use this to calculate α , z in the small angle limit ($\tan \alpha \approx \alpha$)

$$\alpha x2 = \frac{ra2 \tan[\theta2]}{\sqrt{2} za2 \tanh[\sqrt{2} \theta2]} - \frac{ra2 za2}{2 vv};$$

$$zx2 = za2 + \frac{ra2}{\alpha x2}$$

Now calculate $\Delta z / \alpha^2$

$$\Delta zx2 = zx2 - zx0;$$

$$Cs2 = \text{Series}\left[\frac{\Delta zx2}{\alpha x2^2}, \{rc, 0, 0\}\right] // \text{Normal} // \text{Chop}$$

At high enough order v , this has poles in r_C , probably due to rounding errors.

■ C_s / ℓ graphs

```
GraphicsRow[
  {Plot[-Cs2 // Chop, {vv, .65, .99}, PlotLabel -> "Basic Hyperbolic Mirror",
    FrameLabel -> {"v = (V_A-V_C) / (V_A-V_M)", "-C_s/{",
    Frame -> True, Axes -> False, PlotRange -> {0, 160}},
  Plot3D[-Cs2 /. {vv -> (alpha - chi) / (alpha - 1)} // Chop, {chi, .65, .99},
    {alpha, 0, 1}, PlotLabel -> "Basic Hyperbolic Mirror", AxesLabel ->
    {"V_C/V_M", "V_A/V_M", "-C_s/{", PlotRange -> {-10, 160}}], ImageSize -> 800]
```

■ Summary & reproduction of graphs

```
GraphicsRow[{
  Plot[zx0 /. vv -> (1 - x), {x, 0.001, .35}, PlotRange -> {{0, .345}, {0, 8}},
    FrameLabel -> {{Style["z_0/{", Medium], None}, {Style["v", Medium], None}},
    Frame -> True, Axes -> False, FrameTicks -> {{{0, 1, 2, 3, 4, 5, 6, 7, 8}, None},
    {{{0, 1.0}, {0.1, 0.9}, {0.2, 0.8}, {0.3, 0.7}}, None}},
    PlotStyle -> Black, ImageSize -> {250 * 7 / 6.5, 250}, AspectRatio -> 1],

  Plot[{-Cc0 /. vv -> (1 - x),
    (-Cs2 /. vv -> (1 - x)) // Chop, (20 * Cc0 / Cs2 /. vv -> (1 - x)) // Chop},
    {x, 0.005, .35}, PlotRange -> {{0, .3}, {0, 160}},
    FrameLabel -> {{Style["C_c/{", Medium],
      Style["C_c/C_s", Medium],
      Style["v", Medium], None}}, Frame -> True, Axes -> False,
    FrameTicks -> {{{0, {20, -20}, {40, -40}, {60, -60}, {80, -80}, {100, -100},
      {120, -120}, {140, -140}, {160, -160}}, {0, {20, 1}, {40, 2}}},
    {{{0, 1.0}, {0.1, 0.9}, {0.2, 0.8}, {0.3, 0.7}}, None}},
    PlotStyle -> Black, ImageSize -> {290, 250}, AspectRatio -> Full]

}, ImageSize -> 500]
```

Aberration graph to compare to triode model

```
GraphicsRow[{
  ParametricPlot[({-Cc0, (-Cs2)} /. vv -> x) // Re // Chop,
    {x, .65, .996}, PlotRange -> {0, 160}, FrameLabel -> {"Cc/{" , "Cs/{" ,
    FrameTicks -> {{0, {20, -20}, {40, -40}, {60, -60}, {80, -80},
      {100, -100}, {120, -120}, {140, -140}, {160, -160}}, None},
    {{0, {20, -20}, {40, -40}, {60, -60}, {80, -80}, {100, -100},
      {120, -120}, {140, -140}, {160, -160}}, None}}]
  ,
  ParametricPlot[({zx0, Cc0/Cs2} /. vv -> x) // Re // Chop, {x, .65, .996},
    PlotRange -> {{0, 5}, {0, 2}}, FrameLabel -> {"z0/{" , "Cc/Cs"}]
}]
```

Extended Mirror Theory

This incorporates a mirror extension and hopes to find graphs similar to those in the paper

■ Theory

■ Initial region electron trajectory

Only symmetric electron trajectories are considered. At reflection, an electron has coordinate $(r, z, t) = (r_C, z_C, 0)$ and the speed is zero, $\dot{r}_C = \dot{z}_C = 0$.

After traversing the initial region between the mirror electrode at V_M and the adjustable electrode at V_A , an electron has coordinates (r_A, z_A, t_A) . In terms of the turn-around coordinates,

$$\begin{aligned} r_a &= r_c \cos[\theta_i]; \\ z_a &= z_c \cosh[\sqrt{2} \theta_i]; \\ \alpha_a &= \frac{r_a \tan[\theta_i]}{\sqrt{2} z_a \tanh[\sqrt{2} \theta_i]}; \end{aligned}$$

where $\theta_i = \omega_i t$, $\omega_i = \sqrt{2 k_i/m}$, and $k_i = (V_A - V_M)/\ell^2$. θ_i can be approximated as follows:

zero-th order, $z_A = \ell$ and $z_C = \ell \sqrt{1 - \nu}$, where $\nu = (V_A - V_C)/(V_A - V_M)$.


```

Rc[order_] := If[order == 0, 0, rc];

zc[order_] :=  $\sqrt{\{^2 (1 - v) + \frac{Rc[order]^2}{2}}}$ ;

ra[order_] := If[order == 0, 0, Rc[order] Cos[ $\theta_i[order - 1]$ ]];

za[order_] :=  $\sqrt{\{^2 + \frac{ra[order]^2}{2}}}$ ;

 $\theta_i[order_] := \frac{1}{\sqrt{2}} \text{ArcCosh}\left[\frac{za[order]}{zc[order]}\right]$ ;

 $\alpha_a[order_] := \frac{ra[order] \text{Tan}[\theta_i[order]]}{\sqrt{2} za[order] \text{Tanh}[\sqrt{2} \theta_i[order]]}$ ;

 $v = \frac{Va - Vc}{Va - Vm}$ ;

```

■ Aperture A deflection

The aperture at the adjustable electrode acts to deflect the electron trajectory such that $\alpha_A \rightarrow \alpha_A + \delta_A = \alpha_i$, where the deflection is

$$\delta_a[order_] := ra[order] za[order] \frac{(kf - ki)}{2 (Va - Vc)};$$

$$ki = \frac{Va - Vm}{\{^2}; kf = \frac{-Va}{L^2 - \{^2};$$

This deflection will have negligible effect on $\dot{z}$, and $\dot{r} \rightarrow \dot{r}(1 + \delta_A/\alpha_A)$.

$$\delta_{aover\alpha a}[order_] := \frac{\sqrt{2} \text{Tanh}[\sqrt{2} \theta_i[order]]}{\text{Tan}[\theta_i[order]]} \frac{za[order]^2 (kf - ki)}{2 (Va - Vc)};$$

■ Check to see if good single-region results

If the outer region is inactive, the distance z_i at which the trajectory intersects the axis is

$z_i = z_A + \frac{r_A}{\alpha_i}$. Let $q_i/\ell = \alpha_i/r_A$ is

$$zi[order_] := \left(za[order] + \frac{\{ }{qi[order]} \right) /. Va \rightarrow 0;$$

$$qi[order_] := \left\{ \frac{\text{Tan}[\theta_i[order]]}{\sqrt{2} za[order] \text{Tanh}[\sqrt{2} \theta_i[order]]} + za[order] \frac{(kf - ki)}{2 (Va - Vc)} \right\};$$

```

Plot[zi[0] /. {Vm -> -1, { -> 1}, {Vc, -.999, -0.65},
Frame -> True, PlotRange -> {0, 8}, Axes -> False]

```

■ Final region electron trajectory

After traversing the second (final) region potential field, the coordinates are

$$\begin{aligned}
\text{ro}[\text{order\_}] &:= \text{If}[\text{order} == 0, 0, \frac{\text{ra}[\text{order}]}{\text{Cos}[\phi[\text{order}]]} \text{Cos}[\theta f[\text{order} - 1] - \phi[\text{order}]]]; \\
\text{zo}[\text{order\_}] &:= \sqrt{L^2 + \frac{\text{ro}[\text{order}]^2}{2}}; \\
\theta f[\text{order\_}] &:= \frac{1}{\sqrt{2}} \left(\text{ArcCosh}\left[\frac{\text{zo}[\text{order}] \text{Cosh}[\psi[\text{order}]]}{\text{za}[\text{order}]} \right] + \psi[\text{order}] \right); \\
\phi[\text{order\_}] &:= \text{ArcTan}\left[-\sqrt{\frac{\text{ki}}{\text{kf}}} \text{Tan}[\theta i[\text{order}]] (1 + \delta a_{\text{over} \alpha a}[\text{order}])\right]; \\
\psi[\text{order\_}] &:= \text{ArcTanh}\left[-\sqrt{\frac{\text{ki}}{\text{kf}}} \text{Tanh}[\sqrt{2} \theta i[\text{order}]]\right]; \\
\alpha o[\text{order\_}] &:= \frac{\text{ro}[\text{order}] \text{Tan}[\theta f[\text{order}] - \phi[\text{order}]]}{\sqrt{2} \text{zo}[\text{order}] \text{Tanh}[\sqrt{2} \theta f[\text{order}] - \psi[\text{order}]]};
\end{aligned}$$

■ Aperture O deflection

The aperture at the adjustable electrode acts to deflect the electron trajectory such that $\alpha_O \rightarrow \alpha_O + \delta_O = \alpha_f$, where the deflection is

$$\begin{aligned}
\delta o[\text{order\_}] &:= \frac{\text{kf} \text{zo}[\text{order}] \text{ro}[\text{order}]}{2 \text{Vc}}; \\
\alpha f[\text{order\_}] &:= \alpha o[\text{order}] + \delta o[\text{order}];
\end{aligned}$$

The distance z_f at which the trajectory intersects the axis is $z_f = z_O + \frac{r_O}{\alpha_f}$, where $q/\mathcal{L} = \alpha_f/r_O$ is

$$\begin{aligned}
\text{zf}[\text{order\_}] &:= \text{zo}[\text{order}] + \frac{L}{q[\text{order}]}; \\
q[\text{order\_}] &:= \\
&L \left(\frac{\text{Tan}[\theta f[\text{order}] - \phi[\text{order}]]}{\sqrt{2} \text{zo}[\text{order}] \text{Tanh}[\sqrt{2} \theta f[\text{order}] - \psi[\text{order}]]} - \frac{\text{kf} \text{zo}[\text{order}]}{2 \text{Vc}} \right);
\end{aligned}$$

■ Aberration

The chromatic and spherical aberration

$$\begin{aligned}
\text{cc} &= 2 \text{Vc} \partial_{\text{Vc}} (\text{zf}[0]); \\
\text{cs} &= -2 \left(\frac{\frac{1}{2} (D[\text{zf}[1], \{\text{rc}, 2\}] /. \text{rc} \rightarrow 0)}{(D[\alpha f[1], \{\text{rc}, 1\}] /. \text{rc} \rightarrow 0)^2} \right) /. \text{rc} \rightarrow 0;
\end{aligned}$$

Plots

■ 3D Plots to compare to SHM

```

diode3d = ParametricPlot3D[
  Re[Chop[{-Cc0, -Cs2, zx0}]], {vv, .65, .995}
, PlotRange → {{0, 175}, {0, 175}, {0, 2.5}}, PlotPoints → 30,
  MaxRecursion → 3, AxesLabel → {"-Cc/{"", "-Cs/{"", "z0/{"",
  PlotStyle → Thick, ViewVertical → {0, 0, 1},
  ViewPoint → {3, -2.8, 1}, AxesEdge → {{-1, -1}, {1, -1}, {1, 1}},
  BoxRatios → {1, 1, 1}, AspectRatio → .9]

diode2d = ParametricPlot[
  Re[Chop[{Cc0 / Cs2, zx0}]], {vv, .65, .997}
, PlotRange → {{0, 2}, {0, 2.5}}, FrameLabel → {"Cc/Cs", "z0/{"",
  PlotStyle → {Black, Thick}, AspectRatio → 1, GridLines → None]

triode1 = SetAccuracy[
  {-cc, -cs, zf[0]} /. {Vc → 1, L → 1, { → .66, Va → va, Vm → va -  $\frac{(va - 1)}{vv}$ }, 4];

triode3D =
  ParametricPlot3D[
    Chop[Evaluate[triode1]]
  , {vv, .65, .995}, {va, .01, .99}, PlotRange → {{0, 175}, {0, 175}, {0, 2.5}},
    PlotPoints → 50, MaxRecursion → 2, AxesLabel → {"-Cc/{"", "-Cs/{"", "z0/{"",
    PlotStyle → Directive[Opacity[0.7]], ColorFunction → "GrayTones",
    MeshFunctions → {#2 &, #3 &}, Mesh → {Range[5, 175, 10], Range[0.1, 2.5, .2]},
    MeshStyle → {{Opacity[0.7], Thin}, {Opacity[0.7], Thin, GrayLevel[.9]}},
    ViewVertical → {0, 0, 1}, ViewPoint → {3, -2.8, 1},
    AxesEdge → {{-1, -1}, {1, -1}, {1, 1}},
    BoxRatios → {1, 1, 1}, AspectRatio → .9]

triode2 = SetAccuracy[{-Va, cc / cs, zf[0]} /.
  {Vc → 1, L → 1, { → .66, Va → va, Vm → va -  $\frac{(va - 1)}{vv}$ }, 4];

triode2da = ParametricPlot3D[
  Chop[Evaluate[triode2]], {vv, .65, .963}, {va, .0001, .98}
, PlotRange → {{0, -.9}, {0, 4}, {0, 2.5}}, PlotPoints → 50,
  MaxRecursion → 2, AxesLabel → {"VA/VC", "Cc/Cs", "z0/L"},
  PlotStyle → Directive[Opacity[0.7]],
  ColorFunction → "GrayTones", MeshFunctions → {#1 &, #3 &},
  Mesh → {Range[-0.03, -.97, -.09], Range[0, 2.5, .2]},
  MeshStyle → {{Opacity[0.7], Thin}, {Opacity[0.7], Thin, GrayLevel[.9]}},
  BoxRatios → {1, 1, 1}, AspectRatio → .9, PlotLabel → None,
  ViewPoint → {3, 1, .4}, ViewVertical → {0, 0, 1},
  Ticks → {{0, ""}, {-.2, .2}, {-.4, ""}, {-.6, ""}, {-.8, .8}},
  Automatic, Automatic}, AxesEdge → {{1, -1}, {1, -1}, {1, -1}}]

```

```

triode2dc = ParametricPlot3D[
  Chop[Evaluate[triode2]], {vv, .55, .997},
  {va, .01, If[vv < .96, .91, 25 (1 - vv) .91]}
  , PlotRange → {{0, -1}, {0.05, 4}, {0, 2.5}}, PlotPoints → 50,
  MaxRecursion → 2, AxesLabel → {"VA/VC", "Cc/Cs", "z0/L"},
  PlotStyle → {Directive[Opacity[0.7]]},
  ColorFunction → "GrayTones", MeshFunctions → {#1 &, #3 &},
  Mesh → {Range[-0.03, -.97, -.09], Range[0, 2.5, .2]},
  MeshStyle → {{Opacity[0.7], Thin}, {Opacity[0.7], Thin, GrayLevel[.9]}},
  BoxRatios → {1, 1, 1}, AspectRatio → .9, PlotLabel → None,
  ViewPoint → {3, 1, .4}, ViewVertical → {0, 0, 1},
  Ticks → {{0, ""}, {-.2, .2}, {-.4, ""}, {-.6, ""}, {-.8, .8}},
  Automatic, Automatic}, AxesEdge → {{1, -1}, {1, -1}, {1, -1}}]

fb1 = SetAccuracy[
  {-cc, -cs, zf[0]} /. {Vc → 1, L → 1, {→ .3, Va → va, Vm → va -  $\frac{(va - 1)}{vv}$ }, 4}];

fb2 = SetAccuracy[{-cc, -cs, zf[0]} /.
  {Vc → 1, L → 1, {→ .8, Va → va, Vm → va -  $\frac{(va - 1)}{vv}$ }, 4}];

b1 =
ParametricPlot3D[
  Chop[Evaluate[fb1]]
  , {vv, .65, .995}, {va, .01, .99}, PlotRange → {{0, 175}, {0, 175}, {0, 2.5}},
  PlotPoints → 50, MaxRecursion → 2, AxesLabel → {"-Cc/{"", "-Cs/{"", "z0/{"",
  PlotStyle → Directive[Opacity[0.85]], ColorFunction → "GrayTones",
  MeshFunctions → {#2 &, #3 &}, Mesh → {Range[5, 175, 10], Range[0.1, 2.5, .2]},
  MeshStyle → {{Opacity[0.7], Thin}, {Opacity[0.7], Thin, GrayLevel[.3]}},
  ViewVertical → {0, 0, 1}, ViewPoint → {3, -2.8, 1},
  AxesEdge → {{-1, -1}, {1, -1}, {1, 1}},
  BoxRatios → {1, 1, 1}, AspectRatio → .9]

b2 =
ParametricPlot3D[
  Chop[Evaluate[fb2]]
  , {vv, .65, .995}, {va, .012, If[vv < .95, .99, 20 (1 - vv) .99]},
  PlotRange → {{0, 175}, {0, 175}, {0, 2.5}}, PlotPoints → 50,
  MaxRecursion → 2, AxesLabel → {"-Cc/{"", "-Cs/{"", "z0/{"",
  PlotStyle → Directive[Opacity[0.7]], ColorFunction → "GrayTones",
  MeshFunctions → {#2 &, #3 &}, Mesh → {Range[5, 175, 10], Range[0.1, 2.5, .2]},
  MeshStyle → {{Opacity[0.7], Thin, GrayLevel[.7]},
  {Opacity[0.7], Thin, GrayLevel[.9]}}, ViewVertical → {0, 0, 1},
  ViewPoint → {3, -2.8, 1}, AxesEdge → {{-1, -1}, {1, -1}, {1, 1}},
  BoxRatios → {1, 1, 1}, AspectRatio → .9]

Show[b1, b2]

```

■ Plots to show tuning behavior

■ Sample behavior: Aberration plots near ideal geometry & z_0

```

vmF[gf_, va_, z0_] :=
  vm /. FindRoot[Re[zf[0] /. {Vc → 1, L → 1, { → gf, Va → va, Vm → vm}}] == z0,
    {vm, 1.1}, MaxIterations → 12];
z0F[gf_, va_, vm_] := zf[0] /. {Vc → 1, L → 1, { → gf, Va → va, Vm → vm}};
ccF[gf_, va_, vm_] := cc /. {Vc → 1, L → 1, { → gf, Va → va, Vm → vm}};
csF[gf_, va_, vm_] := cs /. {Vc → 1, L → 1, { → gf, Va → va, Vm → vm}};

Ideal geometry,  $z_0$  contours

g = .66;
uu = Table[
  Select[Chop[
    Table[tv = vmF[g, x, y];
    {ccF[g, x, tv], csF[g, x, tv]}, {x, 0.001, 0.999, .002}]
  ], #[[1]] < 0 &]
, {y, .9, 1.25, .05}] // Quiet;

Show[{
  ListLinePlot[-uu // Re, Frame → True, PlotRange → {{0, 30}, {0, 30}},
    AspectRatio → 1, LabelStyle → {FontFamily → "Arial", FontSize → 7},
    FrameLabel → {"-Cc/L", "-Cs/L"},
    PlotStyle → {{GrayLevel[0.4]}, {GrayLevel[0.4], Dashed},
      {GrayLevel[0.4], DotDashed}, {GrayLevel[0.4], Dotted},
      {GrayLevel[0]}, {GrayLevel[0], Dashed},
      {GrayLevel[0], DotDashed}, {GrayLevel[0], Dotted}},
    GridLines → None],
  Graphics[Text[Style["1.25", GrayLevel[0], FontSize → 6],
    {7.5, 12}, {0, 0}, {Cos[74 °], Sin[74 °]}]],
  Graphics[Text[Style["1.20", GrayLevel[0], FontSize → 6],
    {9, 11.5}, {0, 0}, {Cos[70 °], Sin[70 °]}]],
  Graphics[Text[Style["1.15", GrayLevel[0], FontSize → 6],
    {10.7, 11}, {0, 0}, {Cos[67 °], Sin[67 °]}]],
  Graphics[Text[Style["1.10", GrayLevel[0], FontSize → 6],
    {12.8, 10.3}, {0, 0}, {Cos[63 °], Sin[63 °]}]],
  Graphics[Text[Style["1.05", GrayLevel[0.4], FontSize → 6],
    {15, 9}, {0, 0}, {Cos[55 °], Sin[55 °]}]],
  Graphics[Text[Style["1.00", GrayLevel[0.4], FontSize → 6],
    {17.7, 8}, {0, 0}, {Cos[43 °], Sin[43 °]}]],
  Graphics[Text[Style["0.95", GrayLevel[0.4], FontSize → 6],
    {21, 7}, {0, 0}, {Cos[30 °], Sin[30 °]}]],
  Graphics[Text[Style["0.9", GrayLevel[0.4], FontSize → 6],
    {26, 26}, {0, 0}, {Cos[20 °], Sin[20 °]}]]
], TextStyle → {FontFamily → "Arial", FontSize → 7}]

```

```

cand = uu[[4]] ;
ccmax = Min[Transpose[cand][[1]]]
temp1 = Transpose[Select[cand, #[[1]] < .99 ccmax &]][[2]] ;
-Min[temp1]
-Mean[temp1]
-Max[temp1]
Min[temp1] - Max[temp1]
-----
Mean[temp1]
csmax = Min[Transpose[cand][[2]]]
temp2 = Transpose[Select[cand, #[[2]] < .99 csmax &]][[1]] ;
-Min[temp2]
-Mean[temp2]
-Max[temp2]
Min[temp2] - Max[temp2]
-----
Mean[temp2]
Show[
{
ListLinePlot[-uu[[4]] // Re, Frame → True, PlotRange → {{0, 30}, {0, 30}},
AspectRatio → 1, LabelStyle → {FontFamily → "Arial", FontSize → 7},
FrameLabel → {"-Cc/L", "-Cs/L"},
GridLines → None, PlotStyle → {Black, Thick}},
Graphics[Text[Style["z0/L = 1.05", Bold], {25, 27}]],

Graphics[{Thick, GrayLevel[0.5], Line[{{15.31, 21.34}, {12.78, 21.34}}]}],
Graphics[Text[Style["Δ Cc = 18%", Gray // Darker], {14, 21.5}, {0, -1}]],

Graphics[{Thick, GrayLevel[0.5], Line[{{18.11, 14.14}, {18.11, 17.67}}]}],
Graphics[
Text[Style["Δ Cs = 22%", Gray // Darker], {18.5, 16.05}, {-1, 0}]],

Graphics[Text[Style["VM →", Gray, FontSize → 6],
{12.5, 7.3}, {0, 0}, {Cos[44 °], Sin[44 °]}]],
Graphics[Text[Style["← VA", Gray, FontSize → 6],
{10, 3.}, {0, 0}, {Cos[26 °], Sin[26 °]}]]
}, TextStyle → {FontFamily → "Arial", FontSize → 7}]

```

Appendix C   Code, *Mathematica*: mirror theory, updated

The updated code runs more quickly in Mathematica and can generate the same plots as the code given in the previous appendix. In addition, triode solutions with and without an exit aperture are computed, as well as the effect of replacing the outer hyperbolic field with a constant field.

Header

Graphics Options

```

SetOptions[Plot, PlotRange → All,
  PlotStyle → {{Thick, Black}, {Thick, Darker[Red]},
    {Thick, Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, Blend[{Lighter[Gray], Blue}, 1 / 3]}}}, Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[LogPlot, PlotRange → All, PlotStyle →
  {{Thick, Black}, {Thick, Dashed, Black}, {Thick, Dotted, Black}},
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ParametricPlot3D, PlotStyle →
  {{Thick, Black}, {Thick, Dashed, Black}, {Thick, Dotted, Black}},
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350,
  BoxRatios → {1, 1, .5}, Axes → {True, True, False},
  Boxed → False, ViewCenter → {.5, .5, 0},
  ViewVertical → {0, 0, 1}, ViewPoint → {0, -3, 1}];
SetOptions[ListPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.02], Black},
    {Thick, PointSize[.02], Darker[Red]},
    {Thick, PointSize[.02], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.02], Blend[{Lighter[Gray], Blue}, 1 / 3]}}},
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → Gray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListContourPlot, PlotRange → All, Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLinearPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[Large]}}}, Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[Large]}}}, Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLogPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[Large]}}}, Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];

```


Functions

Hyperbolic trajectory functions

$\omega = \sqrt{e k / m}$, k defines shape of hyperbolic potential. Functions of time t

```
rHyp[ω_, r0_, vr0_, θ_] := r0 Cos[θ] + vr0 Sin[θ] / ω;
zHyp[ω_, z0_, vz0_, θ_] := z0 Cosh[√2 θ] + vz0 Sinh[√2 θ] / (√2 ω);
vrHyp[ω_, x0_, v0_, θ_] := ω Derivative[0, 0, 0, 1][rHyp][ω, x0, v0, θ];
vzHyp[ω_, x0_, v0_, θ_] := ω Derivative[0, 0, 0, 1][zHyp][ω, x0, v0, θ];
```

Invert $z(t)$ to get $\theta(z)$

```
ψ[ω_, z0_, vz0_] := ArcTanh[-vz0 / (√2 ω z0)];
θofz[ω_, z0_, vz0_, z_] :=
  2-1/2 (ψ[ω, z0, vz0] + ArcCosh[(z / z0) Cosh[ψ[ω, z0, vz0]]]);
```

Davisson-Calbick approximation

Trajectory through an aperture, from left to right.

```
drdzofzDC[r0_, drdzofz0_, dVdzL_, dVdzR_, VBeam_] :=
  drdzofz0 + (dVdzL - dVdzR) / (4 VBeam) r0;
```

$q = (dr/dz)/r$

```
q[r0_, drdzofz0_, dVdzL_, dVdzR_, VBeam_] :=
  drdzofz0 / r0 + (dVdzL - dVdzR) / (4 VBeam);
```

Constant field trajectory functions

Assumes second electrode is grounded.

```
rConst[r0_, vr0_, t_] := r0 + vr0 t;
zConst[ηdVdz_, z0_, vz0_, t_] := z0 + vz0 t + 2-1 ηdVdz t2;
vrConst[r0_, vr0_, t_] := Derivative[0, 0, 1][rConst][r0, vr0, t];
vzConst[ηdVdz_, z0_, vz0_, t_] :=
  Derivative[0, 0, 0, 1][zConst][ηdVdz, z0, vz0, t];
```

Invert $z(t)$ to get $t(z)$

```
tofzConst[ηdVdz_, z0_, vz0_, z_] :=
  vz0 / ηdVdz (-1 + √(1 + 2 ηdVdz (z - z0) vz0-2));
```

Trajectories

Variables: $v_L = V_L/V_C$, $v_A = V_A/V_C$, $v_M^{-1} = V_M/V_C$.

Constants: $\omega_1 = \sqrt{e k_1/m}$, $k_1 = V_C(v_A - v_M^{-1})/\ell^2$.

Lens half width = s .

Turn-around radial extent, limiting variable r_C

Diode alone

Position and velocity at the aperture

$$\begin{aligned}
 zC[rC\_] &:= \sqrt{\left\{^2 \frac{vM - 1}{vA vM - 1} + rC^2 / 2 \right\}} ; \\
 rA &= \text{Refine}[rHyp[\omega, rC, 0, \theta A[rC]], \omega > 0] \\
 zA &= \text{Refine}[zHyp[\omega, zC[rC], 0, \theta A[rC]], \omega > 0] ; \\
 vrA &= \text{Refine}[vrHyp[\omega, rC, 0, \theta A[rC]], \omega > 0] ; \\
 vzA &= \text{Refine}[vzHyp[\omega, zC[rC], 0, \theta A[rC]], \omega > 0] ; \\
 drdzA &= \text{Refine}[vrA / vzA, \omega > 0] ; \\
 drdzAd &= \text{Refine}[drdzofzDC[rA, drdzA, \\
 &\quad 2 VC (vA - vM^{-1}) \{^{-2} zA, 0, -VC (1 - vA)\}, \{\omega > 0, VC < 0\}] \\
 rC \cos[\theta A[rC]] & \\
 - \frac{1}{2 \ell^2 (1 - vA)} & \\
 rC \left(vA - \frac{1}{vM} \right) \sqrt{\frac{rC^2}{2} + \frac{\ell^2 (-1 + vM)}{-1 + vA vM}} \cos[\theta A[rC]] \cosh[\sqrt{2} \theta A[rC]] - & \\
 \frac{rC \text{Csch}[\sqrt{2} \theta A[rC]] \sin[\theta A[rC]]}{\sqrt{2} \sqrt{\frac{rC^2}{2} + \frac{\ell^2 (-1 + vM)}{-1 + vA vM}}} &
 \end{aligned}$$

Approximations made at the aperture

$$\begin{aligned}
 \theta A0[rC\_] &:= \theta ofz[\omega, zC[rC], 0, \{]; \theta A0[rC] \\
 rA1[rC\_] &:= rHyp[\omega, rC, 0, \theta A0[rC]]; rA1[rC] \\
 \theta A1[rC\_] &:= \theta ofz[\omega, zC[rC], 0, \sqrt{\{^2 + rA1[rC]^2 / 2\}}]; \theta A1[rC]
 \end{aligned}$$

Image location z' and ray angle squared α'^2 .

$$\begin{aligned}
 zDiode &= zA - (\text{Expand}[drdzAd / rA])^{-1} \\
 \alpha\text{SquaredDiode} &= \text{ArcTan}[-drdzAd]^2
 \end{aligned}$$

Paraxial image location z'_0 and first and second order correction terms $z'_1 r_C = 0$ and $z'_2 r_C^2$

```
z0Diode = SeriesCoefficient[zDiode, {rC, 0, 0}]
z0Diode = Block[{θA}, θA[rC_] := θA0[rC];
  Refine[z0Diode, {> 0 && νA > 0 && νA < 1 && νM > 0 && νM < 1}]]

z1Diode = SeriesCoefficient[zDiode, {rC, 0, 1}]
z1Diode = Block[{θA}, θA[rC_] := θA0[rC]; z1Diode]

z2Diode = SeriesCoefficient[zDiode, {rC, 0, 2}]
z2Diode = Block[{θA}, θA[rC_] := θA0[rC];
  Refine[z2Diode, {> 0 && νA > 0 && νA < 1 && νM > 0 && νM < 1}]]
```

Second order angle expansion $\alpha'^2 = (\alpha'^2)_1 r_C + (\alpha'^2)_2 r_C^2 + O(r_C^3)$, $(\alpha'^2)_1 = 0$

```
αSquared1Diode = SeriesCoefficient[αSquaredDiode, {rC, 0, 1}]
αSquared1Diode = Block[{θA}, θA[rC_] := θA0[rC]; αSquared1Diode]

αSquared2Diode = SeriesCoefficient[αSquaredDiode, {rC, 0, 2}]
αSquared2Diode = Block[{θA}, θA[rC_] := θA0[rC];
  Refine[αSquared2Diode, {> 0 && νA > 0 && νA < 1 && νM > 0 && νM < 1}]]
```

Coefficient of chromatic aberration, $C_c = V_C \frac{2 \partial z_0}{\partial V_C} = 2 (\nu_M \partial_{\nu_M} z_0 - \nu_A \partial_{\nu_A} z_0)$

```
CcDiode = 2 (νM ∂νM z0Diode - νA ∂νA z0Diode);
```

Coefficient of spherical aberration, $z' = z_0 - 2^{-1} C_s \alpha'^2 \rightarrow C_s = -2 z'_2 / (\alpha'^2)_2$

```
CsDiode = -2 z2Diode / αSquared2Diode;
```

Plots

```
z0DiodePlotFunction = z0Diode /. {→ 1 /. νA → 0;
Plot[z0DiodePlotFunction, {νM, .65, .995}, PlotRange → {0, 8}]

CcDiodePlotFunction = CcDiode /. {→ 1 /. νA → 0;
Plot[CcDiodePlotFunction, {νM, .7, .995}, PlotRange → {0, -160}]

CsDiodePlotFunction = CsDiode /. {→ 1 /. νA → 0;
Plot[CsDiodePlotFunction, {νM, .7, .996}, PlotRange → {0, -160}]

Plot[CcDiodePlotFunction / CsDiodePlotFunction,
  {νM, .7, .9963}, PlotRange → {0, 2}]
```

Apertureless triode, two hyperbolic regions

Position and velocity at the inner aperture

$$zC[rC\_]:= \sqrt{\left\{^2 \frac{vM-1}{vA vM-1} + rC^2 / 2 \right.};$$

```
Clear[rA]; rA[rC_] := Refine[rHyp[ω1, rC, 0, θA[rC]], ω1 > 0];
Clear[zA]; zA[rC_] := Refine[zHyp[ω1, zC[rC], 0, θA[rC]], ω1 > 0];
Clear[vrA]; vrA[rC_] := Refine[vrHyp[ω1, rC, 0, θA[rC]], ω1 > 0];
Clear[vzA]; vzA[rC_] := Refine[vzHyp[ω1, zC[rC], 0, θA[rC]], ω1 > 0];
drdzA = Refine[vrA[rC] / vzA[rC], ω1 > 0];
```

Aperture deflection

```
drdzAd = drdzofzDC[rA[rC], drdzA, 2 VC (vA - vM-1) {-2 zA[rC],
  2 (-VC vA) (L2 - {2)-1 zA[rC], -VC (1 - vA)}];
factor = (rC Cos[θA[rC]] Cosh[√2 θA[rC]] zC[rC]);
drdzAd = factor Refine[Expand[factor-1 drdzAd], ω1 > 0 && VC < 0]
vzAd =  $\frac{\omega_1}{rC} \left( \frac{(\omega_1)^{-2} vrA[rC]^2 + (\omega_1)^{-2} vzA[rC]^2}{rC^{-2} + rC^{-2} drdzAd^2} \right)^{1/2}$ 
vrAd = drdzAd vzAd
```

Position and velocity at the outer aperture

```
ω2 = ω1  $\left( \frac{-vA vM}{vA vM - 1} \frac{\{^2}{L^2 - \{^2} \right)^{1/2}$ ;
rB = Refine[rHyp[ω2, rA[rC], vrAd, θB[rC]], ω1 > 0]
zB = Refine[zHyp[ω2, zA[rC], vzAd, θB[rC]], ω1 > 0]
vrB = Refine[vrHyp[ω2, rA[rC], vrAd, θB[rC]], ω1 > 0];
vzB = Refine[vzHyp[ω2, zA[rC], vzAd, θB[rC]], ω1 > 0];
drdzB = Refine[vrB / vzB, ω1 > 0]
```

Approximations made at the inner aperture

```
θA0[rC_] := θofz[ω1, zC[rC], 0, {}]; θA0[rC]
rA1[rC_] := rHyp[ω1, rC, 0, θA0[rC]]; rA1[rC]
θA1[rC_] := θofz[ω1, zC[rC], 0, √{2 + rA1[rC]2 / 2}]; θA1[rC]
```

Approximations made at the outer aperture

```
θB0[rC_] := θofz[ω2, zA[rC], vzA[rC], L]; θB0[rC]
rB1[rC_] := rHyp[ω2, rA[rC], vzA[rC], θB0[rC]]; rB1[rC]
θB1[rC_] := θofz[ω2, zA[rC], vzA[rC], √{L2 + rB1[rC]2 / 2}]; θB1[rC]
```

Image location z' and ray angle squared α'^2 . Explicitly using the small angle approximation $\alpha \approx \tan \alpha = -r'$.

```
zTriode = zB - (Expand[drdzB / rB])-1
αSquaredTriode = (-drdzB)2
```

Paraxial image location z'_0 and first and second order correction terms $z'_1 r_C = 0$ and $z'_2 r_C^2$.

```
z0Triode = SeriesCoefficient[zTriode, {rC, 0, 0}]
z0Triode = Refine[z0Triode, { > 0 && L > 0 && L > { &&
    vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
z0Triode = Block[{θA, θB}, θA[rC_] := θA0[rC];
    θB[rC_] := θB0[rC]; z0Triode]
z0Triode = Refine[z0Triode,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }

z1Triode = SeriesCoefficient[zTriode, {rC, 0, 1}]
z1Triode = Refine[z1Triode, { > 0 && L > 0 && L > { &&
    vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
z1Triode = Block[{θA, θB}, θA[rC_] := θA0[rC];
    θB[rC_] := θB0[rC]; z1Triode]
z1Triode = Refine[z1Triode,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }

z2Triode = SeriesCoefficient[zTriode, {rC, 0, 2}]
z2Triode = Refine[z2Triode, { > 0 && L > 0 && L > { &&
    vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
z2Triode = Block[{θA, θB}, θA[rC_] := θA0[rC];
    θB[rC_] := θB0[rC]; z2Triode]
z2Triode = Refine[z2Triode,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }
```

Second order angle expansion $a'^2 = (a'^2)_1 r_C + (a'^2)_2 r_C^2 + O(r_C^3)$, $(a'^2)_1 = 0$

```
αSquared1Triode = SeriesCoefficient[αSquaredTriode, {rC, 0, 1}]
αSquared1Triode = Refine[αSquared1Triode, { > 0 && L > 0 && L > { &&
    vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
αSquared1Triode = Block[{θA, θB}, θA[rC_] := θA0[rC];
    θB[rC_] := θB0[rC]; αSquared1Triode]
αSquared1Triode = Refine[αSquared1Triode,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }

αSquared2Triode = SeriesCoefficient[αSquaredTriode, {rC, 0, 2}]
αSquared2Triode = Refine[αSquared2Triode, { > 0 && L > 0 && L > { &&
    vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
αSquared2Triode = Block[{θA, θB}, θA[rC_] := θA0[rC];
    θB[rC_] := θB0[rC]; αSquared2Triode]
αSquared2Triode = Refine[αSquared2Triode,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 };
```

Coefficient of chromatic aberration, $C_c = V_C \frac{2\partial z_0}{\partial V_C} = 2(\nu_M \partial_{\nu_M} z_0 - \nu_A \partial_{\nu_A} z_0)$

`CcTriode = 2 (νM ∂νM z0Triode - νA ∂νA z0Triode) ;`

Coefficient of spherical aberration, $z' = z_0 - 2^{-1} C_s \alpha'^2 \rightarrow C_s = -2 z'_2 / (\alpha'^2)_2$

`CsTriode = -2 z2Triode / αSquared2Triode ;`

Plots for $\nu_A = 0$ (should give diode behavior)

`z0TriodePlotFunction0 = z0Triode /. { → 1 /. νA → 10-7 /. L → 2 ;`

`Plot[z0TriodePlotFunction0, {νM, .65, .995}, PlotRange → {0, 8}]`

`CcTriodePlotFunction0 = CcTriode /. { → 1 /. νA → 10-7 /. L → 2 ;`

`Plot[CcTriodePlotFunction0, {νM, .7, .995}, PlotRange → {0, -160}]`

`CsTriodePlotFunction0 = CsTriode /. { → 1 /. νA → 10-7 /. L → 2 ;`

`Plot[CsTriodePlotFunction0, {νM, .7, .996}, PlotRange → {0, -160}]`

`Plot[CcTriodePlotFunction0 / CsTriodePlotFunction0,`
`{νM, .7, .9963}, PlotRange → {0, 2}]`

Plots for $\nu_A \neq 0$ and $\ell/\mathcal{L} = 0.783/1.665$ (design triode specs)

`z0TriodePlotFunction = z0Triode /. { → 0.783 /. L → 1.665 ;`

`ParametricPlot[{{νM, z0TriodePlotFunction},`
`{νM, z0TriodePlotFunction0}}, {νM, .65, .995},`
`{νA, 10-7, .8}, PlotRange → {{.65, 1}, {0, 8}}, AspectRatio → 1]`

`CcTriodePlotFunction = CcTriode /. { → 0.783 /. L → 1.665 ;`

`ParametricPlot[{{νM, CcTriodePlotFunction},`
`{νM, CcTriodePlotFunction0}}, {νM, .7, .995}, {νA, 10-7, .8},`
`PlotRange → {{.7, 1}, {0, -160}}, AspectRatio → 1]`

`CsTriodePlotFunction = CsTriode /. { → 0.783 /. L → 1.665 ;`

`ParametricPlot[{{νM, CsTriodePlotFunction},`
`{νM, CsTriodePlotFunction0}}, {νM, .7, .996}, {νA, 10-7, .8},`
`PlotRange → {{.7, 1}, {0, -160}}, AspectRatio → 1]`

`ParametricPlot[{{νM, CcTriodePlotFunction / CsTriodePlotFunction},`
`{νM, CcTriodePlotFunction0 / CsTriodePlotFunction0}}, {νM, .7, .997},`
`{νA, 10-7, .8}, PlotRange → {{.7, 1}, {0, 2}}, AspectRatio → 1]`

Plots for $\nu_A \neq 0$ and $\ell/\mathcal{L} = 0.783/(1.665 + 0.186)$ (front-less triode with lens)

`z0TriodePlotFunctionAlt = z0Triode /. { → 0.783 /. L → (1.665 + 0.186) ;`

`ParametricPlot[{{νM, z0TriodePlotFunctionAlt},`
`{νM, z0TriodePlotFunction0}}, {νM, .65, .995},`
`{νA, 10-7, .8}, PlotRange → {{.65, 1}, {0, 8}}, AspectRatio → 1]`

```

CcTriodePlotFunctionAlt = CcTriode /. { → 0.783 /. L → (1.665 + 0.186) ;
ParametricPlot[{{vM, CcTriodePlotFunctionAlt},
  {vM, CcTriodePlotFunction0}}, {vM, .7, .995}, {vA, 10-7, .8},
  PlotRange → {{.7, 1}, {0, -160}}, AspectRatio → 1]

CsTriodePlotFunctionAlt = CsTriode /. { → 0.783 /. L → (1.665 + 0.186) ;
ParametricPlot[{{vM, CsTriodePlotFunctionAlt},
  {vM, CsTriodePlotFunction0}}, {vM, .7, .996}, {vA, 10-7, .8},
  PlotRange → {{.7, 1}, {0, -160}}, AspectRatio → 1]

ParametricPlot[
  {{vM, CcTriodePlotFunctionAlt / CsTriodePlotFunctionAlt},
   {vM, CcTriodePlotFunction0 / CsTriodePlotFunction0}}, {vM, .7, .997},
  {vA, 10-7, .8}, PlotRange → {{.7, 1}, {0, 2}}, AspectRatio → 1]

ParametricPlot[
  {{vM, CcTriodePlotFunctionAlt / CsTriodePlotFunctionAlt},
   {vM, CcTriodePlotFunction / CsTriodePlotFunction},
   {vM, CcTriodePlotFunction0 / CsTriodePlotFunction0}}, {vM, .7, .997},
  {vA, 10-7, .8}, PlotRange → {{.7, 1}, {0, 2}}, AspectRatio → 1]

```

Apertureless triode, inner hyperbolic region, outer constant field region

Position and velocity at the inner aperture

$$zC[rC\_] := \sqrt{\left\{^2 \frac{vM - 1}{vA vM - 1} + rC^2 / 2 \right. ;}$$

```

Clear[rA]; rA[rC_] := Refine[rHyp[ω, rC, 0, θA[rC]], ω > 0];
Clear[zA]; zA[rC_] := Refine[zHyp[ω, zC[rC], 0, θA[rC]], ω > 0];
Clear[vrA]; vrA[rC_] := Refine[vrHyp[ω, rC, 0, θA[rC]], ω > 0];
Clear[vzA]; vzA[rC_] := Refine[vzHyp[ω, zC[rC], 0, θA[rC]], ω > 0];
Clear[drdzA]; drdzA[rC_] := Refine[vrA[rC] / vzA[rC], ω > 0];

```

Aperture deflection

```

dVdzConst = (-VC vA) (L - { } )-1;
Clear[factor]; factor[rC_] := (rC Cos[θA[rC]]);
Clear[drdzAd]; drdzAd[rC_] :=
  factor[rC] Refine[Expand[factor[rC]-1 drdzofzDC[rA[rC], drdzA[rC], 2
    VC (vA - vM-1) {-2 zA[rC], dVdzConst, -VC (1 - vA)}], ω > 0 && VC < 0];
Clear[vzAd]; vzAd[rC_] := ω  $\left( \frac{(\omega)^{-2} \text{vrA}[rC]^2 + (\omega)^{-2} \text{vzA}[rC]^2}{1 + 1 \text{drdzAd}[rC]^2} \right)^{1/2}$ ; vzAd[rC]
Clear[vrAd]; vrAd[rC_] := drdzAd[rC] vzAd[rC]; vrAd[rC]

```

Position and velocity at the outer aperture

```

ηdVdzConst = ω2  $\frac{\{^2}{L - \{ \text{vA vM} - 1 \}}$ ;
rB = Refine[rConst[rA[rC], vrAd[rC], ω-1 θB[rC]], ω > 0]
zB = L;
vrB = ω Refine[Expand[ω-1 vrConst[rA[rC], vrAd[rC], ω-1 θB[rC]]], ω > 0]
vzB = ω Refine[
  Expand[ω-1 vzConst[ηdVdzConst, zA[rC], vzAd[rC], ω-1 θB[rC]]], ω > 0]
drdzB = Refine[vrB / vzB, ω > 0]

```

Approximations made at the inner aperture

```

θA0[rC_] := θofz[ω1, zC[rC], 0, {}]; θA0[rC]
rA1[rC_] := rHyp[ω1, rC, 0, θA0[rC]]; rA1[rC]
θA1[rC_] := θofz[ω1, zC[rC], 0,  $\sqrt{\{^2 + rA1[rC]^2 / 2}$ ]; θA1[rC]

```

Exact time solution at the outer aperture

```

θBConst[rC_] := ω tofzConst[ηdVdzConst, zA[rC], vzAd[rC], L];
θBConst0 = SeriesCoefficient[
  Block[{θA}, θA[rC_] := θA0[rC]; θBConst[rC]], {rC, 0, 0}]
θBConst1 =
  Series[Block[{θA}, θA[rC_] := θA0[rC]; θBConst[rC21/2]], {rC2, 0, 1}];
θBConst1 = Refine[Normal[θBConst1] /. rC2 → rC2,
  { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }

```

Image location z' and ray angle squared α'^2 . Explicitly using the small angle approximation $\alpha \approx \tan \alpha = -r'$.

```

zTriodeConst = zB - (Expand[drdzB / rB])-1
αSquaredTriodeConst = (-drdzB)2

```

Paraxial image location z'_0 and first and second order correction terms $z'_1 r_C = 0$ and $z'_2 r_C^2$.


```

z0TriodeConst = SeriesCoefficient[zTriodeConst, {rC, 0, 0}]
z0TriodeConst = Refine[z0TriodeConst, { > 0 && L > 0 && L > { &&
    vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
z0TriodeConst = Block[{θA, θB}, θA[rC_] := θA0[rC];
    θB[rC_] := θBConst0; z0TriodeConst]
z0TriodeConst = Refine[z0TriodeConst,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }

z2TriodeConst = SeriesCoefficient[zTriodeConst, {rC, 0, 2}]
z2TriodeConst = Refine[z2TriodeConst, { > 0 && L > 0 && L > { &&
    vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
z2TriodeConst = Block[{θA, θB}, θA[rC_] := θA0[rC];
    θB[ρC_] := Function[rC, Evaluate[θBConst1]] [ρC]; z2TriodeConst]
z2TriodeConst = Refine[z2TriodeConst,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }

```

Second order angle expansion $a'^2 = (\alpha'^2)_1 r_C + (\alpha'^2)_2 r_C^2 + O(r_C^3)$, $(\alpha'^2)_1 = 0$

```

αSquared2TriodeConst =
    SeriesCoefficient[αSquaredTriodeConst, {rC, 0, 2}]
αSquared2TriodeConst = Refine[αSquared2TriodeConst, { > 0 && L > 0 &&
    L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 && θA[0] ≥ 0 && θB[0] ≥ 0 }
αSquared2TriodeConst = Block[{θA, θB}, θA[rC_] := θA0[rC]; θB[ρC_] :=
    Function[rC, Evaluate[θBConst1]] [ρC]; αSquared2TriodeConst]
αSquared2TriodeConst = Refine[αSquared2TriodeConst,
    { > 0 && L > 0 && L > { && vA ≥ 0 && vA < 1 && vM > 0 && vM < 1 }

```

Coefficient of chromatic aberration, $C_c = V_C \frac{2 \partial z_0}{\partial V_C} = 2 (v_M \partial_{v_M} z_0 - v_A \partial_{v_A} z_0)$

```
CcTriodeConst = 2 (vM ∂vM z0TriodeConst - vA ∂vA z0TriodeConst);
```

Coefficient of spherical aberration, $z' = z_0 - 2^{-1} C_s \alpha'^2 \rightarrow C_s = -2 z'_2 / (\alpha'^2)_2$

```
CsTriodeConst = -2 z2TriodeConst / αSquared2TriodeConst;
```

Plots for $v_A = 0$ (should give diode behavior)

```

z0TriodeConstPlotFunction0 = z0TriodeConst /. { → 1 /. vA → 10-7 /. L → 2;
Plot[z0TriodeConstPlotFunction0, {vM, .65, .995}, PlotRange → {0, 8}]

CcTriodeConstPlotFunction0 = CcTriodeConst /. { → 1 /. vA → 10-7 /. L → 2;
Plot[CcTriodeConstPlotFunction0, {vM, .7, .995}, PlotRange → {0, -160}]

CsTriodeConstPlotFunction0 = CsTriodeConst /. { → 1 /. vA → 10-7 /. L → 2;
Plot[CsTriodeConstPlotFunction0, {vM, .7, .996}, PlotRange → {0, -160}]

Plot[CcTriodeConstPlotFunction0 / CsTriodeConstPlotFunction0,
    {vM, .7, .9963}, PlotRange → {0, 2}]

```

Plots for $v_A \neq 0$ and $\ell / \mathcal{L} = 0.783/1.665$ (design triode specs)

```

z0TriodeConstPlotFunction = z0TriodeConst /. {  $\rightarrow$  0.783 /. L  $\rightarrow$  1.665;
ParametricPlot[{{vM, z0TriodeConstPlotFunction},
  {vM, z0TriodeConstPlotFunction0}}, {vM, .65, .995},
  {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.65, 1}, {0, 8}}, AspectRatio  $\rightarrow$  1]

```

```

CcTriodeConstPlotFunction = CcTriodeConst /. {  $\rightarrow$  0.783 /. L  $\rightarrow$  1.665;
ParametricPlot[{{vM, CcTriodeConstPlotFunction},
  {vM, CcTriodeConstPlotFunction0}}, {vM, .7, .995},
  {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.7, 1}, {0, -160}}, AspectRatio  $\rightarrow$  1]

```

```

CsTriodeConstPlotFunction = CsTriodeConst /. {  $\rightarrow$  0.783 /. L  $\rightarrow$  1.665;
ParametricPlot[{{vM, CsTriodeConstPlotFunction},
  {vM, CsTriodeConstPlotFunction0}}, {vM, .7, .996},
  {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.7, 1}, {0, -160}}, AspectRatio  $\rightarrow$  1]

```

```

ParametricPlot[
  {{vM, CcTriodeConstPlotFunction / CsTriodeConstPlotFunction},
   {vM, CcTriodeConstPlotFunction0 / CsTriodeConstPlotFunction0}},
  {vM, .7, .997}, {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.7, 1}, {0, 2}},
  AspectRatio  $\rightarrow$  1]

```

Plots for $v_A \neq 0$ and $\ell/\mathcal{L} = 0.783/(1.665 + 0.186)$ (front-less triode with lens)

```

z0TriodeConstPlotFunctionAlt =
  z0TriodeConst /. {  $\rightarrow$  0.783 /. L  $\rightarrow$  (1.665 + 0.186);
ParametricPlot[{{vM, z0TriodeConstPlotFunctionAlt},
  {vM, z0TriodeConstPlotFunction0}}, {vM, .65, .995},
  {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.65, 1}, {0, 8}}, AspectRatio  $\rightarrow$  1]

```

```

CcTriodeConstPlotFunctionAlt =
  CcTriodeConst /. {  $\rightarrow$  0.783 /. L  $\rightarrow$  (1.665 + 0.186);
ParametricPlot[{{vM, CcTriodeConstPlotFunctionAlt},
  {vM, CcTriodeConstPlotFunction0}}, {vM, .7, .995},
  {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.7, 1}, {0, -160}}, AspectRatio  $\rightarrow$  1]

```

```

CsTriodeConstPlotFunctionAlt =
  CsTriodeConst /. {  $\rightarrow$  0.783 /. L  $\rightarrow$  (1.665 + 0.186);
ParametricPlot[{{vM, CsTriodeConstPlotFunctionAlt},
  {vM, CsTriodeConstPlotFunction0}}, {vM, .7, .996},
  {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.7, 1}, {0, -160}}, AspectRatio  $\rightarrow$  1]

```

```

ParametricPlot[
  {{vM, CcTriodeConstPlotFunctionAlt / CsTriodeConstPlotFunctionAlt},
   {vM, CcTriodeConstPlotFunction0 / CsTriodeConstPlotFunction0}},
  {vM, .7, .997}, {vA,  $10^{-7}$ , .8}, PlotRange  $\rightarrow$  {{.7, 1}, {0, 2}},
  AspectRatio  $\rightarrow$  1]

```

```
ParametricPlot[
  {{vM, CcTriodeConstPlotFunctionAlt / CsTriodeConstPlotFunctionAlt},
   {vM, CcTriodeConstPlotFunction / CsTriodeConstPlotFunction},
   {vM, CcTriodeConstPlotFunction0 / CsTriodeConstPlotFunction0}},
  {vM, .7, .997}, {vA, 10-7, .8}, PlotRange → {{.7, 1}, {0, 2}},
  AspectRatio → 1]
```

Comparison of two apertureless triode models

```
{ParametricPlot[{{vM, z0TriodePlotFunction},
  {vM, z0TriodeConstPlotFunction}, {vM, z0DiodePlotFunction}},
  {vM, .65, .995}, {vA, 10-7, .8}, PlotRange → {{.65, 1}, {0, 8}},
  AspectRatio → 1, ImageSize → 400],
 ParametricPlot[{{vM, CcTriodePlotFunction},
  {vM, CcTriodeConstPlotFunction}, {vM, CcDiodePlotFunction}},
  {vM, .7, .995}, {vA, 10-7, .8}, PlotRange → {{.7, 1}, {0, -160}},
  AspectRatio → 1, ImageSize → 400],
 ParametricPlot[{{vM, CsTriodePlotFunction},
  {vM, CsTriodeConstPlotFunction}, {vM, CsDiodePlotFunction}},
  {vM, .7, .996}, {vA, 10-7, .8}, PlotRange → {{.7, 1}, {0, -160}},
  AspectRatio → 1, ImageSize → 400],
 ParametricPlot[{{vM, CcTriodePlotFunction / CsTriodePlotFunction},
  {vM, CcTriodeConstPlotFunction / CsTriodeConstPlotFunction},
  {vM, CcDiodePlotFunction / CsDiodePlotFunction}},
  {vM, .7, .997}, {vA, 10-7, .8}, PlotRange → {{.7, 1}, {0, 2}},
  AspectRatio → 1, ImageSize → 400]}} // TableForm
```

```
{ { ParametricPlot[ { {vM, z0TriodePlotFunctionAlt},
  {vM, z0TriodeConstPlotFunctionAlt}, {vM, z0DiodePlotFunction} },
  {vM, .65, .995}, {vA, 10-7, .8}, PlotRange -> {{.65, 1}, {0, 8}},
  AspectRatio -> 1, ImageSize -> 400],
  ParametricPlot[ { {vM, CcTriodePlotFunctionAlt},
  {vM, CcTriodeConstPlotFunctionAlt}, {vM, CcDiodePlotFunction} },
  {vM, .7, .995}, {vA, 10-7, .8}, PlotRange -> {{.7, 1}, {0, -160}},
  AspectRatio -> 1, ImageSize -> 400],
  ParametricPlot[ { {vM, CsTriodePlotFunctionAlt},
  {vM, CsTriodeConstPlotFunctionAlt}, {vM, CsDiodePlotFunction} },
  {vM, .7, .996}, {vA, 10-7, .8}, PlotRange -> {{.7, 1}, {0, -160}},
  AspectRatio -> 1, ImageSize -> 400],
  ParametricPlot[ { {vM, CcTriodePlotFunctionAlt /
    CsTriodePlotFunctionAlt}, {vM,
    CcTriodeConstPlotFunctionAlt / CsTriodeConstPlotFunctionAlt},
    {vM, CcDiodePlotFunction / CsDiodePlotFunction} },
  {vM, .7, .997}, {vA, 10-7, .8}, PlotRange -> {{.7, 1}, {0, 2}},
  AspectRatio -> 1, ImageSize -> 400} ] } // TableForm
```

Triode with lens aperture, two hyperbolic regions

Reflection location contour

```
Clear[zC];
```

$$zC[rC\_]:= \left\{ \sqrt{\frac{1-vM}{1-vA vM}} + rC^2 / (2 \{^2\} \right\};$$

Position and velocity at the inner aperture

```
Clear[rA]; rA[rC_] := Refine[rHyp[w1, rC, 0, theta[rC]], w1 > 0]; rA[rC]
```

```
Clear[zA];
```

```
zA[rC_] := Refine[zHyp[w1, zC[rC], 0, theta[rC]], w1 > 0]; zA[rC]
```

```
Clear[vrA];
```

```
vrA[rC_] := Refine[vrHyp[w1, rC, 0, theta[rC]], w1 > 0]; vrA[rC]
```

```
Clear[vzA];
```

```
vzA[rC_] := Refine[vzHyp[w1, zC[rC], 0, theta[rC]], w1 > 0]; vzA[rC]
```

```
Clear[drdzA]; drdzA[rC_] := Refine[vrA[rC] / vzA[rC], w1 > 0]; drdzA[rC]
```

Inner aperture deflection

```

Clear[drdzAd]; drdzAd[rC_] := drdzofzDC[rA[rC], drdzA[rC],
  2 VC (vA - vM-1) {2 zA[rC], 2 (-VC vA) (L2 - {2)-1 zA[rC], -VC (1 - vA)}];
drdzAd[rC]
drdzAd[0]

Clear[vzAd]; vzAd[rC_] := ω1  $\left( \frac{(\omega 1)^{-2} \text{vrA}[rC]^2 + (\omega 1)^{-2} \text{vzA}[rC]^2}{1 + \text{drdzAd}[rC]^2} \right)^{1/2};$ 
vzAd[rC]
vzAd[0]

Clear[vrAd]; vrAd[rC_] := drdzAd[rC] vzAd[rC];
vrAd[rC]
vrAd[0]

```

Position and velocity at the outer aperture

```

ω2 = ω1  $\left( \frac{-vA \, vM}{vA \, vM - 1} \frac{\{^2}{L^2 - \{^2} \right)^{1/2};$ 

Clear[rB];
rB[rC_] := Refine[rHyp[ω2, rA[rC], vrAd[rC], θB[rC]], ω1 > 0]; rB[rC]
Clear[zB];
zB[rC_] := Refine[zHyp[ω2, zA[rC], vzAd[rC], θB[rC]], ω1 > 0]; zB[rC]
Clear[vrB];
vrB[rC_] := Refine[vrHyp[ω2, rA[rC], vrAd[rC], θB[rC]], ω1 > 0];
Clear[vzB];
vzB[rC_] := Refine[vzHyp[ω2, zA[rC], vzAd[rC], θB[rC]], ω1 > 0];
drdzB = Refine[vrB[rC] / vzB[rC], ω1 > 0]

```

Outer aperture deflection

```

drdzBd = drdzofzDC[rB[rC], drdzB,
  2 (-VC vA) (L2 - {2})-1 zB[rC], VC vL / s, -VC] /. VC → 1
qB = q[rB[rC], drdzB, 2 (-VC vA) (L2 - {2})-1 zB[rC], VC vL / s, -VC] /. VC → 1

```

Approximations made at the inner aperture

```

θA0[rC_] := θofz[ω1, zC[rC], 0, {}];
θA0[rC]
θA0[0]
rA1[rC_] := rHyp[ω1, rC, 0, θA0[rC]];
rA1[rC]
rA1[0]
θA1[rC_] := θofz[ω1, zC[rC], 0, {  $\sqrt{1 + rA1[rC]^2 / (2 \{^2)}$  }];
θA1[rC]
θA1[0]

```

Approximations made at the outer aperture

```

 $\theta B0[rC\_]$  :=  $\theta ofz[\omega 2, zA[rC], vzAd[rC], L]$ ;
Block[{ $\theta A$ },  $\theta A[rC\_]$  :=  $\theta A0[rC]$ ;  $\theta B0[0]$ ]
 $rB1[rC\_]$  :=  $rHyp[\omega 2, rA[rC], vrAd[rC], \theta B0[rC]]$ ;
Block[{ $\theta A$ },  $\theta A[rC\_]$  :=  $\theta A1[rC]$ ;  $rB1[rC]$ ]

 $\theta B1[rC\_]$  :=  $\theta ofz[\omega 2, zA[rC], vzAd[rC], L \sqrt{1 + rB1[rC]^2 / (2 L^2)}]$ ;
Block[{ $\theta A$ },  $\theta A[rC\_]$  :=  $\theta A1[rC]$ ;  $\theta B1[0]$ ]

```

Image location z' and ray angle squared α'^2 . Explicitly using the small angle approximation $\alpha \approx \tan \alpha = -r'$.

```

zBTriode =
  Refine[zB[rC], s > 0 && { > 0 && {  $\in$  Reals && L > 0 && L > { && vL > 0 &&
    vL < 2 && vA  $\geq$  0 && vA < 1 && vM > 0 && vM < 1 &&  $\theta A[rC] \geq 0$  &&  $\theta B[rC] \geq 0$  ]
qTriode = Refine[qB, s > 0 && { > 0 && {  $\in$  Reals && L > 0 && L > { && vL > 0 &&
  vL < 2 && vA  $\geq$  0 && vA < 1 && vM > 0 && vM < 1 &&  $\theta A[rC] \geq 0$  &&  $\theta B[rC] \geq 0$  ]
zTriode = zBTriode - qTriode-1;
 $\alpha$ SquaredTriode = (-drdzBd)2;

```

Paraxial image location z'_0 .

```

zB0Triode = SeriesCoefficient[zBTriode, {rC, 0, 0}]
zB0Triode =
  Refine[zB0Triode, s > 0 && { > 0 && {  $\in$  Reals && L > 0 && L > { && vL > 0 &&
    vL < 2 && vA  $\geq$  0 && vA < 1 && vM > 0 && vM < 1 &&  $\theta A[0] \geq 0$  &&  $\theta B[0] \geq 0$  ]
zB0Triode = Block[{ $\theta A$ ,  $\theta B$ },  $\theta A[rC\_]$  :=  $\theta A0[rC]$ ;
   $\theta B[rC\_]$  :=  $\theta B0[rC]$ ; zB0Triode]
zB0Triode = Simplify[zB0Triode, s > 0 && { > 0 && L > 0 &&
  L > { && vL > 0 && vL < 2 && vA  $\geq$  0 && vA < 1 && vM > 0 && vM < 1 ]

rB0 = Normal[Series[rB[rC], {rC, 0, 1}]]
drdzB0 = Normal[Series[drdzB, {rC, 0, 1}]]
qB0Triode =
  q[rB0, drdzB0, 2 (-vC vA) (L2 - {2})-1 zB[0], vC vL / s, -vC] /. vC  $\rightarrow$  1;
qB0Triode = Block[{ $\theta A$ ,  $\theta B$ },  $\theta A[rC\_]$  :=  $\theta A0[rC]$ ;
   $\theta B[rC\_]$  :=  $\theta B0[rC]$ ; qB0Triode]
qB0Triode = Refine[qB0, rC  $\geq$  0 && s > 0 && { > 0 && L > 0 &&
  L > { && vL > 0 && vL < 2 && vA  $\geq$  0 && vA < 1 && vM > 0 && vM < 1 ]

z0Triode = zB0Triode - qB0Triode-1;

z0TriodeLPlotFunction0 =
  z0Triode /. {  $\rightarrow$  1 /. vA  $\rightarrow$  10-7 /. vL  $\rightarrow$  10-7 /. L  $\rightarrow$  2 /. s  $\rightarrow$  .5;
Plot[z0TriodeLPlotFunction0, {vM, .65, .995}, PlotRange  $\rightarrow$  {0, 8}]

```

Aberration coefficients can be evaluated as in other sections

Appendix D Code, simion: swept-back lens

The cylindrical cross-section of lens geometries can be imported in SIMION from the design specification, e.g., App. Appendix A or more precisely App. ???. SIMION 8.0.6 was then used to determine the potential distribution inside the lens. Alternatively, a scale-independent geometry file (GEM) can generate the lens geometry, though at considerably more effort. This latter approach was used in earlier attempts, and below is the Lua code which generates the GEM file, the SIMION potential array (PA), and then refines the array to determine the electric potential distribution. Scaling and refinement options are found on the last line of the code.

```

1  -- intlens_gem.lua
2  -- program to create gem & pa, refine pa of interface lens
3
4  -- write gem, A = mirror-facing electrode
5  function make_gem(Din,inchgu,zoriginin,name)
6      local filename = name .. ".gem"
7      local gem = assert(io.open(filename, "w+"))
8      local tin = 0.05
9      --local Din = 0.275
10     local sAin = 0.125
11     local tAin = 0.025
12     local DAin = 0.05
13     local sBin = 0.125
14     local tBin = 0.025
15     local DBin = 0.1
16
17     -- constants in gu
18     local inch = inchgu
19     local rorigin = 0
20     local zorigin = floor(zoriginin*inch + 0.5)
21     local t = floor(inch*tin + 0.5)
22     local D = floor(inch*Din + 0.5)
23     local sA = floor(inch*sAin + 0.5)
24     local tA = floor(inch*tAin + 0.5)
25     local DA = floor(inch*DAin + 0.5)
26     local sB = floor(inch*sBin + 0.5)
27     local tB = floor(inch*tBin + 0.5)
28     local DB = floor(inch*DBin + 0.5)
29
30     -- size
31     local rsize = floor(1.05*inch + 0.5)
32     local zsize = floor(zorigin + tA + sA + t + sB + tB + inch + zorigin + 0.5)
33
34     -- write out size & definition to gem file
35     gem:write ([[
36     pa_define[] .. zsize .. [[,]] .. rsize .. [[,1,cylindrical,Y,electrostatic)
37     ]])

```

```

38
39 -- electrode A, mirror-facing edge at origin
40     -- polygon outline
41     local rA = floor(DA/2 + 0.5)
42     local pt1z = zorigin
43     local pt1r = rorigin + rA
44     local pt2z = pt1z
45     local pt2r = rorigin + floor(0.2*inch + 0.5)
46     local pt3z = pt1z + floor(0.6*inch + 0.5)
47     local pt3r = rorigin + floor(inch + 0.5)
48     local pt4z = pt1z + floor(0.7*inch + 0.5)
49     local pt4r = pt3r
50     local pt5z = pt1z + tA
51     local pt5r = rorigin + floor(0.17*inch + 0.5)
52     local pt6z = zorigin + tA
53     local pt6r = rorigin + rA
54
55     -- rounding parameters
56     local r1 = floor(tA/2 + 0.5)
57     local cent1z = pt1z + r1
58     local cent1r = pt1r + r1
59     local b11z = pt1z
60     local b11r = cent1r
61     local b12z = pt4z
62     local b12r = pt4r
63
64     gem:write ([[
65     ; electrode A (mirror-facing)
66     electrode(0){ fill{
67         within{
68             polyline([].pt1z..[[],].pt1r..[[],].pt2z..[[],].pt2r..[[],].pt3z
69             ..[[],].pt3r..[[],].pt4z..[[],].pt4r..[[],].pt5z..[[],].pt5r
70             ..[[],].pt6z..[[],].pt6r..[[]]
71             circle([].cent1z..[[],].cent1r..[[],].r1..[[],].r1..[[]] ;aperture
72             rounding
73         }
74         within{
75             polyline([].pt1z..[[],].pt1r..[[],].pt2z..[[],].pt2r..[[],].pt3z
76             ..[[],].pt3r..[[],].pt4z..[[],].pt4r..[[],].pt5z..[[],].pt5r
77             ..[[],].pt6z..[[],].pt6r..[[]]
78             box([].b11z..[[],].b11r..[[],].b12z..[[],].b12r..[[]] ;bulk
79             electrode
80         }
81         notin{
82             box(0,0,[]..zsize..[[],].rA..[[]]
83         }
84     }}
85     ]])
86
87 -- center electrode
88     -- polygon outline
89     local r = floor(D/2 + 0.5)
90     local pt1z = zorigin + tA + sA
91     local pt1r = rorigin + r
92     local pt2z = pt1z
93     local pt2r = rorigin + floor(0.18*inch + 0.5)
94     local pt3z = pt1z + floor(0.5*inch + 0.5)
95     local pt3r = rorigin + floor(0.52*inch + 0.5)
96     local pt4z = pt3z
97     local pt4r = rorigin + floor(0.65*inch + 0.5)
98     local pt5z = pt1z + floor(0.65*inch + 0.5)
99     local pt5r = pt4r
100    local pt6z = pt5z

```



```

96         local pt6r = rorigin + floor(0.8*inch + 0.5)
97         local pt7z = pt1z + floor(0.85*inch + 0.5)
98         local pt7r = pt6r
99         local pt8z = pt7z
100        local pt8r = rorigin + floor(0.7*inch + 0.5)
101        local pt9z = pt1z + floor(0.75*inch + 0.5)
102        local pt9r = pt8r
103        local pt10z = pt9z
104        local pt10r = rorigin + floor(0.55*inch + 0.5)
105        local pt11z = pt1z + t
106        local pt11r = rorigin + floor(0.15*inch + 0.5)
107        local pt12z = pt1z + t
108        local pt12r = pt1r
109
110        -- rounding parameters
111        local r1 = floor(tA/2 + 0.5)
112        local cent1z = pt1z + r1
113        local cent1r = pt1r + r1
114        local r2 = r1
115        local cent2z = pt12z - r1
116        local cent2r = pt12r + r1
117        local b11z = cent1z
118        local b11r = pt1r
119        local b12z = cent2z
120        local b12r = cent2r + r1
121        local r3 = floor(0.05*inch + 0.5)
122        local cent3z = pt2z + r3
123        local cent3r = pt2r - floor(r3/2 + 0.5)
124        local b21z = pt1z
125        local b21r = cent1r
126        local b22z = pt12z
127        local b22r = cent3r
128        local r4 = floor(0.05*inch + 0.5)
129        local cent4z = pt4z + r4
130        local cent4r = pt4r - r4
131        local b31z = cent3z - floor(0.02*inch + 0.5)
132        local b31r = cent3r
133        local b32z = pt7z
134        local b32r = cent4r
135        local r5 = floor(0.05*inch + 0.5)
136        local cent5z = pt6z + r5
137        local cent5r = pt6r - r5
138        local r6 = floor(0.05*inch + 0.5)
139        local cent6z = pt7z - r6
140        local cent6r = pt7r - r6
141        local b41z = cent4z
142        local b41r = cent4r
143        local b42z = cent6z
144        local b42r = cent5r
145        local b51z = cent5z
146        local b51r = cent5r
147        local b52z = cent6z
148        local b52r = pt7r
149
150        gem:write ([[
151        ; center electrode
152        electrode(1){ fill{
153            within{
154                polyline([].pt1z..[[],].pt1r..[[],].pt2z..[[],].pt2r..[[],].pt3z
                    ..[[],].pt3r..[[],].pt4z..[[],].pt4r..[[],].pt5z..[[],].pt5r
                    ..[[],].pt6z..[[],].pt6r..[[],].pt7z..[[],].pt7r..[[],].pt8z
                    ..[[],].pt8r..[[],].pt9z..[[],].pt9r..[[],].pt10z..[[],].
                    pt10r..[[],].pt11z..[[],].pt11r..[[],].pt12z..[[],].pt12r
                    ..[[]])

```

```

155         circle([]..cent1z..[],[]..cent1r..[],[]..r1..[],[]..r1..[] ;aperture
            rounding
156     }
157     within{
158         polyline([]..pt1z..[],[]..pt1r..[],[]..pt2z..[],[]..pt2r..[],[]..pt3z
            ..[],[]..pt3r..[],[]..pt4z..[],[]..pt4r..[],[]..pt5z..[],[]..pt5r
            ..[],[]..pt6z..[],[]..pt6r..[],[]..pt7z..[],[]..pt7r..[],[]..pt8z
            ..[],[]..pt8r..[],[]..pt9z..[],[]..pt9r..[],[]..pt10z..[],[]..
            pt10r..[],[]..pt11z..[],[]..pt11r..[],[]..pt12z..[],[]..pt12r
            ..[])
159         circle([]..cent2z..[],[]..cent2r..[],[]..r2..[],[]..r2..[] ;aperture
            rounding
160     }
161 ]]
162 gem:write ([[
163     within{
164         polyline([]..pt1z..[],[]..pt1r..[],[]..pt2z..[],[]..pt2r..[],[]..pt3z
            ..[],[]..pt3r..[],[]..pt4z..[],[]..pt4r..[],[]..pt5z..[],[]..pt5r
            ..[],[]..pt6z..[],[]..pt6r..[],[]..pt7z..[],[]..pt7r..[],[]..pt8z
            ..[],[]..pt8r..[],[]..pt9z..[],[]..pt9r..[],[]..pt10z..[],[]..
            pt10r..[],[]..pt11z..[],[]..pt11r..[],[]..pt12z..[],[]..pt12r
            ..[])
165         box([]..b11z..[],[]..b11r..[],[]..b12z..[],[]..b12r..[] ;aperture
            rounding, bulk
166     }
167     ;within{
168         ;polyline([]..pt1z..[],[]..pt1r..[],[]..pt2z..[],[]..pt2r..[],[]..
            pt3z..[],[]..pt3r..[],[]..pt4z..[],[]..pt4r..[],[]..pt5z..[],[]..
            pt5r..[],[]..pt6z..[],[]..pt6r..[],[]..pt7z..[],[]..pt7r..[],[]..
            pt8z..[],[]..pt8r..[],[]..pt9z..[],[]..pt9r..[],[]..pt10z
            ..[],[]..pt10r..[],[]..pt11z..[],[]..pt11r..[],[]..pt12z..[],[]..
            pt12r..[])
169         ;box([]..b21z..[],[]..b21r..[],[]..b22z..[],[]..b22r..[] ;near
            aperture bulk electrode
170     ;}
171 ]]
172 gem:write ([[
173     within{
174         polyline([]..pt1z..[],[]..pt1r..[],[]..pt2z..[],[]..pt2r..[],[]..pt3z
            ..[],[]..pt3r..[],[]..pt4z..[],[]..pt4r..[],[]..pt5z..[],[]..pt5r
            ..[],[]..pt6z..[],[]..pt6r..[],[]..pt7z..[],[]..pt7r..[],[]..pt8z
            ..[],[]..pt8r..[],[]..pt9z..[],[]..pt9r..[],[]..pt10z..[],[]..
            pt10r..[],[]..pt11z..[],[]..pt11r..[],[]..pt12z..[],[]..pt12r
            ..[])
175         circle([]..cent3z..[],[]..cent3r..[],[]..r3..[],[]..r3..[] ;lowest
            edge rounding
176     }
177     within{
178         polyline([]..pt1z..[],[]..pt1r..[],[]..pt2z..[],[]..pt2r..[],[]..pt3z
            ..[],[]..pt3r..[],[]..pt4z..[],[]..pt4r..[],[]..pt5z..[],[]..pt5r
            ..[],[]..pt6z..[],[]..pt6r..[],[]..pt7z..[],[]..pt7r..[],[]..pt8z
            ..[],[]..pt8r..[],[]..pt9z..[],[]..pt9r..[],[]..pt10z..[],[]..
            pt10r..[],[]..pt11z..[],[]..pt11r..[],[]..pt12z..[],[]..pt12r
            ..[])
179         box([]..b31z..[],[]..b31r..[],[]..b32z..[],[]..b32r..[] ;lower bulk
            electrode
180     }
181 ]]
182 gem:write ([[
183     within{
184         polyline([]..pt1z..[],[]..pt1r..[],[]..pt2z..[],[]..pt2r..[],[]..pt3z
            ..[],[]..pt3r..[],[]..pt4z..[],[]..pt4r..[],[]..pt5z..[],[]..pt5r
            ..[],[]..pt6z..[],[]..pt6r..[],[]..pt7z..[],[]..pt7r..[],[]..pt8z
            ..[],[]..pt8r..[],[]..pt9z..[],[]..pt9r..[],[]..pt10z..[],[]..

```

```

        pt10r..[,].pt11z..[,].pt11r..[,].pt12z..[,].pt12r
        ..[]
185      circle()[.cent4z..[,].cent4r..[,].r4..[,].r4..[] ;middle
        edge rounding
186    }
187    within{
188      polyline()[.pt1z..[,].pt1r..[,].pt2z..[,].pt2r..[,].pt3z
        ..[,].pt3r..[,].pt4z..[,].pt4r..[,].pt5z..[,].pt5r
        ..[,].pt6z..[,].pt6r..[,].pt7z..[,].pt7r..[,].pt8z
        ..[,].pt8r..[,].pt9z..[,].pt9r..[,].pt10z..[,].pt
        pt10r..[,].pt11z..[,].pt11r..[,].pt12z..[,].pt12r
        ..[]
189      box()[.b41z..[,].b41r..[,].b42z..[,].b42r..[] ;middle bulk
        electrode
190    }
191  ]])
192  gem:write ([[
193    within{
194      polyline()[.pt1z..[,].pt1r..[,].pt2z..[,].pt2r..[,].pt3z
        ..[,].pt3r..[,].pt4z..[,].pt4r..[,].pt5z..[,].pt5r
        ..[,].pt6z..[,].pt6r..[,].pt7z..[,].pt7r..[,].pt8z
        ..[,].pt8r..[,].pt9z..[,].pt9r..[,].pt10z..[,].pt
        pt10r..[,].pt11z..[,].pt11r..[,].pt12z..[,].pt12r
        ..[]
195      circle()[.cent5z..[,].cent5r..[,].r5..[,].r5..[] ;upper
        left edge rounding
196    }
197    within{
198      polyline()[.pt1z..[,].pt1r..[,].pt2z..[,].pt2r..[,].pt3z
        ..[,].pt3r..[,].pt4z..[,].pt4r..[,].pt5z..[,].pt5r
        ..[,].pt6z..[,].pt6r..[,].pt7z..[,].pt7r..[,].pt8z
        ..[,].pt8r..[,].pt9z..[,].pt9r..[,].pt10z..[,].pt
        pt10r..[,].pt11z..[,].pt11r..[,].pt12z..[,].pt12r
        ..[]
199      circle()[.cent6z..[,].cent6r..[,].r6..[,].r6..[] ;upper
        right edge rounding
200    }
201  ]])
202  gem:write ([[
203    within{
204      polyline()[.pt1z..[,].pt1r..[,].pt2z..[,].pt2r..[,].pt3z
        ..[,].pt3r..[,].pt4z..[,].pt4r..[,].pt5z..[,].pt5r
        ..[,].pt6z..[,].pt6r..[,].pt7z..[,].pt7r..[,].pt8z
        ..[,].pt8r..[,].pt9z..[,].pt9r..[,].pt10z..[,].pt
        pt10r..[,].pt11z..[,].pt11r..[,].pt12z..[,].pt12r
        ..[]
205      box()[.b51z..[,].b51r..[,].b52z..[,].b52r..[] ;upper bulk
        electrode
206    }
207  ]])
208  gem:write ([[
209    notin{
210      box(0,0,][.zsize..[,].r..[]
211    }
212  ]])
213 ]])
214
215
216 -- electrode B, magnet-facing
217 -- polygon outline
218 local rB = floor(DB/2 + 0.5)
219 local pt1z = zorigin + tA + sA + t + sB
220 local pt1r = rorigin + rB
221 local pt2z = pt1z

```

```

222     local pt2r = rorigin + floor(0.1*inch + 0.5)
223     local pt3z = pt1z + floor(0.8*inch + 0.5)
224     local pt3r = rorigin + floor(0.42*inch + 0.5)
225     local pt4z = pt3z
226     local pt4r = rorigin + floor(0.58*inch + 0.5)
227     local pt5z = pt1z + floor(0.95*inch + 0.5)
228     local pt5r = pt4r
229     local pt6z = pt5z
230     local pt6r = rorigin + inch
231     local pt7z = pt1z + floor(1.05*inch + 0.5)
232     local pt7r = pt6r
233     local pt8z = pt7z
234     local pt8r = rorigin + floor(0.5*inch + 0.5)
235     local pt9z = pt1z + floor(0.9*inch + 0.5)
236     local pt9r = pt8r
237     local pt10z = pt9z
238     local pt10r = rorigin + floor(0.38*inch + 0.5)
239     local pt11z = pt1z + tB
240     local pt11r = rorigin + floor(0.08*inch + 0.5)
241     local pt12z = pt1z + tB
242     local pt12r = pt1r
243
244     -- rounding parameters
245     local r1 = floor(tB/2 + 0.5)
246     local cent1z = pt1z + r1
247     local cent1r = pt1r + r1
248     local r2 = floor(0.025*inch + 0.5)
249     local cent2z = pt2z + r2
250     local cent2r = pt2r - floor(r2/2 + 0.5)
251     local b11z = pt1z
252     local b11r = cent1r
253     local b12z = pt7z
254     local b12r = cent2r
255     local r3 = floor(0.05*inch + 0.5)
256     local cent3z = pt4z + r3
257     local cent3r = pt4r - r3
258     local b21z = cent2z
259     local b21r = cent2r
260     local b22z = pt7z
261     local b22r = cent3r
262     local b31z = cent3z
263     local b31r = cent3r
264     local b32z = pt7z
265     local b32r = pt7r
266
267     gem:write ([[
268     ; electrode B (magnet-facing)
269     electrode(0){ fill{
270         within{
271             polyline([].pt1z..[[],].pt1r..[[],].pt2z..[[],].pt2r..[[],].pt3z
272                 ..[[],].pt3r..[[],].pt4z..[[],].pt4r..[[],].pt5z..[[],].pt5r
273                 ..[[],].pt6z..[[],].pt6r..[[],].pt7z..[[],].pt7r..[[],].pt8z
274                 ..[[],].pt8r..[[],].pt9z..[[],].pt9r..[[],].pt10z..[[],].
275                 pt10r..[[],].pt11z..[[],].pt11r..[[],].pt12z..[[],].pt12r
276                 ..[[]]
277             circle([].cent1z..[[],].cent1r..[[],].r1..[[],].r1..[[]] ;aperture
278                 rounding
279         }
280     ]])
281     gem:write ([[
282     within{
283         polyline([].pt1z..[[],].pt1r..[[],].pt2z..[[],].pt2r..[[],].pt3z
284             ..[[],].pt3r..[[],].pt4z..[[],].pt4r..[[],].pt5z..[[],].pt5r
285             ..[[],].pt6z..[[],].pt6r..[[],].pt7z..[[],].pt7r..[[],].pt8z

```

```

        ..[[,]]..pt8r..[[,]]..pt9z..[[,]]..pt9r..[[,]]..pt10z..[[,]]..
        pt10r..[[,]]..pt11z..[[,]]..pt11r..[[,]]..pt12z..[[,]]..pt12r
        ..[[
278      box(]]..b11z..[[,]]..b11r..[[,]]..b12z..[[,]]..b12r..[[() ;near
        aperture bulk electrode
279      ]
280  ]])
281  gem:write ([[
282      within{
283      polyline(]]..pt1z..[[,]]..pt1r..[[,]]..pt2z..[[,]]..pt2r..[[,]]..pt3z
        ..[[,]]..pt3r..[[,]]..pt4z..[[,]]..pt4r..[[,]]..pt5z..[[,]]..pt5r
        ..[[,]]..pt6z..[[,]]..pt6r..[[,]]..pt7z..[[,]]..pt7r..[[,]]..pt8z
        ..[[,]]..pt8r..[[,]]..pt9z..[[,]]..pt9r..[[,]]..pt10z..[[,]]..
        pt10r..[[,]]..pt11z..[[,]]..pt11r..[[,]]..pt12z..[[,]]..pt12r
        ..[[
284      circle(]]..cent2z..[[,]]..cent2r..[[,]]..r2..[[,]]..r2..[[() ;lower
        edge rounding
285      ]
286  ]])
287  gem:write ([[
288      within{
289      polyline(]]..pt1z..[[,]]..pt1r..[[,]]..pt2z..[[,]]..pt2r..[[,]]..pt3z
        ..[[,]]..pt3r..[[,]]..pt4z..[[,]]..pt4r..[[,]]..pt5z..[[,]]..pt5r
        ..[[,]]..pt6z..[[,]]..pt6r..[[,]]..pt7z..[[,]]..pt7r..[[,]]..pt8z
        ..[[,]]..pt8r..[[,]]..pt9z..[[,]]..pt9r..[[,]]..pt10z..[[,]]..
        pt10r..[[,]]..pt11z..[[,]]..pt11r..[[,]]..pt12z..[[,]]..pt12r
        ..[[
290      box(]]..b21z..[[,]]..b21r..[[,]]..b22z..[[,]]..b22r..[[() ;middle bulk
        electrode
291      ]
292  ]])
293  gem:write ([[
294      within{
295      polyline(]]..pt1z..[[,]]..pt1r..[[,]]..pt2z..[[,]]..pt2r..[[,]]..pt3z
        ..[[,]]..pt3r..[[,]]..pt4z..[[,]]..pt4r..[[,]]..pt5z..[[,]]..pt5r
        ..[[,]]..pt6z..[[,]]..pt6r..[[,]]..pt7z..[[,]]..pt7r..[[,]]..pt8z
        ..[[,]]..pt8r..[[,]]..pt9z..[[,]]..pt9r..[[,]]..pt10z..[[,]]..
        pt10r..[[,]]..pt11z..[[,]]..pt11r..[[,]]..pt12z..[[,]]..pt12r
        ..[[
296      circle(]]..cent3z..[[,]]..cent3r..[[,]]..r3..[[,]]..r3..[[() ;upper
        edge rounding
297      ]
298  ]])
299  gem:write ([[
300      within{
301      polyline(]]..pt1z..[[,]]..pt1r..[[,]]..pt2z..[[,]]..pt2r..[[,]]..pt3z
        ..[[,]]..pt3r..[[,]]..pt4z..[[,]]..pt4r..[[,]]..pt5z..[[,]]..pt5r
        ..[[,]]..pt6z..[[,]]..pt6r..[[,]]..pt7z..[[,]]..pt7r..[[,]]..pt8z
        ..[[,]]..pt8r..[[,]]..pt9z..[[,]]..pt9r..[[,]]..pt10z..[[,]]..
        pt10r..[[,]]..pt11z..[[,]]..pt11r..[[,]]..pt12z..[[,]]..pt12r
        ..[[
302      box(]]..b31z..[[,]]..b31r..[[,]]..b32z..[[,]]..b32r..[[() ;upper bulk
        electrode
303      ]
304  ]])
305  gem:write ([[
306      notin{
307      box(0,0,]]..zsize..[[,]]..rB..[[()
308      ]
309  ]}
310  ]])
311
312
313  -- grounding can

```

```

314         local inner = inch
315         local outer = rsize
316     gem:write ([[
317     ; grounding can & interface lens face
318     electrode(0){
319         fill{
320             within{box[]}..(zorigin + floor(0.6*inch + 0.5))..[[,]]..inner..[[,]]..zsize
321                 ..[[,]]..outer..[[,]]}
322         }
323     ]])
324 ]])
325
326
327
328     gem:close()
329
330         return(filename)
331 end
332
333
334 -- make & refine the .PA
335 function make_pa(Din,inchgu,zoriginin,name,convergence)
336     -- create GEM file of proper dimensions
337     local gem_filename = make_gem(Din,inchgu,zoriginin,name)
338
339     -- convert GEM file to PA# file.
340     local pasharp_filename = string.gsub(gem_filename, ".gem", ".pa#")
341     simion.command("gem2pa " .. gem_filename .. " " .. pasharp_filename)
342
343     -- refine PA# file.
344     simion.command("refine --convergence=" .. convergence .. " " ..
345         pasharp_filename)
346
347 end
348
349 make_pa(0.264,25*254,0.5,"intlens",5e-5)

```

Electron trajectory data is collected in SIMION following a procedure similar to the experimental characterization described in Ref. [60]. Trajectory data was written to file according to a user program written in Lua. The following code is an example of the user program used to analyze trajectories in a swept-back lens. With only a few details specific to the design, it can be readily adapted to other lens geometries.

```

1  =====
2  -- intlens.lua version
3  -- simulation: adjust VL and VC
4  -- then record z', a'
5  -- Cc calculated by changing electron energy by +/-1 eV
6  =====
7  simion.workbench_program()
8
9  ===== variables
10 -- record VC & max angle for analysis (set in .fly file)

```

```

11 adjustable electronsperun = 35
12 local VC = -20000
13
14 adjustable dVC = 1
15 adjustable VCruns = 2
16 local VCmin = VC - dVC
17 local VCmax = VC + dVC
18 local VCdelta = (VCmax - VCmin)/(VCruns - 1)
19 local E = -VCmin
20 local E0 = -VC
21 local VCn = 0 -- electron energy counter
22
23 -- adjust VL
24 adjustable VLmax = -10000
25 adjustable VLmin = -24000
26 adjustable VRuns = 140*4+1
27 local VL = VLmin
28 local VLdelta = (VLmax - VLmin)/(VRuns - 1)
29 local VLn = 0 --counter
30
31 -- define z0 & bound range
32 local z0 = 17*25
33
34 -- find z' and a'
35 local zprimeset = -17
36 local px_prev = 0
37 local py_prev = 0
38 local axisn = 0
39 local A = 1
40 local a = {}
41 local m = {}
42 local zprime = {}
43 local aprime2 = {}
44 local z0_prev = 0
45 local z0_pprev = 0
46
47 -- save data
48 local data
49 local first = 1
50 local fullfilename
51
52 -- count runs
53 local total = VRuns
54 local current_i = 0
55 local V_count = 0
56
57
58 -- (1) initializes all electrons' (without flying them)
59 -- can output messages and control rerun looping
60 function segment.initialize()
61
62     sim_trajectory_quality = 99
63
64     -- first time only: print simulation parameters,
65     --     make output filenames (with current date/time),
66     --     one for Cs data, one for Cs & Cc data
67     --     open output file for writing, and print column headings.
68     if first == 1 then
69         local total_runs = VRuns
70         local folder = "../..data/"
71         local name = "swept-back-lens,D=0.264"
72         local filetype = "csv"
73         fullfilename = os.date(folder .. name .. ". " .. "%Y-%m-%d-%H%M" .. ". " ..
            .. filetype)

```

```

74         local dataheader = assert(io.open(fullfilename,"a"))
75         dataheader:write("VL,VC,Z,a,Z0',a'\n")
76         dataheader:close()
77         print("Running simulation: will take at least ".. total_runs .."
              simulation runs.")
78         print("Data file: " .. fullfilename)
79
80         first = 0
81     end
82
83     -- set z0 and electron energy
84     -- (sets y, off-axis distance; actual start location set in "fly2" file)
85     local speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm, ion_vz_mm)
86     E0 = speed_to_ke(speed,ion_mass)
87     E = E0*(VCmin + VCdelta*VCn)/VC
88     local speed = ke_to_speed(E,ion_mass)
89     ion_vx_mm, ion_vy_mm, ion_vz_mm = polar3d_to_rect3d(speed, az, el)
90     ion_py_mm = (ion_px_mm - z0)*ion_vy_mm/ion_vx_mm
91     a[ion_number] = atan2(ion_vy_mm,-ion_vx_mm)
92
93 end
94
95
96 -- (2) initializes electrodes & scales array before electrons fly
97 function segment.init_p_values()
98
99     -- set VL
100     VL = VLmin + VLn*VLdelta
101     adj_elect01 = VL
102
103     -- print some trial information
104     if VCn == 0 then current_i = current_i + 1 end
105     print("( "..current_i.." / "..total.." ) VL = "..VL.." V, VC = "..-E.." V")
106
107     redraw_screen() -- show new contours(?)
108
109 end
110
111
112 -- (3) measures/adjusts electron conditions after each time step
113 -- can output messages
114 function segment.other_actions()
115
116     -- correct for non-zero potential at start point
117     if ion_time_of_flight <= 1.0*ion_time_step then
118         local speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm,
            ion_vz_mm)
119         local E_corrected = E + ion_volts
120         speed = ke_to_speed(E_corrected,ion_mass)
121         ion_vx_mm, ion_vy_mm, ion_vz_mm = polar3d_to_rect3d(speed, az, el)
122     end
123
124
125     -- marks axis crossing (if it occurs)
126     if abs(py_prev + ion_py_mm) < abs(py_prev) + abs(ion_py_mm) then mark() end
127
128     -- measure location (y',z') at z' = z'set
129     if (abs(zprimeset - ion_px_mm) < abs(px_prev - ion_px_mm)) then
130         ap = atan2(ion_vy_mm,-ion_vx_mm)
131         axisn = axisn + 1
132         local zp = ion_px_mm - ion_vx_mm*ion_py_mm/ion_vy_mm
133         data = assert(io.open(fullfilename,"a"))
134         data:write(VL.."","..(-E).."","..z0.."","..a[ion_number].."","..zp.."","..
            ap.."\\n")

```



```
135             data:close()
136             ion_splat = -1
137         end
138
139         -- records electron position for use in next time step
140         px_prev = ion_px_mm
141         py_prev = ion_py_mm
142     end
143
144
145     -- (4) measures electron conditions after every one has died
146     -- can output messages and control rerun looping
147     function segment.terminate()
148         -- analyze z' & a'^2 to find z0, reset z0
149         if ion_number == electronsperrun then
150
151             -- reset variables
152             m = {}
153             axisn = 0
154             zprime = {}
155             aprime2 = {}
156
157             -- increment VC & VL run counters
158             VCn = VCn + 1
159             if VCn >= VCruns then VCn = 0 end
160
161             if VCn == 0 then VLn = VLn + 1 end
162
163         end
164
165         -- check if this is the last run
166         if VLn >= VLruns then sim_rerun_flym = 0 else sim_rerun_flym = 1 end
167     end
```

Appendix E   Code, *Mathematica*: swept-back lens

Electron trajectory data collected from SIMION according to App. Appendix D is then analyzed in Mathematica 9 with the following code to determine the optical properties f , g , S_f , S_g , C_f , and C_g , as defined in Ref. [60]. While this code is applied to the swept-back lens design, it is general enough to be applied to any lens with good SIMION data.

Header

Graphics Options

```

SetOptions[Plot, PlotRange → All,
  PlotStyle → {{Thick, Black}, {Thick, Darker[Red]}},
  {Thick, Blend[{Darker[Gray], Green}, 1 / 4]},
  {Thick, Blend[{Lighter[Gray], Blue}, 1 / 3]}}], Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ParametricPlot, PlotRange → All,
  PlotStyle → {{Dashed, Thin, Black}, {Dashed, Thin, Darker[Red]}},
  {Dashed, Thin, Blend[{Darker[Gray], Green}, 1 / 4]},
  {Dashed, Thin, Blend[{Lighter[Gray], Blue}, 1 / 3]}}], Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[LogPlot, PlotRange → All,
  PlotStyle → {{Thick, Black}, {Thick, Darker[Red]}},
  {Thick, Blend[{Darker[Gray], Green}, 1 / 4]},
  {Thick, Blend[{Lighter[Gray], Blue}, 1 / 3]}}], Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[LogLogPlot, PlotRange → All, PlotStyle → {{Thick, Black},
  {Thick, Darker[Red]}, {Thick, Blend[{Darker[Gray], Green}, 1 / 4]},
  {Thick, Blend[{Lighter[Gray], Blue}, 1 / 3]}}], Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ParametricPlot3D, PlotStyle →
  {{Thick, Black}, {Thick, Dashed, Black}, {Thick, Dotted, Black}},
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350,
  BoxRatios → {1, 1, .5}, Axes → {True, True, False},
  Boxed → False, ViewCenter → {.5, .5, 0},
  ViewVertical → {0, 0, 1}, ViewPoint → {0, -3, 1}];
SetOptions[ListPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.02], Black},
  {Thick, PointSize[.02], Darker[Red]},
  {Thick, PointSize[.02], Blend[{Darker[Gray], Green}, 1 / 4]},
  {Thick, PointSize[.02], Blend[{Lighter[Gray], Blue}, 1 / 3]}}],
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → Gray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListPointPlot3D, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.01], Black},
  {Thick, PointSize[.01], Darker[Red]}},

```

```

    {Thick, PointSize[.01], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.01], Blend[{Lighter[Gray], Blue}, 1 / 3]}}},
BoxRatios → 1, BaseStyle → {FontFamily → "Arial", FontSize → 14},
ImageSize → 350];
SetOptions[ListContourPlot, PlotRange → All, Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLinearPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.02], Black},
    {Thick, PointSize[.02], Darker[Red]}},
    {Thick, PointSize[.02], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.02], Blend[{Lighter[Gray], Blue}, 1 / 3]}}},
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.02], Black},
    {Thick, PointSize[.02], Darker[Red]}},
    {Thick, PointSize[.02], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.02], Blend[{Lighter[Gray], Blue}, 1 / 3]}}},
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLogPlot, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.02], Black},
    {Thick, PointSize[.02], Darker[Red]}},
    {Thick, PointSize[.02], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.02], Blend[{Lighter[Gray], Blue}, 1 / 3]}}},
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];

```

Characterization

Thick lens equations for focal length and distance from Rempfer 1985

```

Clear[z, zp, m]
f[z_, zp_, m_] := (z - zp) / (1 / m - m);
g[z_, zp_, m_] := (zp / m - m z) / (1 / m - m);

```

Aberration formulas at the Gaussian plane (not circle of least confusion)

```

Clear[m, f, Sf, Sg, Cf, Cg]
Csp[m_, f_, Sf_, Sg_] := -((1 + m^2) Sg + 2 m Sf) (1 + m)^2 f;
Ccp[m_, f_, Cf_, Cg_] := ((1 + m^2) Cg + 2 m Cf) f;

```

D = 0.264 in

```

Import data, format : VL, VC, z, alpha, z', alpha'

SetDirectory[$HomeDirectory<>
  "/Dropbox/Electron optics/Simion/swept-back lenses"];
data0 = ({1, 1, 1, 1, -1, 1} Drop[
  Import["swept-back-lens,D=0.264.2014-10-08-1249.csv"], 1]<)<;
data0[[
  1,
  3]]

VLsets = GatherBy[data0, #[[1]] &];
VLCsets0 =
  Select[Table[Select[GatherBy[VLsets[[i]], #[[2]] &], Length[#] > 8 &],
    {i, Length[VLsets]}], Length[#] == 2 &];
data0 = Flatten[VLCsets0, 2];

VLCsets1 = Table[Block[{set = VLCsets0[[i, j]], hplane, rofξfunctions},
  hplane = Table[
    rofξfunctions = ({ξ, -ξ} + set[[k, {3, 5}]] Tan[set[[k, {4, 6}]]];
    sol = FindRoot[rofξfunctions[[1]] == -rofξfunctions[[1]],
      {ξ, 0}] // Quiet;
    {set[[k, 4]], ξ} /. sol
    , {k, Length[set]}];
  Block[{αatmaxξ = SortBy[hplane, -#[[1]] &] [[1, 1]],
    Select[set, #[[4]] > 1.3 αatmaxξ &]]
  ], {i, Length[VLCsets0]}, {j, Length[VLCsets0[[i]]]}] // Quiet;

VLCsets = Select[VLCsets1, # == Re[#] && Length#[[1]] > 10 &&
  Length#[[1]] > 10 && Max[#[[1]]<[[5]] - Min[#[[1]]<[[5]]]] > 1 × 10-4 &&
  Max[#[[1]]<[[5]] - Min[#[[1]]<[[5]]]] > 1 × 10-4 &];
data = Flatten[VLCsets, 2];
{{Length[data0], Length[data]}, {Length[VLCsets0], Length[VLCsets]}}
```

```

Block[{sets = SortBy[RandomSample[GatherBy[data, #[[1 ;; 2]] &], 11],
  #[[1, 1]] &]}, dzvsa2sets =
  Table[Union[{sets[[i]]<[[4]]2, sets[[i]]<[[5]] - Min[sets[[i]]<[[5]]]}<],
    {i, Length[sets]}];
hplanes = Table[functions =
  ({ξ, -ξ} + sets[[i, k, {3, 5}]) Tan[sets[[i, k, {4, 6}]]];
  sol = FindRoot[functions[[1]] == -functions[[-1]], {ξ, 0}] // Quiet;
  {sets[[i, k, 4]], ξ} /. sol
  , {i, Length[sets]}, {k, Length[sets[[i]]]}];
hplanesrel =
  Table[Union[{hplanes[[i, All, 1]], hplanes[[i, All, -1]] - Min[
    hplanes[[i, All, -1]]}<], {i, Length[hplanes]}];
{{TableForm[Round[sets[[All, 1, 1]] / sets[[All, 1, 2]], .001]],
  ListPlot[dzvsa2sets, Joined → True],
  Show[ListPlot[hplanesrel], ListPlot[hplanesrel, Joined → True]],
  {Histogram[data0<[[1]], ImageSize → 300, AspectRatio → .55],
  Histogram[data<[[1]], ImageSize → 300,
  AspectRatio → .55]}}} // TableForm]

```

```

Clear[sets, set, Ccpts, as, aps, ms, zps,
      fs, gs, zpfite, mfit, Sffite, Sgfit, v0, m0, m1, zp1,
      f1, g1, Cs, Sf, Sg, zp0, f0, g0, Sf0, Sg0, Cc, Cf, Cg];
properties0 = Union[Table[
  Block[{sets, set, Ccpts, as, aps, ms, zps,
        fs, gs, zpfite, mfit, Sffite, Sgfit, v0, m0, m1, zp1, f1,
        g1, Cs, Sf, Sg, zp0, f0, g0, Sf0, Sg0, Cc, Cf, Cg},
    sets = VLCsets[[i]];
    Ccpts = Table[set = sets[[j]];
      as = set[[4]];
      aps = -set[[6]];
      ms = as / aps;
      zps = set[[5]];
      fs = f[set[[3]], set[[5]], ms];
      gs = g[set[[3]], set[[5]], ms];
      zpfite = Fit[{aps, zps} <, {1,  $\alpha^2$ ,  $\alpha^4$ },  $\alpha$ ];
      mfit = Fit[{as, ms} <, {1,  $\alpha^2$ ,  $\alpha^4$ },  $\alpha$ ];
      Sffite = Fit[{as, fs} <, {1,  $\alpha^2$ ,  $\alpha^4$ },  $\alpha$ ];
      Sgfit = Fit[{as, gs} <, {1,  $\alpha^2$ ,  $\alpha^4$ },  $\alpha$ ];
      {zp0, m0, f0, g0} = {zpfite, mfit, Sffite, Sgfit} /.  $\alpha \rightarrow 0$ ;
      {zp1, m1, f1, g1} =
        SeriesCoefficient[{zpfite, mfit, Sffite, Sgfit}, { $\alpha$ , 0, 2}];
      Cs = -zp1;
      {Sf, Sg} = {f1, g1} / (f0 (1 + m0-1)2);
      {Mean[set[[1]] / set[[2]], zp0, m0, f0, g0, Cs, Sf, Sg, m1}
      , {j, Length[sets]}}];
  {v0, zp0, m0, f0, g0, Cs, Sf0, Sg0, m1} = Mean[Ccpts];
  {Cc, Cf, Cg} =
    (Ccpts[[1, {2, 4, 5}]] - Ccpts[[2, {2, 4, 5}]]) / {1, f0, f0}
    / (Ccpts[[2, 1]] - Ccpts[[1, 1]]) / v0
  {v0, zp0, m0, f0, g0, Cs, Sf0, Sg0, Cc, Cf, Cg}
], {i, Length[VLCsets]}}];

```

```

{{ListLogPlot[
  {properties0[[All, {1, 2}]], (properties0[[All, {1, 2}]] < {1, -1}) <},
  Joined → True, ImageSize → 250],
ListLogPlot[{properties0[[All, {1, 3}]],
  (properties0[[All, {1, 3}]] < {1, -1}) <},
  Joined → True, ImageSize → 250],
ListLogPlot[{{properties0[[1]], properties0[[6]] <},
  {properties0[[1]], Csp[properties0[[3]], properties0[[4]],
    properties0[[7]], properties0[[8]]} <},
  Joined → True, ImageSize → 250, PlotRange → Automatic],
ListLogPlot[{{properties0[[1]], properties0[[9]] <},
  {properties0[[1]], Ccp[properties0[[3]], properties0[[4]],
    properties0[[10]], properties0[[11]]} <}, Joined → True,
  ImageSize → 250, PlotRange → Automatic]}} // TableForm

properties =
  Select[properties0, Abs[#[[3]]] < 100 && Norm[#[[4 ;; 5]]] < 1000 &];

{{ListLogPlot[{properties[[All, {1, 4}]], properties[[All, {1, 5}]]},
  Joined → True], ListLogPlot[{{properties[[1]], -properties[[7]]} <},
  {properties[[1]], -properties[[8]]} <}, Joined → True],
ListPlot[{properties[[All, {1, 10}]], properties[[All, {1, 11}]]},
  Joined → True]},
{"", ListLogLogPlot[{{properties[[4]], -properties[[7]]} <},
  {properties[[4]], -properties[[8]]} <}, Joined → True],
ListLogLogPlot[{properties[[All, {4, 10}]], properties[[All, {4, 11}]]},
  Joined → True]}} // TableForm

L264propertyData = properties;

```

Fit properties to analytic functions

D = 0.264 in

```

properties = L264propertyData;

{Table[Block[
  {vs = properties[[1]], sum = .5 (properties[[i]] + properties[[i + 1]]),
  dif = -.5 (properties[[i]] - properties[[i + 1]])},
  {ListLogPlot[{vs, Abs[sum]} <, AspectRatio → .55],
  ListPlot[Select[{vs, dif} <, #[[1]] > .2 &], AspectRatio → .55]}}],
{i, 4, 10, 3}]] // TableForm

```



```

{Table[Block[
  {vs = properties[[1]], sum = .5 (properties[[i]] + properties[[i + 1]]),
    dif = -.5 (properties[[i]] - properties[[i + 1]]), sumfit, diffit},
  sumfit = LinearModelFit[{vs, Log[If[i == 7, -1, 1] sum]}<,
    vRange[0, 4], v];
  diffit = LinearModelFit[Select[
    {vs, If[i == 7, Log[dif + Ceiling[Abs[Min[dif]]], .1]], dif]}<,
    #[[1]] > .2 &], vRange[0, 4], v];
  functions = {Abs[If[i == 7, -1, 1] Exp[sumfit[v]]], If[i == 7,
    Exp[diffit[v]] - Ceiling[Abs[Min[dif]]], .1], diffit[v]};
  {sumfit["ParameterTable"], Show[ListLogPlot[{vs, Abs[sum]}<,
    AspectRatio → .55], LogPlot[functions[[1]], {v, .1, 1.3}]],
    diffit["ParameterTable"], Show[ListPlot[
    Select[{vs, dif}<, #[[1]] > .2 &], AspectRatio → .55],
    Plot[functions[[-1]], {v, .1, 1.3}]]]}, {i, 4, 10, 3}]] // TableForm

propertyFits = Table[Block[
  {vs = properties[[1]], sum = .5 (properties[[i]] + properties[[i + 1]]),
    dif = -.5 (properties[[i]] - properties[[i + 1]]), sumfit, diffit},
  sumfit = LinearModelFit[{vs, Log[If[i == 7, -1, 1] sum]}<,
    vRange[0, 4], v];
  diffit = LinearModelFit[Select[
    {vs, If[i == 7, Log[dif + Ceiling[Abs[Min[dif]]], .1]], dif]}<,
    #[[1]] > .2 &], vRange[0, 4], v];
  {If[i == 7, -1, 1] Exp[sumfit[v]] - If[i == 7,
    Exp[diffit[v]] - Ceiling[Abs[Min[dif]]], .1], diffit[v]},
  If[i == 7, -1, 1] Exp[sumfit[v]] + If[i == 7, Exp[diffit[v]] -
    Ceiling[Abs[Min[dif]]], .1], diffit[v]}}], {i, 4, 10, 3}]

{Table[Show[ListPlot[
  {properties[[All, {1, 1 + 3 i}]], properties[[All, {1, 2 + 3 i}]]}],
  Plot[{propertyFits[[i, 1]], propertyFits[[i, -1]]},
  {v, .1, 1.25}]], {i, 3}],
  Table[ListPlot[{Select[{properties[[All, 1]],
    1 - propertyFits[[i, 1]] / standard /. {v → properties[[All, 1]],
    standard → properties[[All, 1 + 3 i}]]}<, #[[1]] > .6 &], Select[
  {properties[[All, 1]], 1 - propertyFits[[i, -1]] / standard /. {v →
    properties[[All, 1]], standard → properties[[All, 2 + 3 i}]]}<,
  #[[1]] > .6 &}]], {i, 3}]] // TableForm

Export["Swept-back lens properties, D=0.264in.wdx",
  {properties, propertyFits}]

```

Appendix F Code, *Mathematica*: objective branch

After characterizing the swept-back lens and auxiliary lens (of the projection design), they can be combined with the estimated aberration coefficients of the cathode to provide a complete model of the objective branch of our PEEM. The following code computes the focusing curves that maintain constant magnification, with $0.1\times$ increments given. The spherical and chromatic aberration in transfer space is also computed.

Header

Graphics Options

```

colors = {Black, Darker[Red], Blend[{Darker[Gray], Green}, 1 / 4],
  Blend[{Lighter[Gray], Blue}, 1 / 3]};
SetOptions[Plot, PlotRange → All,
  PlotStyle → Table[{Thick, colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1,
  GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ParametricPlot, PlotRange → All,
  PlotStyle → Table[{Dashed, colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1,
  GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[LogPlot, PlotRange → All,
  PlotStyle → Table[{Thick, colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1,
  GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[LogLogPlot, PlotRange → All, PlotStyle →
  Table[{Thick, colors[[i]]}, {i, Length[colors]}], Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ParametricPlot3D, PlotStyle →
  {{Thick, Black}, {Thick, Dashed, Black}, {Thick, Dotted, Black}},
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350,
  BoxRatios → {1, 1, .5}, Axes → {True, True, False},
  Boxed → False, ViewCenter → {.5, .5, 0},
  ViewVertical → {0, 0, 1}, ViewPoint → {0, -3, 1}];
SetOptions[ListPlot, PlotRange → All, PlotStyle →
  Table[{Thick, PointSize[.02], colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → Gray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListPointPlot3D, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.01], Black},
    {Thick, PointSize[.01], Darker[Red]},
    {Thick, PointSize[.01], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.01], Blend[{Lighter[Gray], Blue}, 1 / 3]}}},
  BoxRatios → 1, BaseStyle → {FontFamily → "Arial", FontSize → 14},
  ImageSize → 350];
SetOptions[ListContourPlot, PlotRange → All, Frame → True,

```

```

    AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLinearPlot, PlotRange → All,
    PlotStyle → {{Thick, PointSize[.02], Black},
        {Thick, PointSize[.02], Darker[Red]},
        {Thick, PointSize[.02], Blend[{Darker[Gray], Green}, 1 / 4]},
        {Thick, PointSize[.02], Blend[{Lighter[Gray], Blue}, 1 / 3]}}},
    Frame → True, AspectRatio → 1, GridLines → Automatic,
    GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogPlot, PlotRange → All, PlotStyle →
    Table[{Thick, PointSize[.02], colors[[i]]}, {i, Length[colors]}],
    Frame → True, AspectRatio → 1, GridLines → Automatic,
    GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLogPlot, PlotRange → All, PlotStyle →
    Table[{Thick, PointSize[.02], colors[[i]]}, {i, Length[colors]}],
    Frame → True, AspectRatio → 1, GridLines → Automatic,
    GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];

```

Analysis

Measurements (pixels)

Measurements taken from PEEM CAD diagram PDF, 90 pixels/in.

Front of cathode

$Cf[z] = 2550.192;$

Alternate cathode front measurements (diagram unclear).

2548.748

2549.649;

2550.192;

Front aperture of objective lens

```

{Of[r, left, front], Of[z, left, front]} = {1773.243, 2535.472};
{Of[r, right, front], Of[z, right, front]} = {1777.745, 2535.472};
{Of[r, left, back], Of[z, left, back]} = {1773.243, 2533.222};
{Of[r, right, back], Of[z, right, back]} = {1777.745, 2533.222};

```

$Of[z, front] = Mean[{Of[z, left, front], Of[z, right, front]}];$

$Of[z, back] = Mean[{Of[z, left, back], Of[z, right, back]}];$

$Of[z, center] = Mean[{Of[z, front], Of[z, back]}]$

Center aperture of objective lens

```

{Oc[r, left, front], Oc[z, left, front]} = {1766.497, 2521.974};
{Oc[r, right, front], Oc[z, right, front]} = {1784.491, 2521.974};
{Oc[r, left, back], Oc[z, left, back]} = {1766.497, 2517.477};
{Oc[r, right, back], Oc[z, right, back]} = {1784.491, 2517.477};

Oc[z, front] = Mean[{Oc[z, left, front], Oc[z, right, front]}];
Oc[z, back] = Mean[{Oc[z, left, back], Oc[z, right, back]}];
Oc[z, center] = Mean[{Oc[z, front], Oc[z, back]}];

DO = Abs[Mean[{Oc[r, left, front], Oc[r, left, back]}] -
  Mean[{Oc[r, right, front], Oc[r, right, back]}]]
tO = Abs[Oc[z, front] - Oc[z, back]]

Back aperture of objective lens

{Ob[r, left, front], Ob[z, left, front]} = {1770.994, 2506.224};
{Ob[r, right, front], Ob[z, right, front]} = {1779.989, 2506.224};
{Ob[r, left, back], Ob[z, left, back]} = {1770.994, 2503.974};
{Ob[r, right, back], Ob[z, right, back]} = {1779.989, 2503.974};

Ob[z, front] = Mean[{Ob[z, left, front], Ob[z, right, front]}];

Objective lens spacing

sOf = Abs[Of[z, back] - Oc[z, front]]
sOb = Abs[Oc[z, back] - Ob[z, front]]
sO = Mean[{sOf, sOb}]

Front aperture of auxiliary lens

{Xf[r, left, front], Xf[z, left, front]} = {1768.742, 2094.474};
{Xf[r, right, front], Xf[z, right, front]} = {1782.242, 2094.474};
{Xf[r, left, back], Xf[z, left, back]} = {1768.742, 2089.978};
{Xf[r, right, back], Xf[z, right, back]} = {1782.242, 2089.978};

Xf[z, back] = Mean[{Xf[z, left, back], Xf[z, right, back]}];

Center aperture of auxiliary lens

{Xc[r, left, front], Xc[z, left, front]} = {1768.288, 2078.733};
{Xc[r, right, front], Xc[z, right, front]} = {1782.695, 2078.733};
{Xc[r, left, back], Xc[z, left, back]} = {1768.288, 2065.231};
{Xc[r, right, back], Xc[z, right, back]} = {1782.695, 2065.231};

Xc[z, front] = Mean[{Xc[z, left, front], Xc[z, right, front]}];
Xc[z, back] = Mean[{Xc[z, left, back], Xc[z, right, back]}];
Xc[z, center] = Mean[{Xc[z, front], Xc[z, back]}];

DX = Abs[Mean[{Xc[r, left, front], Xc[r, left, back]}] -
  Mean[{Xc[r, right, front], Xc[r, right, back]}]]
tX = Abs[Xc[z, front] - Xc[z, back]]

```

Back aperture of auxiliary lens

```
{Xb[r, left, front], Xb[z, left, front]} = {1772.119, 2053.980};
{Xb[r, right, front], Xb[z, right, front]} = {1778.869, 2053.980};
{Xb[r, left, back], Xb[z, left, back]} = {1772.119, 2049.479};
{Xb[r, right, back], Xb[z, right, back]} = {1778.869, 2049.479};

Xb[z, front] = Mean[{Xb[z, left, front], Xb[z, right, front]}];
```

Auxiliary lens spacing

```
sXf = Abs[Xf[z, back] - Xc[z, front]]
sXb = Abs[Xc[z, back] - Xb[z, front]]
sX = Mean[{sXf, sXb}]
```

Center of magnet A

```
MAc[z] = Mean[{1874.793, 1869.395}];
```

Relevant lengths (mm)

l_a = cathode length, distance from the sample surface to the front electrode

```
lamm = la 25.4 / 90
```

Measured l_a

```
lamm = 3.95;
```

D_O = objective lens center aperture diameter

```
DOmm = DO 25.4 / 90
```

D_X = auxiliary lens center aperture diameter

```
DXmm = DX 25.4 / 90
```

CO = distance from cathode sample plane to center of objective lens

```
Cf[z] - Oc[z, center]
```

```
COmm = Abs[Cf[z] - Oc[z, center]] 25.4 / 90
```

OX = distance from center of objective lens to center of auxiliary lens

```
OXmm = Abs[Oc[z, center] - Xc[z, center]] 25.4 / 90
```

XA = distance from center of auxiliary lens to center of magnet A

```
XAm = Abs[Xc[z, center] - MAc[z]] 25.4 / 90
```

Objective lens properties from Simlon

Import swept-back lens property fits

```

SetDirectory[
  $HomeDirectory<> "/Dropbox/Electron optics/PEEM optical models";
{propertiesO, propertyFitsO} =
  Import["Swept-back lens properties, D=0.264in.wdx"];
{{fOofvO, gOofvO}, {SfOofvO, SgOofvO}, {CfOofvO, CgOofvO}} =
  propertyFitsO / {DOmm, 1, 1} /. v -> vO

```

Auxiliary lens properties from Simlon

Import swept-back lens property fits

```

SetDirectory[
  $HomeDirectory<> "/Dropbox/Electron optics/PEEM optical models";
{propertiesX, propertyFitsX} =
  Import["Projection lens properties.wdx"];
{{fXofvX, gXofvX}, {SfXofvX, SgXofvX}, {CfXofvX, CgXofvX}} =
  propertyFitsX / {DXmm, 1, 1} /. v -> vX

```

Optics, focusing as function of z_C (mm)

Thick lens equations

```

Clear[f, g, z, zp, m];

z[f_, g_, zp_] := g +  $\frac{f^2}{zp - g}$ ;

zp[f_, g_, z_] := g +  $\frac{f^2}{z - g}$ ;

m[f_, g_, z_, zp_] :=  $\sqrt{\frac{zp - g}{z - g}}$ ;

```

Accelerating field virtual image location, measured from sample surface.

Magnification of accelerating field and first aperture.

```

zCp = -lamm +  $\delta z_C$ 
mC = 2 / 3;

```

Objective lens object and image locations.

```

zO = COmm - zCp
zOp = zp[fOofvO DOmm, gOofvO DOmm, zO];
mO = -Simplify[m[fOofvO DOmm, gOofvO DOmm, zO, zOp], 0 < vO < 2];
mO /. vO -> {.96, .99} /.  $\delta z_C \rightarrow 0$ 

```

```

Block[{ $\delta z_C = 0$ }, {{LogPlot[{zOp, OXmm + XAmm}, {vO, .965, 1.01}],
  LogPlot[{ $-mO$ ,  $mC^{-1} 9$ }, {vO, .965, 1.01}],
  Show[ParametricPlot[{zOp, mO}, {vO, .965, 1.01}],
  ListPlot[{OXmm + XAmm,  $-mC^{-1} 9$ }]}}} // TableForm]

Auxiliary lens object and image locations, with image centered in magnet A (where
possible).

zXp = XAmm;
zX = z[fXofvX DXmm, gXofvX DXmm, zXp];
mX = Simplify[m[fXofvX DXmm, gXofvX DXmm, zX, zXp], 0 < vX < 2];
mX /. vX → {.2, .4}

{{LogPlot[{ $-zX$ , XAmm}, {vX, .2, .43}, PlotRange → Automatic],
  LogPlot[{mX, 6 mC / 9}, {vX, .2, .43}, PlotRange → Automatic],
  Show[ParametricPlot[{zX, mX}, {vX, .2, .43}],
  ListPlot[{ $-XAmm$ , 6 mC / 9}]}]} // TableForm

focusData0 = ParallelTable[
  Block[{sol = Quiet[FindMinimum[(zX - (OXmm - zOp))2, { $\delta z_C$ , 0}]]][[-1]],
    {vO, vX,  $\delta z_C$ , mC mO mX, (zX - (OXmm - zOp))} /. sol],
  {vO, .95, 1.01, .0005}, {vX, .25, .45, .0005}];
focusData0 = Select[Table[Select[focusData0[[i]], Abs[#[-1]] < 10-6 &],
  {i, Length[focusData0]}], Length[#] > 0 &][[All, All, 1 ;; -2]];
Histogram[Flatten[focusData0, 1]<[[4]]]

focusDataMs =
  Select[Table[Select[Table[SortBy[focusData0[[i]], Abs[#[[4]] + m] &][[1]],
    {i, Length[focusData0]}], Abs[#[[4]] + m] < .01 &],
    {m, 3.5, 7, .1}], Length[#] > 1 &];
Length[focusDataMs]

{{Show[ListPlot[focusDataMs[[All, All, {1, 2}]], Joined → True,
  FrameLabel → {"vO", "vX"}, ImageSize → 400], Graphics[Table[
  Text[Style[ToString[-Round[Mean[focusDataMs[[i, All, 4]]], .1]] <>
    "x", colors[[tmp = Mod[i, Length[colors]]];
    If[tmp == 0, Length[colors], tmp]]],
  Mean[focusDataMs[[i, All, {1, 2}]], {0, 1}],
  {i, Length[focusDataMs]}]]],
  ListPlot[focusDataMs[[All, All, {3, 1}]], Joined → True,
  FrameLabel → {" $\delta z_C$  (mm)", "vO"}, ImageSize → 400]}] // TableForm

```



```
Show[ListPlot[focusDataMs[[1 ;; -1 ;; 5, All, {1, 2}]],
Joined → True, FrameLabel → {"Vo/Vc", "Vx/Vc"},
ImageSize → 300, GridLines → None], Graphics[Table[Text[Style[
ToString[-Round[Mean[focusDataMs[[i, All, 4]], .1]] <> "x", colors[
tmp = Mod[i, Length[colors]]; If[tmp == 0, Length[colors], tmp]]],
Mean[focusDataMs[[i, All, {1, 2}]], {0, 1}],
{i, 1, Length[focusDataMs], 5}]]]
```

Optics, focusing as function of z_C , aberration (mm)

Cathode object magnification and aberration for Cu illuminated with 4.83 eV light

$$CsC = \left(\frac{1\text{mm} + \delta zC}{4} \right) 807.$$

$$CcC = \left(\frac{1\text{mm} + \delta zC}{4} \right) 844.$$

Lens image aberration formulas

```
Clear[m, f, Sf, Sg]
Csp[m_, f_, Sf_, Sg_] := -((1 + m^2) Sg + 2 m Sf) (1 + m)^2 f;
Ccp[m_, f_, Cf_, Cg_] := ((1 + m^2) Cg + 2 m Cf) f;

CsSys = mC^4 mO^4 mX^4 CsC + mX^4 Csp[mO, fOofvO D0mm, SfOofvO, SgOofvO] +
  Csp[mX, fXofvX D0mm, SfXofvX, SgXofvX];
CsSysNoC = mX^4 Csp[mO, fOofvO D0mm, SfOofvO, SgOofvO] +
  Csp[mX, fXofvX D0mm, SfXofvX, SgXofvX];
CcSys = mC^2 mO^2 mX^2 CcC + mX^2 Ccp[mO, fOofvO D0mm, CfOofvO, CgOofvO] +
  Ccp[mX, fXofvX D0mm, CfXofvX, CgXofvX];
CcSysNoC = mX^2 Ccp[mO, fOofvO D0mm, CfOofvO, CgOofvO] +
  Ccp[mX, fXofvX D0mm, CfXofvX, CgXofvX];

focusAberDataMs =
Table[Block[{vO = focusDataMs[[i, j, 1]], vX = focusDataMs[[i, j, 2]],
  dzC = focusDataMs[[i, j, 3]], m = focusDataMs[[i, j, 4]],
Join[focusDataMs[[i, j]], {CsSys, CcSys}, {CsSys/m^4, CcSys/m^2},
{CsSysNoC, CcSysNoC}, {CsSysNoC/m^4, CcSysNoC/m^2}]]],
{i, Length[focusDataMs]}, {j, Length[focusDataMs[[i]]]}];

{{Show[ListLogLogPlot[focusAberDataMs[[All, All, {5, 6}]]/10^3,
Joined → True, FrameLabel → {"C's (m)", "C'c (m)"}, ImageSize → 400],
ParametricPlot[Log[{CsC 6^4, CcC 6^2}/10^3], {dzC, 0, .5},
PlotStyle → {{Thick, Red}}], Graphics[Table[Text[
Style[ToString[-Round[Mean[focusAberDataMs[[i, All, 4]], .1]] <>
"x", colors[tmp = Mod[i, Length[colors]]];
If[tmp == 0, Length[colors], tmp]]],
```

```

Log[Mean[focusAberDataMs[[i, All, {5, 6}]]/103]],
{0, If[i == 4, 1, -1]}], {i, Length[focusAberDataMs]}]],
Graphics[{Red, Text["Cathode\nm = 6×",
Log[{CsC 64, CcC 62}/103 /.  $\delta zC \rightarrow 0.$ ], {1.1, -0.5}]}]],
Show[ListPlot[focusAberDataMs[[All, All, {7, 8}]]/103,
Joined → True, FrameLabel → {"Cs = C's/M4 (m)", "Cc = C'c/M2 (m)"},
ImageSize → 400], Plot[{CsC, CcC}/103,
{ $\delta zC$ , 0, .5}, PlotStyle → {{Thick, Red}}],
Graphics[{Red, Text["Cathode", {CsC, CcC}/103 /.  $\delta zC \rightarrow 0.5$ ,
{-.2, -1}]}]],
Show[ListPlot[focusAberDataMs[[All, All, {1, 8}]],
Joined → True, FrameLabel → {"v0", "Cc = C'c/M2 (mm)"},
ImageSize → 400], Graphics[Table[Text[
Style[ToString[-Round[Mean[focusAberDataMs[[i, All, 4]]], .1]] <>
"x", colors[[tmp = Mod[i, Length[colors]]];
If[tmp == 0, Length[colors], tmp]]],
Mean[focusAberDataMs[[i, All, {1, 8}]]], {-1, -.5}],
{i, Length[focusAberDataMs]}]]],
{Show[ListLogLogPlot[focusAberDataMs[[All, All, {9, 10}]]/103,
Joined → True, FrameLabel →
{"Obj & aux (no cath) C's (m)", "Obj & aux (no cath) C'c (m)"},
ImageSize → 400], Graphics[Table[Text[Style[
ToString[-Round[Mean[focusAberDataMs[[i, All, 4]]], .1]] <> "x",
colors[[tmp = Mod[i, Length[colors]]];
If[tmp == 0, Length[colors], tmp]]],
Log[Mean[focusAberDataMs[[i, All, {9, 10}]]/103]], {.5, -1}],
{i, Length[focusAberDataMs]}]]],
Show[ListPlot[focusAberDataMs[[All, All, {11, 12}]]/103,
Joined → True, FrameLabel → {"Obj & aux (no cath) Cs = C's/M4 (m)",
"Obj & aux (no cath) Cc = C'c/M2 (m)"},
ImageSize → 400], Graphics[Table[Text[Style[
ToString[-Round[Mean[focusAberDataMs[[i, All, 4]]], .1]] <> "x",
colors[[tmp = Mod[i, Length[colors]]];
If[tmp == 0, Length[colors], tmp]]],
Mean[focusAberDataMs[[i, All, {11, 12}]]/103],
{.8 If[i == 4, -1, 1], If[i == 4, .5, -1]}],
{i, Length[focusAberDataMs]}]]],
Show[ListPlot[focusAberDataMs[[All, All, {1, 12}]], Joined → True,
FrameLabel → {"v0", "Obj & aux (no cath) Cc = C'c/M2 (mm)"},
ImageSize → 400], Graphics[Table[Text[
Style[ToString[-Round[Mean[focusAberDataMs[[i, All, 4]]], .1]] <>

```

```

"x", colors[[tmp = Mod[i, Length[colors]]];
If[tmp == 0, Length[colors], tmp]]],
Mean[focusAberDataMs[[i, All, {1, 12}]]], {-1, -.5}],
{i, Length[focusAberDataMs]]}] // TableForm

Show[ListPlot[
  focusAberDataMs[[6 ;; -1 ;; 10, All, {7, 8}]] / 103, Joined → True,
  FrameLabel → {"Cs,tot = C's,tot/M4 (m)", "Cc,tot = C'c,tot/M2 (m)"},
  ImageSize → 350, GridLines → None,
  PlotRange → {{2.4, 6.6}, {.7, 1.4}}],
Graphics[{Text[Style[
  ToString[-Round[Mean[focusDataMs[[6, All, 4]]], .1]] <> "x",
  colors[[1]], {Min[focusAberDataMs[[6, All, 7]]],
  Max[focusAberDataMs[[6, All, 8]]] / 103, {0, -1}}], Text[
  ToString[-Round[Mean[focusDataMs[[16, All, 4]]], .1]] <> "x",
  colors[[2]], {Min[focusAberDataMs[[16, All, 7]]],
  Max[focusAberDataMs[[16, All, 8]]] / 103, {0, -1}}}],
Graphics[Table[Text[Style[ToString[
  -Round[Mean[focusDataMs[[i, All, 4]]], .1]] <> "x",
  colors[[tmp = -Mod[i, Length[colors]]]; If[tmp == 0,
  Length[colors], tmp]]], {Max[focusAberDataMs[[i, All, 7]]],
  Min[focusAberDataMs[[i, All, 8]]] / 103, {0, 1}},
{i, 6, Length[focusDataMs], 10}][[-2 ;; -1]]]

```

```
Show[ListPlot[Table[{focusAberDataMs[[i, All, 1],
  (2.12 + (106 focusAberDataMs[[i, All, 7] (0.0025)3 / 4)2 +
    (106 focusAberDataMs[[i, All, 8]
      (2 × .125 / 20 000.5) (0.0025) / 2)2)1/2}<,
  {i, 6, Length[focusAberDataMs], 10}], Joined →
  True,
FrameLabel → {"Vo/Vc", "<Ra+o+x>ap (nm)"},
ImageSize → 350,
GridLines → None,
PlotRange → {17, 24}],
Graphics[{Text[Style[
  ToString[-Round[Mean[focusDataMs[[6, All, 4]], .1]] <> "x",
  colors[[1]], {.975, 20.}],
  Text[Style[ToString[-Round[Mean[focusDataMs[[16, All, 4]], .1]] <>
  "x", colors[[2]], {.97, 18}],
  Text[Style[ToString[-Round[Mean[focusDataMs[[26, All, 4]], .1]] <>
  "x", colors[[3]], {1.003, 20.9}],
  Text[Style[ToString[-Round[Mean[focusDataMs[[36, All, 4]], .1]] <>
  "x", colors[[4]], {.974, 22.5}]]]]]
```

Aberration comparison to diode

Hyperbolic trajectory functions

$\omega = \sqrt{e k / m}$, k defines shape of hyperbolic potential. Functions of time t

```
rHyp[ $\omega$ _, r0_, vr0_,  $\theta$ _] := r0 Cos[ $\theta$ ] + vr0 Sin[ $\theta$ ] /  $\omega$ ;
zHyp[ $\omega$ _, z0_, vz0_,  $\theta$ _] := z0 Cosh[ $\sqrt{2}$   $\theta$ ] + vz0 Sinh[ $\sqrt{2}$   $\theta$ ] / ( $\sqrt{2}$   $\omega$ );
vrHyp[ $\omega$ _, x0_, v0_,  $\theta$ _] :=  $\omega$  Derivative[0, 0, 0, 1][rHyp][ $\omega$ , x0, v0,  $\theta$ ];
vzHyp[ $\omega$ _, x0_, v0_,  $\theta$ _] :=  $\omega$  Derivative[0, 0, 0, 1][zHyp][ $\omega$ , x0, v0,  $\theta$ ];
```

Invert $z(t)$ to get $\theta(z)$

```
 $\psi$ [ $\omega$ _, z0_, vz0_] := ArcTanh[-vz0 / ( $\sqrt{2}$   $\omega$  z0)];
thetafz[ $\omega$ _, z0_, vz0_, z_] :=
  2-1/2 ( $\psi$ [ $\omega$ , z0, vz0] + ArcCosh[(z / z0) Cosh[ $\psi$ [ $\omega$ , z0, vz0]]]);
```

Davisson-Calbick approximation

Trajectory through an aperture, from left to right.

```
drdzofzDC[r0_, drdzofz0_, dVdzL_, dVdzR_, VBeam_] :=
  drdzofz0 +  $\frac{dVdzL - dVdzR}{4 VBeam}$  r0;
```

$q = (dr/dz)/r$

```
q[r0_, drdzofz0_, dVdzL_, dVdzR_, VBeam_] :=  $\frac{drdzofz0}{r0} + \frac{dVdzL - dVdzR}{4 VBeam}$ ;
```

Put it all together

Variables: $v_L = V_L/V_C$, $v_A = V_A/V_C$, $v_M^{-1} = V_M/V_C$.

Constants: $\omega_1 = \sqrt{e k_1/m}$, $k_1 = V_C(v_A - v_M^{-1})/\ell^2$.

Lens half width = s.

Turn-around radial extent, limiting variable r_C

Position and velocity at the aperture

```
zC[rC_] :=  $\sqrt{\left\{^2 \frac{vM - 1}{vA vM - 1} + rC^2 / 2\right\}}$ ;
```

```
rA = Refine[rHyp[ $\omega$ , rC, 0,  $\theta A[rC]$ ],  $\omega > 0$ ];
zA = Refine[zHyp[ $\omega$ , zC[rC], 0,  $\theta A[rC]$ ],  $\omega > 0$ ];
vrA = Refine[vrHyp[ $\omega$ , rC, 0,  $\theta A[rC]$ ],  $\omega > 0$ ];
vzA = Refine[vzHyp[ $\omega$ , zC[rC], 0,  $\theta A[rC]$ ],  $\omega > 0$ ];
drdzA = Refine[vrA / vzA,  $\omega > 0$ ];
drdzAd = Refine[drdzofzDC[rA, drdzA,
  2 VC (vA - vM-1) {-2 zA, 0, -VC (1 - vA)}], { $\omega > 0$ , VC < 0}]
```

Approximations made at the aperture

```
 $\theta A0[rC_] := \theta ofz[\omega, zC[rC], 0, \{]; \theta A0[rC]$ 
rA1[rC_] := rHyp[ $\omega$ , rC, 0,  $\theta A0[rC]$ ]; rA1[rC]
 $\theta A1[rC_] := \theta ofz[\omega, zC[rC], 0, \sqrt{\{^2 + rA1[rC]^2 / 2\}}]; \theta A1[rC]$ 
```

Image location z' and ray angle squared α'^2 .

```
zDiode = zA - (Expand[drdzAd / rA])-1;
 $\alpha SquaredDiode = ArcTan[-drdzAd]^2$ ;
```

Paraxial image location z'_0 and first and second order correction terms $z'_1 r_C = 0$ and $z'_2 r_C^2$

```
z0Diode = SeriesCoefficient[zDiode, {rC, 0, 0}];
z0Diode = Block[{ $\theta A$ },  $\theta A[rC_] := \theta A0[rC]$ ;
  Refine[z0Diode, {> 0 && vA > 0 && vA < 1 && vM > 0 && vM < 1}];

z1Diode = SeriesCoefficient[zDiode, {rC, 0, 1}];
z1Diode = Block[{ $\theta A$ },  $\theta A[rC_] := \theta A0[rC]$ ; z1Diode];
```

```

z2Diode = SeriesCoefficient[zDiode, {rC, 0, 2}];
z2Diode = Block[{θA}, θA[rC_] := θA0[rC];
  Refine[z2Diode, { > 0 && νA > 0 && νA < 1 && νM > 0 && νM < 1}];

Second order angle expansion  $a'^2 = (\alpha'^2)_1 r_C + (\alpha'^2)_2 r_C^2 + O(r_C^3)$ ,  $(\alpha'^2)_1 = 0$ 

αSquared2Diode = SeriesCoefficient[αSquaredDiode, {rC, 0, 2}];
αSquared2Diode = Block[{θA}, θA[rC_] := θA0[rC];
  Refine[αSquared2Diode, { > 0 && νA > 0 && νA < 1 && νM > 0 && νM < 1}];

Coefficient of chromatic aberration,  $C_c = V_C \frac{2 \partial z_0}{\partial V_C} = 2 (\nu_M \partial_{\nu_M} z_0 - \nu_A \partial_{\nu_A} z_0)$ 

CcDiode = 2 (νM ∂νM z0Diode - νA ∂νA z0Diode);

Coefficient of spherical aberration,  $z' = z_0 - 2^{-1} C_s \alpha'^2 \rightarrow C_s = -2 z'_2 / (\alpha'^2)_2$ 

CsDiode = -2 z2Diode / αSquared2Diode;

Import interface lens properties

SetDirectory[
  $HomeDirectory <> "/Dropbox/Electron optics/PEEM optical models";
{propertiesL, propertyFitsL} =
  Import["Swept-back lens properties, D=0.242in.wdx"];
{{fI, gI}, {SfI, SgI}, {CfI, CgI}} = propertyFitsL /. ν → νI

MImm = (715.250 - 558.565) 25.4 / 90
IBmm = (972.102 - 715.250) 25.4 / 90

Thick lens equations for focal length and distance from Rempfer 1985

Clear[f, g, z, zp, m];

z[f_, g_, zp_] := g +  $\frac{f^2}{zp - g}$ ;

zp[f_, g_, z_] := g +  $\frac{f^2}{z - g}$ ;

m[f_, g_, z_, zp_] :=  $\sqrt{\frac{zp - g}{z - g}}$ ;

mo[f_, g_, z_] := f / (z - g);
mi[f_, g_, zp_] := (zp - g) / f;

Aberration formulas at the Gaussian plane (not circle of least confusion)

```

```

Clear[m0, f0, Sf, Sg, Cf, Cg]
Cs[m0_, f0_, Sf_, Sg_] :=
  - ((1 + (1 / m0)^2) Sg + 2 (1 / m0) Sf) (1 + (1 / m0))^2 f0;
Csp[m0_, f0_, Sf_, Sg_] := - ((1 + m0^2) Sg + 2 m0 Sf) (1 + m0)^2 f0;
Cc[m0_, f0_, Cf_, Cg_] := ((1 + (1 / m0)^2) Cg + 2 (1 / m0) Cf) f0;
Ccp[m0_, f0_, Cf_, Cg_] := ((1 + m0^2) Cg + 2 m0 Cf) f0;

diodeAberData = ParallelTable[Block[{m, cs, cc},
  {vM, vI, m = mo[fI, gI, z[fI, gI, IBmm]],
   cs = (CsDiode /. { -> 25.4 /. vA -> 0) + 2 Cs[m, fI, SfI, SgI],
   cc = (CcDiode /. { -> 25.4 /. vA -> 0) + 2 Cc[m, fI, SfI, SgI],
   m^4 cs, m^2 cc} /. FindRoot[
    z[fI, gI, IBmm] == MImm - (z0Diode /. { -> 25.4 /. vA -> 0}), {vI, 1}]
  ], {vM, .85, .98, .001}];

ListPlot[-diodeAberData[[All, 6 ;; 7]] / 10^3,
  Joined -> True, PlotStyle -> {{Thick, Darker[Gray]}}]

Plots

Show[ListPlot[
  focusAberDataMs[[6 ;; -1 ;; 10, All, {5, 6}]] / 10^3, Joined -> True,
  FrameLabel -> {"C'_{s,aox} & -C'_{s,MI} (m)", "C'_{c,aox} & -C'_{c,MI} (m)"},
  ImageSize -> 350, GridLines -> None, PlotRange -> {{0, 16000}, {0, 80}}],
ListPlot[-diodeAberData[[All, 6 ;; 7]] / 10^3, Joined -> True,
  PlotStyle -> {{Thick, Darker[Gray]}}],
Graphics[Text[Style["Diode mirror + lens", Darker[Gray]],
  {8500, 68}, {0, -1}, {1, .4}]],
Graphics[{Text[Style[
  ToString[-Round[Mean[focusDataMs[[6, All, 4]], .1]] <> "x",
  colors[[1]], {Min[focusAberDataMs[[6, All, 5]],
    Max[focusAberDataMs[[6, All, 6]]} / 10^3, {0, -1}], Text[
  Style[ToString[-Round[Mean[focusDataMs[[16, All, 4]], .1]] <> "x",
  colors[[2]], {Min[focusAberDataMs[[16, All, 5]],
    Max[focusAberDataMs[[16, All, 6]]} / 10^3, {0, -1}]]],
Graphics[Table[Text[Style[ToString[
  -Round[Mean[focusDataMs[[i, All, 4]], .1]] <> "x",
  colors[[tmp = -Mod[i, Length[colors]]]; If[tmp == 0,
    Length[colors], tmp]]], {Max[focusAberDataMs[[i, All, 5]],
    Min[focusAberDataMs[[i, All, 6]]} / 10^3, {0, 1}],
  {i, 6, Length[focusDataMs], 10}]] [-2 ;; -1]]]

```

Aberration comparison to triode

```

SetDirectory[
  $HomeDirectory<> "/Dropbox/Electron optics/PEEM optical models";
triodeTable = Sort[Import["triode Cs and Cc data fits.wdx"]];

SetDirectory[
  $HomeDirectory<> "/Dropbox/Electron optics/PEEM optical models";
triodepts = Import["triode primary range Cc vs Cs, mm.wdx"]<;

Show[ListLogLogPlot[focusAberDataMs[[All, All, {5, 6}]]/103,
  Joined → True, FrameLabel → {"Cs' (m)", "Cc' (m)"},
  ImageSize → 400, PlotRange → All],
Array[ParametricPlot[Log[-10-3 triodeTable[[#, 2 ;; 3]]],
  {vA, triodeTable[[#, 4]], triodeTable[[#, 5]]},
  PlotStyle → Gray] &, Length[triodeTable]],
ListLogLogPlot[focusAberDataMs[[All, All, {5, 6}]]/103, Joined → True],
Graphics[Table[Text[Style[
  ToString[-Round[Mean[focusAberDataMs[[i, All, 4]], .1]] <> "x",
  colors[[tmp = Mod[i, Length[colors]]];
  If[tmp == 0, Length[colors], tmp]]],
  Log[Mean[focusAberDataMs[[i, All, {5, 6}]]/103],
  {0, If[i == 4, 1, -1]}], {i, Length[focusAberDataMs]}]],
Graphics[Text["Csc = " <> ToString[Round[Csc /. δzC → 0]] <>
  " mm\nCcc = " <> ToString[Round[CcC /. δzC → 0]] <> " mm",
  Scaled[{.95, .05}], {1, -1}, Background → White]]]

Show[ListLogLogPlot[focusAberDataMs[[All, All, {5, 6}]]/103,
  Joined → True, FrameLabel → {"Cs' (m)", "Cc' (m)"},
  ImageSize → 400, PlotRange → All],
ListLogLogPlot[-10-3 triodepts, PlotStyle → Gray],
ListLogLogPlot[focusAberDataMs[[All, All, {5, 6}]]/103, Joined → True],
Graphics[Table[Text[Style[
  ToString[-Round[Mean[focusAberDataMs[[i, All, 4]], .1]] <> "x",
  colors[[tmp = Mod[i, Length[colors]]];
  If[tmp == 0, Length[colors], tmp]]],
  Log[Mean[focusAberDataMs[[i, All, {5, 6}]]/103],
  {0, If[i == 4, 1, -1]}], {i, Length[focusAberDataMs]}]],
Graphics[Text["Csc = " <> ToString[Round[Csc /. δzC → 0]] <>
  " mm\nCcc = " <> ToString[Round[CcC /. δzC → 0]] <> " mm",
  Scaled[{.95, .05}], {1, -1}, Background → White]]]

```



```
Show[
  ListLogLogPlot[focusAberDataMs[[All, All, {5, 6}]]/103, Joined → True,
    FrameLabel → {"Cs' (m)", "Cc' (m)"}, ImageSize → 400, PlotRange → All,
    PlotStyle → Table[{colors[[i]]}, {i, Length[colors]}]],
  ListLogLogPlot[-10-3 triodepts, PlotStyle → Gray],
  ListLogLogPlot[focusAberDataMs[[All, All, {5, 6}]]/103, Joined → True,
    PlotStyle → Table[{colors[[i]]}, {i, Length[colors]}]],
  ListLogLogPlot[Array[SortBy[focusAberDataMs[[#1]], Abs[#[[3]]] &] [[{1}] &,
    Length[focusAberDataMs]] [[All, All, {5, 6}]]/103, PlotStyle →
    Table[{PointSize[Large], colors[[i]]}, {i, Length[colors]}]],
  Graphics[Table[Text[Style[ToString[
    -Round[Mean[focusAberDataMs[[i, All, 4]]], .1]] <> "x", colors[[
    tmp = Mod[i, Length[colors]]]; If[tmp == 0, Length[colors], tmp]]],
    Log[Mean[focusAberDataMs[[i, All, {5, 6}]]/103]],
    {0, If[i == 4, 1, -1]}], {i, Length[focusAberDataMs]}]],
  Graphics[Text["CsC = " <> ToString[Round[CsC /.  $\delta zC \rightarrow 0$ ]] <>
    " mm\nCcC = " <> ToString[Round[CcC /.  $\delta zC \rightarrow 0$ ]] <> " mm",
    Scaled[ {.95, .05}], {1, -1}, Background → White]]]
```

Export tables

Fit focus data to polynomials of νO

```
labels = {"Mag", "VO/VC", "VX/VC",
  " $\delta z_c$  ( $\mu m$ )", "Cs' (no cath) (mm)", "Cc' (no cath) (mm)"};
filelabels = {"Mag", "VO", "VX", "dzC",
  "Csp, no cath,", "Ccp, no cath,"};
exportlabels = {"Mag", "VO/VC", "VX/VC", "dzC ( $\mu m$ )",
  "Csp (no cath) (mm)", "Ccp (no cath) (mm)"};
data = focusAberDataMs[[All, All, {4, 1, 2, 3, 9, 10}]];
data = Array[(data[[#]] < {1, 1, 1, 103, 1, 1}) < &, Length[data]];
Length[data]
```

```

Table[Block[{set = data[[i, All, {2, j}]],
  m = Round[-Mean[data[[i, All, 1]], .1], fit, rank},
  rank = 2; If[j == 5 && m > 4, rank = 3]; If[j == 5 && m > 5.5, rank = 4];
  If[j == 6 && m > 5.5, rank = 3];
  fit = LinearModelFit[set, vRange[0,rank], v];
  {m,
   labels[[j]],
   fit["ParameterTable"],
   Show[ListPlot[set, ImageSize → 275,
     AspectRatio → .7, FrameLabel → {"vo", labels[[j]]}],
     function = fit[v]; Plot[function, {v, .9575, 1.0125}]]}],
  {i, Length[data]}, {j, 3, 6}] // TableForm

```

Tables with all magnifications

```

exportfilenames =
  Table[filelabels[[j]] <> " of " <> filelabels[[2]] <> ".txt", {j, 3, 6}]

exporttables = Table[Block[{headercol, params},
  headercol = {Join[{exportlabels[[j]], "Mag"},
    Array["(VO/VC)^( " <> ToString[# - 1] &, 5]]}],
  params = Table[
    Block[{set = data[[i, All, {2, j}]],
      m = Round[-Mean[data[[i, All, 1]], .1], fit, rank},
      rank = 2; If[j == 5 && m > 4, rank = 3]; If[j == 5 && m > 5.5, rank = 4];
      If[j == 6 && m > 5.5, rank = 3];
      fit = LinearModelFit[set, vRange[0,rank], v];
      Join[{"", m}, Array[
        If[# ≤ rank + 1, fit["ParameterTableEntries"][[#, 1], 0] &, 5]]
      ], {i, Length[data]}];
    Join[headercol, params]
  ], {j, 3, 6}]

```

```

SetDirectory[
  $HomeDirectory <> "/Dropbox/Electron optics/PEEM optical models"]
SetDirectory["./focus functions, multiple magnifications"]
Array[Export[exportfilenames[[#]], exporttables[[#]], "TSV"] &,
  Length[exportfilenames]]

```

Tables separated by magnification

```

exportfilenames =
  Table[Block[{m = SetAccuracy[-Mean[data[[i, All, 1]], 2]},
    filelabels[[j]] <> " of " <> filelabels[[2]] <> ", mag " <>
    ToString[m] <> ".txt"}, {i, Length[data]}, {j, 3, 6}]

```

```

exporttables = Table[Block[
  {set = data[[i, All, {2, j}]], m = Round[-Mean[data[[i, All, 1]]], .1],
  min, max, fit, rank, header, params},
  min = Min[set[[1]]; max = Max[set[[1]]];
  rank = 2; If[j == 5 && m > 4, rank = 3];
  If[j == 5 && m > 5.5, rank = 4]; If[j == 6 && m > 5.5, rank = 3];
  fit = LinearModelFit[set,  $\sqrt{\text{Range}[0, \text{rank}]}$ , v];
  header = {{exportlabels[[j]]},
    {"Mag", m},
    {"Range VO/VC", min, max}};
  params = Array[{"(VO/VC)^(# - 1)"} <> ToString[# - 1],
    If[# ≤ rank + 1, fit["ParameterTableEntries"][[#, 1], 0]] &, 5];
  Join[header, params]
], {i, Length[data]}, {j, 3, 6}]

SetDirectory[
  $HomeDirectory <> "/Dropbox/Electron optics/PEEM optical models"
SetDirectory["./focus functions, single magnifications"]
Array[Export[exportfilenames[[#1, #2]], exporttables[[#1, #2]], "TSV"] &,
  {Length[exportfilenames], Length[exportfilenames]}]

```

Fit focus data to polynomials of δzC

```

labels = {"Mag", " $\delta z_c$  ( $\mu\text{m}$ )", "Vx/Vc",
  "Vo/Vc", "C's (no cath) (mm)", "C'c (no cath) (mm)"};
filelabels = {"Mag", "dzC", "VX", "VO",
  "Csp, no cath,", "Ccp, no cath,"};
exportlabels = {"Mag", "dzC ( $\mu\text{m}$ )", "VX/VC", "VO/VC",
  "Csp (no cath) (mm)", "Ccp (no cath) (mm)"};
data = focusAberDataMs[[All, All, {4, 3, 2, 1, 9, 10}]];
data = Array[(data[[#]] < {1, 103, 1, 1, 1, 1}) < &, Length[data]];

Length[data]

Table[Block[{set = data[[i, All, {2, j}]],
  m = Round[-Mean[data[[i, All, 1]]], .1], fit, rank},
  rank = 2; If[j > 4 && m > 6, rank = 3];
  fit = LinearModelFit[set,  $\text{dz}^{\text{Range}[0, \text{rank}]}$ , dz];
  {m,
  labels[[j]],
  fit["ParameterTable"],
  Show[ListPlot[set, ImageSize → 275,
    AspectRatio → .7, FrameLabel → {labels[[2]], labels[[j]]}],
    function = fit[dz]; Plot[function, {dz, -1000, 1000}]]}
], {i, Length[data]}, {j, 3, 6}] // TableForm

```

Tables with all magnifications

```
exportfilenames =
  Table[filelabels[[j]] <> " of " <> filelabels[[2]] <> ".txt", {j, 3, 6}]

exporttables = Table[Block[{headercol, params},
  headercol = {Join[{exportlabels[[j]], "Mag"},
    Array["(dzC)^( " <> ToString[# - 1] &, 4]]];
  params = Table[
    Block[{set = data[[i, All, {2, j}]],
      m = Round[-Mean[data[[i, All, 1]]], .1], fit, rank},
      rank = 2; If[j > 4 && m > 6, rank = 3];
      fit = LinearModelFit[set, dzRange[0,rank], dz];
      Join[{"", m}, Array[
        If[# ≤ rank + 1, fit["ParameterTableEntries"][[#, 1], 0] &, 4]]
      ], {i, Length[data]}}];
  Join[headercol, params] <
], {j, 3, 6}]

SetDirectory[
  $HomeDirectory <> "/Dropbox/Electron optics/PEEM optical models"]
SetDirectory["./focus functions, multiple magnifications"]
Array[Export[exportfilenames[[#]], exporttables[[#]], "TSV"] &,
  Length[exportfilenames]]
```

Tables separated by magnification

```
exportfilenames =
  Table[Block[{m = SetAccuracy[-Mean[data[[i, All, 1]]], 2]},
    filelabels[[j]] <> " of " <> filelabels[[2]] <> ", mag " <>
    ToString[m] <> ".txt"], {i, Length[data]}, {j, 3, 6}]

exporttables = Table[Block[
  {set = data[[i, All, {2, j}]], m = Round[-Mean[data[[i, All, 1]]], .1],
  min, max, fit, rank, header, params},
  min = Min[set[[1]]]; max = Max[set[[1]]];
  rank = 2; If[j > 4 && m > 6, rank = 3];
  fit = LinearModelFit[set, dzRange[0,rank], dz];
  header = {{exportlabels[[j]]},
    {"Mag", m},
    {"Range dzC um", min, max}}];
  params = Array[{"(dzC)^( " <> ToString[# - 1],
    If[# ≤ rank + 1, fit["ParameterTableEntries"][[#, 1], 0] &, 4];
  Join[header, params]
], {i, Length[data]}, {j, 3, 6}]
```

```
SetDirectory[
  $HomeDirectory<> "/Dropbox/Electron optics/PEEM optical models"]
SetDirectory["./focus functions, single magnifications"]
Array[Export[exportfilenames[[#1, #2]], exporttables[[#1, #2]], "TSV"] &,
  {Length[exportfilenames], Length[exportfilenames<]>}]
```

Appendix G Code, simion: diode hyperbolic mirror

It was necessary to characterize the diode hyperbolic mirror to compare the strength of the SIMION analysis to the theory in a situation where the theory was known to be at least approximately accurate. In addition, the diode mirror characterization allowed a simple estimation of the aberration in our PEEM. By running the calculation at the same potentials as used in the instrument, the aberration correction of the diode could be measured. Assuming that the diode mirror is operating as designed, this is the also the aberration of our PEEM. It was later determined that the diode mirror may not be correcting aberration as well as hoped—see Fig. 3.5. The interface lens is not included with diode mirror since the separation between the two is sufficiently large that they do not influence each other.

The following code calculates the optical properties of the mirror in SIMION. by first finding the symmetric mode object distance, and then determining the paraxial image distance and spherical aberration coefficient. The incident beam energy is then adjusted, and the symmetric paraxial image distance and spherical aberration coefficient are measured again. The chromatic aberration coefficient is calculated from the difference between the two image distances, and spherical aberration is taken as the mean of the two spherical aberration coefficients. For the immersion triode mirror and lens this method was significantly refined, so it is worth looking at the code there as well. The Mathematica code compiling the data is fairly straightforward, so it is not included here.

```

1  =====
2  -- diode.lua version
3  -- simulation: adjust VM, then find symmetric z0
4  -- then calculate z0, Cs, Cc
5  -- Cc calculated by decreasing electron energy by 5 eV
6  =====
7  simion.workbench_program()
```

```

8
9  ===== variables
10 -- record VC & max angle for analysis (set in .fly file)
11 adjustable electronsperun = 35
12 local VC = -20000
13
14 adjustable dVC = 5
15 adjustable VCruns = 2
16 local VCmin = VC - dVC
17 local VCmax = VC + dVC
18 local VCdelta = (VCmax - VCmin)/(VCruns - 1)
19 local E = -VCmin
20 local E0 = -VC
21 local VCn = 0 -- electron energy counter
22
23 -- adjust VM/VC
24 adjustable VMmin = -24200
25 adjustable VMmax = -20200
26 adjustable VMruns = 41
27 local VM = VC
28 local VMdelta = (VMmax-VMmin)/(VMruns - 1)
29 local VMn = 0 --counter
30
31 -- define z0 (impacts width of beam in mirror)
32 local z0 = 50
33
34 -- find z0' & Cs
35 local minpts = math.floor(electronsperun*.5)
36 local zprimeset = 35
37 local px_prev = 0
38 local py_prev = 0
39 local vx_prev = 0
40 local vy_prev = 0
41 local V_prev = 0
42 local axisn = 0
43 local a = {}
44 local m = {}
45 local zprime = {}
46 local aprime2 = {}
47
48 -- calculate Cc
49 local z0prime_prev = 0
50 local M_prev = 0
51 local cs_prev = 0
52 local VM_prev = 10000000
53 local E_prev = 100000000
54
55 -- save data
56 local data
57 local fullfilename = "diode.csv"
58 local first = 1
59
60 -- count runs
61 local total = VMruns
62 local current_i = 0
63
64
65 -- (1) initializes all electrons' (without flying them)
66 -- can output messages and control rerun looping
67 function segment.initialize()
68
69     sim_trajectory_quality = 99
70
71     -- first time only: print simulation parameters,

```

```

72      --      make output filenames (with current date/time),
73      --      one for Cs data, one for Cs & Cc data
74      --      open output file for writing, and print column headings.
75      if first == 1 then
76          local total_runs = VMruns*VCruns
77          print("Running simulation: may take ".. total_runs .." simulation
              runs.")
78
79          local folder = "./"
80          local name = "diode"
81          local filetype = "csv"
82          fullfilename = os.date(folder .. name ..".. "%Y-%m-%d-%H%M" .. ". "
              .. filetype)
83          local dataheader = assert(io.open(fullfilename,"a"))
84          dataheader:write("VM,z0,Cs,Cc\n")
85          dataheader:flush()
86          dataheader:close()
87          print("Data file: " .. fullfilename)
88
89          first = 0
90      end
91
92      -- set z0 and electron energy
93      -- (sets y, off-axis distance; actual start location set in "fly2" file)
94      local speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm, ion_vz_mm)
95      E0 = speed_to_ke(speed,ion_mass)
96      E = E0*(VCmin + VCdelta*VCn)/VC
97      local speed = ke_to_speed(E,ion_mass)
98      ion_vx_mm, ion_vy_mm, ion_vz_mm = polar3d_to_rect3d(speed, az, el)
99      ion_py_mm = (ion_px_mm - z0)*ion_vy_mm/ion_vx_mm
100     a[ion_number] = abs(atan(ion_vy_mm/ion_vx_mm))
101
102 end
103
104
105 -- (2) initializes electrodes & scales array before electrons fly
106 function segment.init_p_values()
107
108     -- set VM
109     VM = VMmin + VMn*VMdelta
110     adj_elect01 = VM
111
112     -- print some trial information
113     if (VCn == 0) then
114         current_i = current_i + 1
115         print(("..current_i.."/"..total..") VM = "..VM.." V")
116     end
117
118     redraw_screen() -- show new contours(?)
119
120 end
121
122
123 -- (3) measures/adjusts electron conditions after each time step
124 -- can output messages
125 function segment.other_actions()
126     -- correct for non-zero potential at start point
127     if ion_time_of_flight < 1.1*ion_time_step then
128         local speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm,
            ion_vz_mm)
129         E_current = speed_to_ke(speed,ion_mass)
130         E_correction = -ion_volts
131         E_corrected = E_current - E_correction
132         local speed = ke_to_speed(E,ion_mass)

```



```

133         ion_vx_mm, ion_vy_mm, ion_vz_mm = polar3d_to_rect3d(speed, az, el)
134     end
135
136     -- set radial speed to zero at turn-around point
137     if (abs(ion_vx_mm) < abs(ion_vx_mm - vx_prev) and ion_vx_mm > 0) then
138         -- local speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm,
139             ion_vz_mm)
140         -- E_current = speed_to_ke(speed, ion_mass)
141         -- print(ion_number..", "..ion_volts..", "..E_current..", ("..
142             ion_vx_mm..", "..ion_vy_mm.."))
143         ion_vy_mm = 0
144         -- speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm, ion_vz_mm)
145         -- E_current = speed_to_ke(speed, ion_mass)
146         -- print(ion_number..", "..ion_volts..", "..E_current..", ("..
147             ion_vx_mm..", "..ion_vy_mm.."))
148     end
149
150     -- marks axis crossing (if it occurs)
151     if abs(py_prev + ion_py_mm) < abs(py_prev) + abs(ion_py_mm) then mark() end
152
153     -- measure location (y', z') at z' = z'set
154     if (ion_vx_mm > 0 and abs(zprimeset - ion_px_mm) < abs(px_prev - ion_px_mm))
155     then
156         local ap = abs(atan(ion_vy_mm/ion_vx_mm))
157         axisn = axisn + 1
158         aprime2[axisn] = ap*ap
159         zprime[axisn] = ion_px_mm - ion_vx_mm*ion_py_mm/ion_vy_mm
160         ion_splat = -1
161     end
162
163     -- records electron position and potential for use in next time step
164     px_prev = ion_px_mm
165     py_prev = ion_py_mm
166     vx_prev = ion_vx_mm
167     vy_prev = ion_vy_mm
168     V_prev = ion_volts
169 end
170
171 -- (4) measures electron conditions after every one has died
172 -- can output messages and control rerun looping
173 function segment.terminate()
174     -- analyze z' & a'^2 to find z0, reset z0
175     if ion_number == electronsperrun then
176
177         if axisn >= minpts then
178
179             -- fit z' vs a'^2 to get Cs and z0'
180             local fit = require "fit" -- opens fitting code
181             local z0prime, cs = fit.linear(aprime2, zprime)
182             cs = -2*cs
183
184             -- calculate Cc
185             if VCn > 0 then
186                 local dz0p = z0prime - z0prime_prev
187                 local de = (E - E_prev)/E0
188                 local cc = 2*dz0p/de
189                 if de == 0 then cc = 0 end
190                 print(" Success! z0 = "..floor(1000*z0prime+.5)
191                     /1000 .." mm, Cs = "..floor(1000*cs+.5)/1000 .."
192                     mm, Cc = "..floor(1000*cc+.5)/1000 .." mm")
193                 data = assert(io.open(fullfilename, "a"))
194                 data:write(VM.."", "..(0.5*z0prime+0.5*z0prime_prev)

```

```

191         ..", "..(0.5*cs+0.5*cs_prev).."", "..cc.."\"n")
192         data:flush()
193         data:close()
194         VCn = 0
195     else
196         VCn = VCn + 1
197     end
198     -- z0 = z0prime
199     z0prime_prev = z0prime
200     cs_prev = cs
201     E_prev = E
202     VM_prev = VM
203     VA_prev = VA
204
205 end
206
207 -- reset variables
208 m = {}
209 axisn = 0
210 zprime = {}
211 aprime2 = {}
212
213
214 -- increment VM & VA run & z0 guess counters
215 if VCn >= VCruns then VCn = 0 end
216 if VCn == 0 then VMn = VMn + 1 end
217
218 end
219
220 -- check if this is the last run
221 if VMn >= VMruns then sim_rerun_flym = 0 else sim_rerun_flym = 1 end
222 end

```

Appendix H Code, simion: triode hyperbolic mirror

It was necessary to fully characterize the triode hyperbolic mirror and interface lens in SIMION to very high degree in order to provide sufficient control of aberration correction and focus of the mirror branch. The triode mirror was installed without a grounded front electrode, such that there is a significant potential gradient between the center electrode at V_A and the outer grounded electrode of the interface lens. As such, it was necessary to model the triode mirror and lens together to capture the complex interaction between them.

The final implementation of this analysis includes several refinements over the initial code. First, the object distance is fixed, and symmetric mode is determined by tuning the lens potential. Over the range in interest, this potential is fairly linear; however, over wider ranges this method could break down. Second, three beam energies are used: the central energy, one below, and one above. Third, the computation only obtains a symmetric mode image distance for the central beam energy. It was found that tuning object position for symmetric mode in the other cases introduces chromatic aberration into the point source object. The desired model is one in which the object has no aberration and the image has all the aberration, instead of some in the image and some in the object, as here. This led to faster analysis, and less uncertainty in the computation. Finally, this code dumps basic trajectory data into the data file, and Mathematica is used to calculate the optical properties.

```

1  =====
2  -- triode+intlens.lua version
3  -- simulation: adjust VC, VM, VA, & VL
4  -- then calculate z0, Cs
5  =====
6  simion.workbench_program()
7
8  ===== variables
9  -- record VC & max angle for analysis (set in .fly file)
```

```

10 adjustable electronsperun = 49
11 local VC = -20000
12
13 adjustable dVC = 1
14 adjustable VCruns = 2
15 local VCmin = VC - dVC
16 local VCmax = VC + dVC
17 local VCdelta = (VCmax - VCmin)/(VCruns - 1)
18 local E = -VC
19 local E0 = -VC
20 local VCn = 0 -- electron energy counter
21
22 -- adjust VL
23 adjustable VLmax = -21500
24 adjustable VLmin = -19000
25 --adjustable VRuns = 1 + abs(VLmax - VLmin)/10
26 local VL = -20400
27 --local VLdelta = (VLmax - VLmin)/(VRuns - 1)
28 --local VLn = 0 --counter
29
30 -- adjust VA
31 adjustable VAmix = -17000
32 adjustable VAmix = -500
33 adjustable VAruns = 1 + abs(VAmix - VAmix)/10
34 local VA = VAmix
35 local VAdelta = (VAmix - VAmix)/(VAruns - 1)
36 local VAn = VAruns --counter
37
38 -- adjust VM
39 adjustable VMmax = -22500
40 adjustable VMmin = -21700
41 adjustable VMruns = 1 + abs(VMmax - VMmin)/20
42 local VM = VMmin
43 local VMdelta = (VMmax - VMmin)/(VMruns - 1)
44 local VMn = 0 --counter
45
46 -- exclude some VM values
47 local vm_exclude_list = {-23480, -23470, -23460}
48
49 -- define z0 & bound range
50 local z0 = 84.5032 + 25.4*(1.04+1.1/2)
51 local Dz0 = 0
52 local VLn = 0
53 local VLnmax = 2
54
55 -- find z0' & Cs
56 local zprimeset = 84
57 local px_prev = 0
58 local py_prev = 0
59 local vx_prev = 0
60 local vy_prev = 0
61 local vx_pprev = 0
62 local volts_prev = 0
63 local speed_prev = 81507.1849
64 local speed_pprev = speed_prev
65 local axisn = 0
66 local A = 1
67 local a = {}
68 local m = {}
69 local zprime = {}
70 local aprime2 = {}
71
72 -- ion status at turn-around
73 local zC, rC, vrC, vzC, tC, VCC = 0, 0, 0, 0, 0, 0

```

```

74 local zCp, rCp, vrCp, vzCp, tCp, VCCp = 0, 0, 0, 0, 0, 0
75 local zCm, rCm, vrCm, vzCm, tCm, VCCm = 0, 0, 0, 0, 0, 0
76
77 -- tune z0 to find symmetric mode
78 local symm_maxsearches = 20
79 local symmn = 30
80 adjustable dz0 = .005
81 local tuning = false
82 local z0_prev = 0
83 local z0_pprev = 0
84
85 -- save data
86 local data
87 local first = 1
88 local fullfilename
89
90 -- count runs
91 local total = VMruns*VAruns
92 local current_i = 0
93 local V_count = 0
94
95
96 -- (1) initializes all electrons' (without flying them)
97 -- can output messages and control rerun looping
98 function segment.initialize()
99
100     sim_trajectory_quality = 99
101
102     -- first time only: print simulation parameters,
103     --     make output filenames (with current date/time),
104     --     one for Cs data, one for Cs & Cc data
105     --     open output file for writing, and print column headings.
106     if first == 1 then
107         local total_runs = VMruns*VAruns
108         local folder = "../data/"
109         local name = "triode_no_front+intlens-no_fit-vl_var"
110         local filetype = "csv"
111         fullfilename = os.date(folder .. name .. ".%. " .. "%Y-%m-%d-%H%M" .. ". " ..
            .. filetype)
112         local dataheader = assert(io.open(fullfilename,"a"))
113         dataheader:write("VM,VA,VL,VC,z,a,z',a',tC,zC,rC,vzC,vrC,VCC,tC1,zC1,
            rC1,vzC1,vrC1,VCC1,tC-1,zC-1,rC-1,vzC-1,vrC-1,VCC-1\n")
114         dataheader:close()
115         print("Running simulation: will take at least ".. total_runs .."
            simulation runs.")
116         print("Data file: " .. fullfilename)
117
118         first = 0
119     end
120
121     -- set z0 (if tuning, z0 computed in "terminate") and electron energy
122     -- (sets y, off-axis distance; actual start location set in "fly2" file)
123     local speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm, ion_vz_mm)
124     E0 = speed_to_ke(speed,ion_mass)
125     if VCn == 0 then E = E0 else E = E0*(VCmin + VCdelta*(VCn-1))/VC end
126     local speed = ke_to_speed(E,ion_mass)
127     ion_vx_mm, ion_vy_mm, ion_vz_mm = polar3d_to_rect3d(speed, az, el)
128     ion_py_mm = (ion_px_mm - z0)*ion_vy_mm/ion_vx_mm
129     a[ion_number] = atan2(ion_vy_mm,-ion_vx_mm)
130
131 end
132
133
134 -- (2) initializes electrodes & scales array before electrons fly

```

```

135 function segment.init_p_values()
136
137     -- set VL
138     --VL = VLmin + VAn*VLdelta
139     adj_elect03 = VL
140
141     -- set VM
142     VM = VMmin + VMn*VMdelta
143     adj_elect01 = VM
144
145     --set VA
146     VA = VAmin + VAdelta*VAn
147     adj_elect02 = VA
148
149     -- print some trial information
150     if (not tuning and VCn == 0) then
151         current_i = current_i + 1
152         local V_count_prev = V_count
153         V_count = 1 + VAn + VMn*VAruns
154         skip_n = V_count - V_count_prev
155         print("(..V_count../"..total.." (..current_i..)") VM = "..VM.."V,
156             VA = "..floor(VA+.5).." V, VL = "..floor(VL+.5).." V")
157         if skip_n > 1 then print(" (skipped "..(skip_n-1).." voltage settings
158             )") end
159     end
160     if (not tuning) then
161         print(" VC = "..(-E).." V")
162     end
163     --print(" init_p z0 = "..z0.." mm")
164     redraw_screen() -- show new contours(?)
165
166
167 -- (3) measures/adjusts electron conditions after each time step
168 -- can output messages
169 function segment.other_actions()
170     local speed, az, el = rect3d_to_polar3d(ion_vx_mm, ion_vy_mm, ion_vz_mm)
171
172     -- correct for non-zero potential at start point
173     if ion_time_of_flight <= 1.0*ion_time_step then
174         if abs(Dz0) > 5 and axisn > 7 then ion_splat = -1 end
175         if abs(Dz0) > 1 and axisn > 19 then ion_splat = -1 end
176         local E_corrected = E + ion_volts
177         speed = ke_to_speed(E_corrected,ion_mass)
178         ion_vx_mm, ion_vy_mm, ion_vz_mm = polar3d_to_rect3d(speed, az, el)
179     end
180
181     -- greatest radial extent at turn-around
182     -- check that ion is greater than 5 gu from axis to experience curvature of
183     field
184     -- check that ion is less than 0.6 mm from axis to get paraxial field
185     if abs(ion_vx_mm) > abs(vx_prev) and abs(vx_pprev) > abs(vx_prev) and
186         ion_px_mm < 25 then
187         mark()
188         zC, rC, vrC, vzC = px_prev, py_prev, vy_prev, vx_prev
189         tC, VCC = time_prev, volts_prev
190
191         zCp, rCp, vrCp, vzCp = ion_px_mm, ion_py_mm, ion_vy_mm, ion_vx_mm
192         tCp, VCCp = ion_time_of_flight, ion_volts
193
194         zCm, rCm, vrCm, vzCm = px_pprev, py_pprev, vy_pprev, vx_pprev
195         tCm, VCCm = time_, volts_pprev
196     end

```

```

195         if (abs(ion_py_gu) < 5 or abs(ion_py_mm) > 0.6) then ion_splat = -1
196             end
197     end
198     -- marks axis crossing (if it occurs)
199     if abs(py_prev + ion_py_mm) < abs(py_prev) + abs(ion_py_mm) then mark() end
200
201     -- measure location (y',z') at z' = z'set
202     if (ion_vx_mm > 0 and abs(zprimeiset - ion_px_mm) < abs(px_prev - ion_px_mm))
203         then
204             axisn = axisn + 1
205             zprime[axisn] = ion_px_mm - ion_vx_mm*ion_py_mm/ion_vy_mm
206             local ap = atan2(ion_vy_mm,ion_vx_mm)
207             data = assert(io.open(fullfilename,"a"))
208             data:write(VM.." "..VA.." "..VL.." ..(-E).." ..z0.." ..a[
209                 ion_number].." ..zprime[axisn].." ..ap.." ..zC.." ..rC.." ..
210                 vzC.." ..vrC.." ..VCC.." ..zCp.." ..rCp.." ..vzCp.." ..vrCp
211                 .." ..VCCp.." ..zCm.." ..rCm.." ..vzCm.." ..vrCm.." ..VCCm
212                 .."\n")
213             data:close()
214             if abs(ap) > 1 then ap = atan2(-ion_vy_mm,ion_vx_mm) end
215             m[axisn] = abs(ap/a[ion_number])
216             aprime2[axisn] = ap*ap
217             ion_splat = -1
218         end
219
220     -- kills electrons 1mm before hitting mirror electrode
221     if ion_px_mm < sqrt(2)*ion_py_mm + 1 then ion_splat = -1 end
222
223     -- records electron position for use in next time step
224     px_pprev = px_prev
225     py_pprev = py_prev
226     px_prev = ion_px_mm
227     py_prev = ion_py_mm
228     volts_pprev = volts_prev
229     time_pprev = time_prev
230     vx_pprev = vx_prev
231     vy_pprev = vy_prev
232     time_prev = ion_time_of_flight
233     vx_prev = ion_vx_mm
234     vy_prev = ion_vy_mm
235     speed_pprev = speed_prev
236     speed_prev = speed
237     volts_prev = ion_volts
238 end
239
240 -- (4) measures electron conditions after every one has died
241 -- can output messages and control rerun looping
242 function segment.terminate()
243     -- analyze z' & a'^2 to find z0, reset z0
244     if ion_number == electronsperun then
245         z0_pprev = z0_prev
246         z0_prev = z0
247
248         if axisn >= 7 then
249             local fit = require "fit" -- opens fitting code
250
251             -- compute paraxial magnification
252             local M, slope, aprime4coeff = fit.parabola(aprime2, m)
253
254             -- fit z' vs a'^2 to get Cs and z0'
255             local z0prime, cs, aprime4coeff = fit.parabola(aprime2,
256                 zprime)

```

```

252         cs = -cs
253
254         -- tune z0 only if E = E0
255         -- if not tuning then change E and set z0
256         if (VCn == 0 and abs(z0 - z0prime) > dz0) then
257             if symmn >= symmn_maxsearches then -- too many
258                 searches, move on
259                 print(" max tuning searches hit!")
260                 tuning = false
261                 symmn = 0
262                 VCn = VCruns + 1
263             else -- tune for symmetric z0
264                 tuning = true
265                 symmn = symmn + 1
266                 Dz0 = 0.5*(z0prime-z0) -- assign new start
267                     position
268                 if symmn < 2 then Dz0 = Dz0 + 0.3*(z0prime-z0
269                     ) end -- accelerate convergence for first
270                     tuning
271                 dVL = -15*Dz0
272                 print(" (".symmn.."") searching for
273                     symmetric mode... dz = "..floor(1000*Dz0
274                     +.5)/1000 .." mm, VL = "..floor(VL+.5)
275                     .." V, VL' = "..floor((VL+dVL)+.5) .." V
276                     ")
277                 VL = VL + dVL
278                 local vlmax, vlmin = max(VLmin,VLmax), min(
279                     VLmin,VLmax)
280                 if VL > vlmax then
281                     VL = vlmin + 100*(simion.rand())
282                     VLn = VLn + 1
283                 end
284                 if VL < vlmin then
285                     VL = vlmax - 100*(simion.rand())
286                     VLn = VLn + 1
287                 end
288                 end
289             elseif ((VCn == 0 and abs(z0 - z0prime) < dz0)) or VCn > 0
290                 then -- symmetric mode found
291                 tuning = false
292                 symmn = 0
293                 print(" M = "..floor(1000*M+.5)/1000 ..", z0 = "..
294                     floor(100*z0+.5)/100 ..", z0' = "..floor(100*
295                     z0prime+.5)/100 .." mm, Cs = "..floor(cs+.5) .."
296                     mm")
297             end
298         end
299
300         end
301
302         if tuning == true and (axisn < 7 or VLn >= VLnmax) then -- move on
303             if axisn < 7 then print(" .. no particles") else print("
304                 .. trouble") end
305             tuning = false
306             VCn = VCruns + 1
307             VLn = 0
308             symmn = 0
309         end
310
311         -- reset variables
312         m = {}
313         axisn = 0
314         zprime = {}
315         aprime2 = {}

```

```

302      -- increment VC, VL, VA, & VM run counters
303      if not tuning then
304          VCn = VCn + 1
305          if VCn > VCruns then
306              VCn = 0
307              repeat -- keep within target range of VA
308                  if abs(Dz0) < 5 then VAn = VAn + 1 else VAn =
                      VAn + 3 end
309                  local VAtest = VAmn + VAdelta*VAn
310                  local VAtarget = -21940 - 7.23*(VM+20000)
                      -0.000319*((VM+20000)^2)
311                  until (abs(VAtest - VAtarget) < 1500 or VAn >= VAruns
                      )
312                  if VAn >= VAruns then
313                      VAn = 0
314                      local is_excluded = false
315                      repeat -- exclude specific VMs
316                          VMn = VMn + 1
317                          local VMtest = VMmin + VMdelta*VMn
318                          is_excluded = false
319                          for _, value in pairs(vm_exclude_list
                      ) do
320                              if value == VMtest then
321                                  is_excluded = true
322                              end
323                          end
324                          until not is_excluded
325                          is_excluded = false
326                      end
327                  end
328              end
329          end
330      end
331
332      -- check if this is the last run
333      if VMn >= VMruns then sim_rerun_flym = 0 else sim_rerun_flym = 1 end
334  end

```

Appendix I Code, *Mathematica*: triode hyperbolic mirror

The SIMION trajectory information from executing the previous Lua code is analyzed and sifted through to characterize the mirror branch with Mathematica. SIMION uses a stochastic process to determine the symmetric mode paraxial image distance, introducing some random uncertainty to the properties calculated with that data set. In this Mathematica code, data is sorted by constant mirror potential V_M and fit to analytic curves which average out this stochastic noise in order to obtain more accurate control parameters for the mirror branch. Finally, a grid of correction values of spherical and chromatic aberration coefficients is generated for computer control.

Header

Graphics Options

```

colors = {Black, Darker[Red], Blend[{Darker[Gray], Green}, 1 / 4],
  Blend[{Lighter[Gray], Blue}, 1 / 3]};
SetOptions[Plot, PlotRange → All,
  PlotStyle → Table[{Thick, colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1,
  GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ContourPlot, PlotRange → All,
  ContourStyle → Table[{Thick, colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1,
  GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ParametricPlot, PlotRange → All,
  PlotStyle → Table[{Dashed, colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1,
  GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[LogPlot, PlotRange → All,
  PlotStyle → Table[{Thick, colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1,
  GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[LogLogPlot, PlotRange → All, PlotStyle →
  Table[{Thick, colors[[i]]}, {i, Length[colors]}], Frame → True,
  AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ParametricPlot3D, PlotStyle →
  {{Thick, Black}, {Thick, Dashed, Black}, {Thick, Dotted, Black}},
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350,
  BoxRatios → {1, 1, .5}, Axes → {True, True, False},
  Boxed → False, ViewCenter → {.5, .5, 0},
  ViewVertical → {0, 0, 1}, ViewPoint → {0, -3, 1}];
SetOptions[ListPlot, PlotRange → All, PlotStyle →
  Table[{Thick, PointSize[.02], colors[[i]]}, {i, Length[colors]}],
  Frame → True, AspectRatio → 1, GridLines → Automatic,
  GridLinesStyle → Gray,
  BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListPointPlot3D, PlotRange → All,
  PlotStyle → {{Thick, PointSize[.01], Black},
  {Thick, PointSize[.01], Darker[Red]}},

```

```

    {Thick, PointSize[.01], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.01], Blend[{Lighter[Gray], Blue}, 1 / 3]}},
    BoxRatios → 1, BaseStyle → {FontFamily → "Arial", FontSize → 14},
    ImageSize → 350];
SetOptions[ListPlot3D, PlotRange → All, BoxRatios → 1,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListContourPlot, PlotRange → All, Frame → True,
    AspectRatio → 1, GridLines → Automatic, GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLinearPlot, PlotRange → All,
    PlotStyle → {{Thick, PointSize[.02], Black},
    {Thick, PointSize[.02], Darker[Red]}},
    {Thick, PointSize[.02], Blend[{Darker[Gray], Green}, 1 / 4]},
    {Thick, PointSize[.02], Blend[{Lighter[Gray], Blue}, 1 / 3]}},
    Frame → True, AspectRatio → 1, GridLines → Automatic,
    GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogPlot, PlotRange → All, PlotStyle →
    Table[{Thick, PointSize[.02], colors[[i]]}, {i, Length[colors]}],
    Frame → True, AspectRatio → 1, GridLines → Automatic,
    GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];
SetOptions[ListLogLogPlot, PlotRange → All, PlotStyle →
    Table[{Thick, PointSize[.02], colors[[i]]}, {i, Length[colors]}],
    Frame → True, AspectRatio → 1, GridLines → Automatic,
    GridLinesStyle → LightGray,
    BaseStyle → {FontFamily → "Arial", FontSize → 14}, ImageSize → 350];

```

Thick lens equations

Thick lens equations for focal length and distance from Rempfer 1985

```

Clear[z, zp, m]
f[z_, zp_, m_] := (z - zp) / (1 / m - m);
g[z_, zp_, m_] := (zp / m - m z) / (1 / m - m);

```

```

Clear[f, g, z, zp, m];

z[f_, g_, zp_] := g +  $\frac{f^2}{zp - g}$ ;

zp[f_, g_, z_] := g +  $\frac{f^2}{z - g}$ ;

m[f_, g_, z_, zp_] :=  $\sqrt{\frac{zp - g}{z - g}}$ ;

mo[f_, g_, z_] := f / (z - g);
mi[f_, g_, zp_] := (zp - g) / f;

```

Aberration formulas at the Gaussian plane (not circle of least confusion)

```

Clear[m0, f0, Sf, Sg, Cf, Cg]
Cs[m0_, f0_, Sf_, Sg_] :=
  - ((1 + (1 / m0)^2) Sg + 2 (1 / m0) Sf) (1 + (1 / m0))^2 f0;
Csp[m0_, f0_, Sf_, Sg_] := - ((1 + m0^2) Sg + 2 m0 Sf) (1 + m0)^2 f0;
Cc[m0_, f0_, Cf_, Cg_] := ((1 + (1 / m0)^2) Cg + 2 (1 / m0) Cf) f0;
Ccp[m0_, f0_, Cf_, Cg_] := ((1 + m0^2) Cg + 2 m0 Cf) f0;

```

Relative focal length and magnification variations, $\delta f = (f - f_0)/f_0$ and $\delta g = (g - g_0)/f_0$ and $\delta m = (m - m_0)/m_0$, and object/image distance changes, Δz & $\Delta z'$, with spherical and chromatic aberration

```

Clear[α, m0, f0, Sf, Sg, Cf, Cg, Δf, Δg, Δz, Δzp]
δfs[α_, m0_, Sf_] := Sf (1 + 1 / m0)^2 α^2;
δgs[α_, m0_, Sg_] := Sg (1 + 1 / m0)^2 α^2;
δms[α_, m0_, Sf_, Sg_] := - (Sg / m0 + Sf) (1 + 1 / m0)^2 α^2;
δfc[E1_, E2_, Cf_] := Cf (E1 - E2) / (2^-1 (E1 + E2));
δgc[E1_, E2_, Cg_] := Cg (E1 - E2) / (2^-1 (E1 + E2));
δmc[m0_, E1_, E2_, Cf_, Cg_] :=
  - (Cg / m0 + Cf) (E1 - E2) / (2^-1 (E1 + E2));
Δzp[m0_, Δf_, Δg_, Δz_] := (1 + m0^2) Δg + 2 m0 Δf - m0^2 Δz;
Δz[m0_, Δf_, Δg_, Δzp_] := (1 + m0^-2) Δg + 2 m0^-1 Δf - m0^-2 Δzp;

```

Triode mirror and lens measurement (mm)

LM = lens center to mirror cone vertex

ℓ = AM = mirror center electrode aperture to mirror cone vertex

LA = LM - ℓ = lens center to mirror center electrode

$\mathcal{L}$ = distance from lens front aperture to mirror cone vertex

Z = distance from mirror cone vertex to magnet B center

```

LM = (1.665 + 0.13 + 0.056 + 0.025 + 0.125 + 0.05 / 2) 25.4
AM = 0.783 × 25.4
LA = LM - AM
LA = (1.665 + 0.13 + 0.056) 25.4
Z = 124.8892

```

Objective lens properties from previous Simlon analysis

Import swept-back lens property fits

```

SetDirectory[$HomeDirectory<>
  "/Dropbox/Electron optics/Simion/triode mirror and lens"];
{propertiesL, propertyFitsL} =
  Import["Swept-back lens properties, D=0.242in.wdx"];
{{fL242, gL242}, {SfL242, SgL242}, {CfL242, CgL242}} =
  propertyFitsL /. v → vL

SetDirectory[$HomeDirectory<>
  "/Dropbox/Electron optics/Simion/triode mirror and lens"];
{propertiesL, propertyFitsL} =
  Import["Swept-back lens properties, D=0.220in.wdx"];
{{fL220, gL220}, {SfL220, SgL220}, {CfL220, CgL220}} =
  propertyFitsL /. v → vL

SetDirectory[$HomeDirectory<>
  "/Dropbox/Electron optics/Simion/triode mirror and lens"];
{propertiesL, propertyFitsL} =
  Import["Swept-back lens properties, D=0.200in.wdx"];
{{fL200, gL200}, {SfL200, SgL200}, {CfL200, CgL200}} =
  propertyFitsL /. v → vL

Plot[{z[fL242, gL242, Z - LM],
  z[fL220, gL220, Z - LM], z[fL200, gL200, Z - LM]}, {vL, .9, 1.2}]

Block[{zL242 = z[fL242, gL242, Z - LM], zL220 = (z[fL220, gL220, Z - LM]),
  mL242 = mi[fL242, gL242, Z - LM], mL220 = mi[fL220, gL220, Z - LM],
  CsL242, CsL220, CcL242, CcL220},
CsL242 = Cs[mL242, fL242, SfL242, SgL242];
CsL220 = Cs[mL220, fL220, SfL220, SgL220];
CcL242 = Cc[mL242, fL242, CfL242, CgL242];
CcL220 = Cc[mL220, fL220, CfL220, CgL220];
{{ParametricPlot[{{zL242, mL242}, {zL220, mL220}},
  {vL, .9, 1.2}, FrameLabel → {"zL", "mL"}],
ParametricPlot[{{zL242, CsL242}, {zL220, CsL220}},
  {vL, .9, 1.2}, FrameLabel → {"zL", "CsL"}],
ParametricPlot[{{zL242, CcL242}, {zL220, CcL220}},
  {vL, .9, 1.2}, FrameLabel → {"zL", "CcL"}]}} // TableForm]

```

```

Block[{zL242 = z[fL242, gL242, Z - LM],
  zL220 = (z[fL220, gL220, Z - LM] /. vL → vLp),
  mL242 = mi[fL242, gL242, Z - LM],
  mL220 = mi[fL220, gL220, Z - LM] /. vL → vLp,
  CsL242, CsL220, CcL242, CcL220},
CsL242 = Cs[mL242, fL242, SfL242, SgL242];
CsL220 = Cs[mL220, fL220, SfL220, SgL220] /. vL → vLp;
CcL242 = Cc[mL242, fL242, CfL242, CgL242];
CcL220 = Cc[mL220, fL220, CfL220, CgL220] /. vL → vLp;
ContourPlot[
  {zL242 == zL220, mL242 == mL220, CsL242 == CsL220, CcL242 == CcL220},
  {vL, .9, 1.2}, {vLp, .9, 1.2}, FrameLabel → {"vL,242", "vL,220"}]]

vL220ofvL242 = Block[{zL242 = z[fL242, gL242, Z - LM],
  zL220 = (z[fL220, gL220, Z - LM] /. vL → vLp), table},
  table = ParallelTable[{vL, vLp} /. FindRoot[zL242 == zL220, {vLp, vL}],
    {vL, .9, 1.2, .0005}];
  vL220ofvL242fit = LinearModelFit[table, vL242Range[0,5], vL242];
  Print[vL220ofvL242fit["ParameterTable"]];
  Print[ListPlot[vL220ofvL242fit["FitResiduals"]]];
  vL220ofvL242fit["BestFit"]]

Block[{zL242 = z[fL242, gL242, Z - LM], zL220 = (z[fL200, gL200, Z - LM]),
  mL242 = mi[fL242, gL242, Z - LM], mL220 = mi[fL200, gL200, Z - LM],
  CsL242, CsL220, CcL242, CcL220},
CsL242 = Cs[mL242, fL242, SfL242, SgL242];
CsL220 = Cs[mL220, fL200, SfL200, SgL200];
CcL242 = Cc[mL242, fL242, CfL242, CgL242];
CcL220 = Cc[mL220, fL200, CfL200, CgL200];
{{ParametricPlot[{zL242, mL242}, {zL220, mL220}],
  {vL, .8, 1.2}, FrameLabel → {"zL", "mL"}],
ParametricPlot[{zL242, CsL242}, {zL220, CsL220}],
  {vL, .8, 1.2}, FrameLabel → {"zL", "CsL"}],
ParametricPlot[{zL242, CcL242}, {zL220, CcL220}],
  {vL, .8, 1.2}, FrameLabel → {"zL", "CcL"}]] // TableForm]

```

```

Block[{zL242 = z[fL242, gL242, Z - LM],
  zL220 = (z[fL200, gL200, Z - LM] /. vL → vLp),
  mL242 = mi[fL242, gL242, Z - LM],
  mL220 = mi[fL200, gL200, Z - LM] /. vL → vLp,
  CsL242, CsL220, CcL242, CcL220},
CsL242 = Cs[mL242, fL242, SfL242, SgL242];
CsL220 = Cs[mL220, fL200, SfL200, SgL200] /. vL → vLp;
CcL242 = Cc[mL242, fL242, CfL242, CgL242];
CcL220 = Cc[mL220, fL200, CfL200, CgL200] /. vL → vLp;
ContourPlot[
  {zL242 == zL220, mL242 == mL220, CsL242 == CsL220, CcL242 == CcL220},
  {vL, .9, 1.2}, {vLp, .8, 1.1}, FrameLabel → {"vL,242", "vL,220"}]]

vL200ofvL242 = Block[{zL242 = z[fL242, gL242, Z - LM],
  zL200 = (z[fL200, gL200, Z - LM] /. vL → vLp), table},
table = ParallelTable[{vL, vLp} /. FindRoot[zL242 == zL200, {vLp, vL}],
  {vL, .9, 1.2, .0005}];
vL200ofvL242fit = LinearModelFit[table, vL242Range[0,5], vL242];
Print[vL200ofvL242fit["ParameterTable"]];
Print[ListPlot[vL200ofvL242fit["FitResiduals"]]];
vL200ofvL242fit["BestFit"]]

```

Triode mirror and lens Simlon data

Import data

```

import[filename_] := Block[{data = Import[filename], VMs},
  Print[TableForm[Join[data[[{1}]], RandomSample[data, 5]]]];
  data = Select[Drop[data, 1], # == Re[#] &];
  VMs = Tally[Union[data[[All, 1 ;; 2]]<[[1]]];
  Print[TableForm[{VMs<[[1]], VMs<[[2]], "",
    {Length[data], Length[VMs]}}]];
  data];

SetDirectory["M:/fit/simion/data"];
simiondata[1] =
  import["triode_no_front+intlens.2014-10-29-0320.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[2] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-29-1538.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[3] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-29-1122.csv"];

```



```

SetDirectory["M:/fit/simion/data"];
simiondata[4] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-29-2141.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[5] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-29-2216.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[6] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-29-2217.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[7] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-30-1100.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[8] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-30-1152.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[9] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-30-1400.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[10] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-30-1906.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[11] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-30-1907.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[12] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-30-1908.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[13] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-31-1336.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[14] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-31-1337.csv"];

SetDirectory["M:/fit/simion/data"];
simiondata[15] = import[
  "triode_no_front+intlens-no_fit-vl_var.2014-10-31-1338.csv"];

Consolidate data

```

```

data0 = Flatten[Delete[Array[simiondata[#] &, 15], {{5}, {6}, {10}}],
  1]; Length[data0]

dz0Tolerance = 0.005;
{Cs0guess, Cc0guess} = {-994 652., -23 120.5};
ap2cutoff =  $1.4 \times 10^{-7}$ ;

data1 = Select[data0, #[[8]]2 > ap2cutoff &];
Length[data1]

Gather symmetric sets

VMALsets = GatherBy[data1, #[{1, 2, 3}]] &;
VMALCsets = Select[Array[GatherBy[VMALsets[[#]], #1[[4]] &],
  Length[VMALsets]], Length[#1] == 3 &];
VMALCsets = Array[SortBy[VMALCsets[[#1, #2]], #[[6]] &],
  {Length[VMALCsets], 3}];
data2 = Flatten[VMALCsets, 2];
{Length[VMALsets], Length[VMALCsets], Length[data2]}

tmp = GatherBy[Union[data1[[All, 1 ;; 2]]], #[[1]] &]; tmp0 = tmp;
tmp = Array[{tmp[[#, 1, 1]], Length[tmp[[#]]],
  Max[tmp[[#, All, 2]] - Min[tmp[[#, All, 2]]] &, Length[tmp]]];
{{ListPlot[tmp0], ListPlot[tmp[[All, {1, 2}]]],
  ListPlot[tmp[[All, {2, 3}]]]} // TableForm

tmp = GatherBy[Union[data2[[All, 1 ;; 2]]], #[[1]] &]; tmp0 = tmp;
tmp = Array[{tmp[[#, 1, 1]], Length[tmp[[#]]],
  Max[tmp[[#, All, 2]] - Min[tmp[[#, All, 2]]] &, Length[tmp]]];
{{ListPlot[tmp0], ListPlot[tmp[[All, {1, 2}]]],
  ListPlot[tmp[[All, {2, 3}]]]} // TableForm

tmp2 = 10-3 Sort[Select[tmp[[All, {1, 3}]],
  #[[2]] < 2600 && (#[[1]] < -23 000 || #[[1]] > -21 500 || #[[2]] > 1250) &]];
ListPlot[{tmp2, tmp2}, FrameLabel → {"VM (kV)", "VA Range (kV)"},
  Joined → {True, False}, Filling → Bottom]

```

Organize and calculate optical properties of full column

Organize data & calculate Z'_0 , M_0 , C'_s , C'_c

```

VMs0 = Union[data2[[1]]]; VAs0 = Union[data2[[2]]];
VCs0 = Union[data2[[4]]];
{Nsets0, NVMs0, NVAs0, NVCs0} =
  {Length[VMALCsets], Length[VMs0], Length[VAs0], Length[VCs0]}

```

```

{"VM (V)", "VA (V)", "VL (V)", "VC (V)", "Z0 (mm)"};
Zdata0 = VMALCsets[All, 1, 1, 1 ;; 5];

{"VM (V)", "VA (V)", "VL (V)", "VC (V)", "Z0 (mm)"};
Zdata0C = Array[VMALCsets[All, #, 1, 1 ;; 5] &, NVCs0];

{"Z (mm)", "α"};
Zdata0C0 = Array[VMALCsets[All, #, All, 5 ;; 6] &, NVCs0];

{"Z' (mm)", "α'"};
Zpdata0C0 = Array[VMALCsets[All, #, All, 7 ;; 8] &, NVCs0];

{"Z'0 (mm)", "M0", "C's (mm)", "VC (V)"};
Zpdata0C =
  ParallelTable[Block[{set = VMALCsets[[i, j]], VC0 = Zdata0[[i, 4]],
    VC, αs, Zps, αps, fit, α2, M0, dMs, d2Ms, Z0p, Csp, Cs2p},
    VC = set[[1, 4]]; {αs, Zps, αps} = set[All, {6, 7, 8}];
    fit = FindFit[{αps2, -αs / αps} <,
      M0 - dMs α2 - d2Ms α22, {M0, dMs, d2Ms}, α2]; M0 = M0 /. fit;
    fit = FindFit[{αps2, Zps} <, Z0p - Csp α2 - Cs2p α22, {Z0p, Csp, Cs2p},
      α2]; {Z0p, Csp, Cs2p} = {Z0p, Csp, Cs2p} /. fit;
    {Z0p, M0, Csp, VC}
  ], {j, NVCs0}, {i, Nsets0}];

{"Z'0 (mm)", "M0", "C's (mm)", "C'c (mm)"};
Zpdata0 =
  ParallelTable[Block[{set = Zpdata0C[All, i], Z0p0, M00, Csp0, VC0,
    Z0ps, M0s, Csps, VCs, Z0p, M0, Csp, δVCs, fit, Ccp, δVC, χ},
    {Z0ps, M0s, Csps, VCs} = set; VC0 = -20 000; δVCs = (VCs / VC0 - 1);
    fit = FindFit[{δVCs, Z0ps} <, Z0p + Ccp δVC, {Z0p, Ccp}, δVC];
    {Z0p, Ccp} = {Z0p, Ccp} /. fit;
    fit = FindFit[{δVCs, M0s} <, M0 + χ δVC, {M0, χ}, δVC]; M0 = M0 /. fit;
    fit = FindFit[{δVCs, Csps} <, Csp + χ δVC, {Csp, χ}, δVC];
    Csp = Csp /. fit;
    {Z0p, M0, Csp, Ccp}
  ], {i, Nsets0}];

outlierPositions = Block[{set = Zdata0<[5] - Zpdata0<[1], subset},
  subset = Select[set, Abs[#] > 20 dz0Tolerance &];
  Flatten[Array[Position[set, subset[[#]]] &, Length[subset]], 1]];
outlierPositionsj = Flatten[Array[Join[{#1}, outlierPositions[[#2]]] &,
  {NVCs0, Length[outlierPositions]}], 1];
Length[outlierPositions]

```

```

dataC0 = Delete[VMALCsets, outlierPositions];
Zdata = Delete[Zdata0, outlierPositions];
Zpdata = Delete[Zpdata0, outlierPositions];
ZZpdata = Join[Zdata<, Zpdata<]<;

ZdataC = Delete[Zdata0C, outlierPositionsj];
ZdataC0 = Delete[Zdata0C0, outlierPositionsj];
ZpdataC = Delete[Zpdata0C, outlierPositionsj];
ZpdataC0 = Delete[Zpdata0C0, outlierPositionsj];

VMs = Union[Zdata<[[1]]]; VAs = Union[Zdata<[[2]]];
VCs = Union[ZdataC[[All, All, 4]]];
{Nsets, NVMs, NVAs, NVCs} =
  {Length[Zdata], Length[VMs], Length[VAs], Length[VCs]}

```

Analysis

```

Block[{set = Flatten[Select[GatherBy[Union[Zdata[[All, 1 ;; 2]]], #[[1]] &],
  Length[#] > 30 &], 1], fit, vm, dv},
  fit = LinearModelFit[set, (vm + 20 000)Range[0,2], vm];
  {{fit["ParameterTable"], Show[ListPlot[set],
    fit = {{vm, Normal[fit]}, {vm, Normal[fit] + dv}}; ParametricPlot[
      fit, {vm, -25 000, -20 500}, {dv, -7000, 7000}]]}} // TableForm]

Block[
  {set = Flatten[Select[GatherBy[Union[Zdata[[All, {1, 3}]]], #[[1]] &],
    Length[#] > 60 &], 1], fit, vm, dv},
  {{ListPlot[set]}} // TableForm]

Block[{set = {Zpdata<[[2]] - 1, Zpdata<[[1]] - Zdata<[[5]]<}, dM},
  dZfit = LinearModelFit[set, dMRange[0,2], dM];
  {{dZfit["ParameterTable"], Show[ListPlot[set],
    Plot[dZfit[dM], {dM, -.001, .001}]]}} // TableForm]

```

Analysis by constant VM

```

{"VM (V)", "VA (V)", "VL (V)", "VC (V)", "Z0 (mm)", "Z'0 (mm)", "M0",
 "C's (mm)", "C'c (mm)", "fL (mm)", "gL (mm)", "mL", "z0L (mm)"};
L0data = ParallelTable[
  Block[{zpL = Zdata[[i, 5]] - LM, v = Zdata[[i, 3]] / Zdata[[i, 4]],
    {fL, gL, mi[fL, gL, zpL], LM - z[fL, gL, zpL]}], {i, Nsets}];
VMsets = Select[GatherBy[Select[Join[ZZpdata<, L0data<],
  #[[8]] < .2 Cs0guess &], #[[1]] &], Length[#] > 30 &];
NVMS = Length[VMsets]
{{TableForm[
  Sort[Array[{VMsets[[#, 1, 1]], Length[VMsets[[#]]] &, NVMS}]],
  ListPlot[Array[Sort[{VMsets[[#, All, 8]], VMsets[[#, All, 9]] /
    {Cs0guess, Cc0guess} - 1}<], NVMS], FrameLabel →
    {"δ Cs", "δ Cc"}, GridLines → {2Range[-5, 5, .2], 2Range[-5, 5, .2]/2} - 1],
  ListPlot[Array[{10-3 VMsets[[#, 1, 1]],
    SortBy[VMsets[[#]], Abs[#[[8]] - Cs0guess] &][[1, 9]] / Cc0guess - 1} &,
    NVMS], FrameLabel → {"VM (kV)", "δ Cc @ Cs,sys"},
  ListPlot[{Array[SortBy[VMsets[[#]], -Abs[#[[8]] / Cs0guess] &][[
    1, {3, 8}]] {10-3, 1 / Cs0guess} - {0, 1} &, NVMS],
    Array[SortBy[VMsets[[#]], Abs[#[[8]] / Cs0guess] &][[1, {3, 8}]]
    {10-3, 1 / Cs0guess} - {0, 1} &, NVMS}],
  FrameLabel → {"VL (kV)", "δ Cs,extrm"}]] // TableForm

Block[{set = Array[{10-3 VMsets[[#, 1, 1]],
  SortBy[VMsets[[#]], Abs[#[[8]] - Cs0guess] &][[1, 9]] / Cc0guess - 1} &,
  NVMS], fit, model, a, b, vm0, c, vm},
fit = FindFit[set, model = a - b (vm - vm0)-1 + c vm,
  {a, b, {vm0, Max[set<[[1]]] + .1}, {c, 0}}, vm];
Print[fit]; fit = model /. fit;
Show[ListPlot[set, FrameLabel → {"VM (kV)", "δ Cc @ Cs,sys"},
  GridLines → {Range[-25, -20, 1], 2Range[-5, 5, .2]/2} - 1],
  Plot[fit, {vm, -25, -20.8}]]]

Sort[VMsets[[All, 1, 1]]]

Sort[Select[VMsets, Max[#[[All, 8]] / Cs0guess] > 2 &][[All, 1, 1]]]

vLofvAfits = ParallelTable[Block[{set = VMsets[[i]], fit, vA},
  fit = LinearModelFit[set[[All, 2 ;; 3]] / set[[All, 4]], vARange[0, 6], vA];
  {set[[1, 1]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVMS}];

```

```

CspofvAfits = ParallelTable[Block[{set = VMsets[[i]], fit, vA},
  fit =
    LinearModelFit[{set[[2]] / set[[4]], set[[8]]}<, vARange[0,6], vA];
  {set[[1, 1]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVMs}];

CcpofvAfits = ParallelTable[Block[{set = VMsets[[i]], fit, vA},
  fit =
    LinearModelFit[{set[[2]] / set[[4]], set[[9]]}<, vARange[0,6], vA];
  {set[[1, 1]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVMs}];

{ListPlot[
  Array[Sort[{VMsets[[#, All, 3]] / -20 000, VMsets[[#, All, 7]] - 1}<] &,
    NVMs], Joined → True, AspectRatio → .5],
  ListPlot[Array[Sort[{VMsets[[#, All, 3]] / -20 000, CspofvAfits[[
    #, 4]]}<] &, NVMs], Joined → True, AspectRatio → .5],
  ListPlot[Array[Sort[{VMsets[[#, All, 3]] / -20 000, CcpofvAfits[[
    #, 4]]}<] &, NVMs], Joined → True, AspectRatio → .5]],
  {ListPlot[Array[Sort[{VMsets[[#, All, 3]] / -20 000,
    20 000 vLofvAfits[[#, 4]]}<] &,
    NVMs], Joined → True, AspectRatio → .5],
  ListPlot[Array[Sort[{VMsets[[#, All, 3]] / -20 000,
     $\frac{\text{CspofvAfits}[[\#, 4]]}{\text{VMsets}[[\#, \text{All}, 8]]}$ }<] &,
    NVMs], Joined → True, AspectRatio → .5],
  ListPlot[Array[Sort[{VMsets[[#, All, 3]] / -20 000,
     $\frac{\text{CcpofvAfits}[[\#, 4]]}{\text{VMsets}[[\#, \text{All}, 9]]}$ }<] &,
    NVMs], Joined → True, AspectRatio → .5]}],
  {ListPlot[Array[Sort[{VMsets[[#, All, 7]] - 1,
    20 000 vLofvAfits[[#, 4]]}<] &,
    NVMs], Joined → True, AspectRatio → .5],
  ListPlot[Array[Sort[{VMsets[[#, All, 7]] - 1,
     $\frac{\text{CspofvAfits}[[\#, 4]]}{\text{VMsets}[[\#, \text{All}, 8]]}$ }<] &,
    NVMs], Joined → True, AspectRatio → .5],
  ListPlot[Array[Sort[{VMsets[[#, All, 7]] - 1,
     $\frac{\text{CcpofvAfits}[[\#, 4]]}{\text{VMsets}[[\#, \text{All}, 9]]}$ }<] &,
    NVMs], Joined → True, AspectRatio → .5]}] // TableForm

```

```

SetDirectory[$HomeDirectory<>
"/Dropbox/Electron optics/Simion/triode mirror and lens"];
tmp = Sort[Array[{VMsets[[#, 1, 1]], CspofvAfits[[#, 2]],
  CcpofvAfits[[#, 2]], Min[VMsets[[#, All, 2]] / -20 000.],
  Max[VMsets[[#, All, 2]] / -20 000.]} &, NVMs]];
Export["triode Cs and Cc data fits.wdx", tmp];

tmp = Array[
{10.-3 VMsets[[#, 1, 1]],
  Length[VMsets[[#]]], 3 Mean[(20 000 vLofvAfits[[#, 4]]2)1/2,
  3 Mean[100 (CspofvAfits[[#, 4]]2 / VMsets[[#, All, 8]])1/2,
  3 Mean[100 (CcpofvAfits[[#, 4]]2 / VMsets[[#, All, 9]])1/2,
  3 Mean[(CspofvAfits[[#, 4]]2)1/2,
  3 Mean[(CcpofvAfits[[#, 4]]2)1/2} &, NVMs];
{{TableForm[Join[{{"VM (kV)", "N pts", "3σVL (V)", "3σCs (%)",
  "3σCc (%)", "3σCs (mm)", "3σCc (mm)"}}, Sort[tmp]]], Show[
ListLogPlot[{tmp[[All, {1, 3}]], tmp[[All, {1, 4}]], tmp[[All, {1, 5}]]},
  FrameLabel → {"VM (kV)", "3σ uncertainty (V, %)"},
Graphics[{colors[[1]], Text["3σ(VL) (V)",
  {tmp[[1, 1]], Log[tmp[[1, 3]]}], {1, 1}, Background → White],
  colors[[2]], Text["3σ(Cs) (%)", {tmp[[-1, 1]], Log[tmp[[-1, 4]]}],
  {-1, 1}, Background → White],
  colors[[3]], Text["3σ(Cc) (%)", {tmp[[-1, 1]], Log[tmp[[-1, 5]]}],
  {-1, -1}, Background → White}}]] // TableForm

```

Aberration sensitivity to voltage fluctuations at constant focus

```

VAsets = Select[GatherBy[Select[ZZpdata, #[[8]] < .2 Cs0guess &],
  Round[#[[2]], 100] &], Length[#] > 25 &];
NVAs = Length[VAsets]
{{ListPlot[
  Array[Sort[(VAsets[[#, All, 8]], VAsets[[#, All, 9]]) / {Cs0guess,
    Cc0guess} - 1) <] &, NVAs], FrameLabel → {"δ Cs", "δ Cc"},
  GridLines → {2Range[-5,5,.2], 2Range[-5,5,.2]/2} - 1, Joined → True],
ListPlot[Array[{10-3 VAsets[[#, 1, 2]],
  SortBy[VAsets[[#]], Abs[#[[8]] - Cs0guess] &][[1, 9]] / Cc0guess - 1} &,
  NVAs], FrameLabel → {"VA (kV)", "δ Cc @ Cs,sys"}]],
ListPlot[{Array[SortBy[VAsets[[#]], -Abs[#[[8]] / Cs0guess] &][[
  1, {3, 8}]] {10-3, 1 / Cs0guess} - {0, 1} &, NVAs],
  Array[SortBy[VAsets[[#]], Abs[#[[8]] / Cs0guess] &][[1, {3, 8}]]
    {10-3, 1 / Cs0guess} - {0, 1} &, NVAs]],
  FrameLabel → {"VL (kV)", "δ Cs,extrm"}]]} // TableForm

```

90

```

Block[{set = VAsets[[RandomInteger[{1, NVAs}]]]},
  {{ListPlot[{ $\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}$ ,  $\frac{\text{set}[[3]]}{\text{set}[[4]]}$ ]} <],
  ListPlot[{ $\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}$ , set[[8]]]} <],
  ListPlot[{ $\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}$ , set[[9]]]} <]},
  {ListPlot[{ $\frac{\text{set}[[1]]}{\text{set}[[4]]}$ ,  $\frac{\text{set}[[3]]}{\text{set}[[4]]}$ ]} <], ListPlot[{ $\frac{\text{set}[[1]]}{\text{set}[[4]]}$ , set[[8]]]} <],
  ListPlot[{ $\frac{\text{set}[[1]]}{\text{set}[[4]]}$ , set[[9]]]} <]}} // TableForm]

vLofvfits = ParallelTable[Block[{set = VAsets[[i]], fit, v},
  fit = LinearModelFit[{ $\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}$ ,  $\frac{\text{set}[[3]]}{\text{set}[[4]]}$ ]} <, vRange[0,6], v];
  {set[[1, 2]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVAs}];

```



```

Cspofvfits = ParallelTable[Block[{set = VAsets[[i]], fit, v},
  fit = LinearModelFit[ $\left\{\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}, \text{set}[[8]]\right\}$ , vRange[0,6], v];
  {set[[1, 2]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVAs}];

Ccpofvfits = ParallelTable[Block[{set = VAsets[[i]], fit, v},
  fit = LinearModelFit[ $\left\{\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}, \text{set}[[9]]\right\}$ , vRange[0,6], v];
  {set[[1, 2]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVAs}];

VLsets = Select[GatherBy[Select[ZZpdata, #[[2]] / #[[4]] < .6 &],
  Round[#[[3]], 10] &], Length[#] > 50 &];
NVls = Length[VLsets]
ListPlot[Array[
  Sort[(VLsets[[#, All, 8]], VLsets[[#, All, 9]]] / {Cs0guess, Cc0guess} -
    1)<] &, NVls], FrameLabel → {"δ Cs", "δ Cc"},
  GridLines → {2Range[-5,5,.2], 2Range[-5,5,.2]/2} - 1, Joined → True]

Block[{set = VLsets[[RandomInteger[{1, NVls}]]]},
  {ListPlot[ $\left\{\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}, \frac{\text{set}[[2]]}{\text{set}[[4]]}\right\}$ ],
  ListPlot[ $\left\{\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}, \text{set}[[8]]\right\}$ ],
  ListPlot[ $\left\{\frac{\text{set}[[2]] - \text{set}[[4]]}{\text{set}[[2]] - \text{set}[[1]]}, \text{set}[[9]]\right\}$ ]},
  {ListPlot[ $\left\{\frac{\text{set}[[2]]}{\text{set}[[4]]}, \frac{\text{set}[[1]]}{\text{set}[[4]]}\right\}$ ], ListPlot[ $\left\{\frac{\text{set}[[2]]}{\text{set}[[4]]}, \text{set}[[8]]\right\}$ ],
  ListPlot[ $\left\{\frac{\text{set}[[2]]}{\text{set}[[4]]}, \text{set}[[9]]\right\}$ ]} // TableForm]

vMofvAconstVLfits = ParallelTable[Block[{set = VLsets[[i]], fit, vA},
  fit = LinearModelFit[ $\left\{\frac{\text{set}[[2]]}{\text{set}[[4]]}, \frac{\text{set}[[1]]}{\text{set}[[4]]}\right\}$ , vARange[0,6], vA];
  {set[[1, 3]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVls}];

```

```

CspofvAconstVLfits = ParallelTable[Block[{set = VLsets[[i]], fit, vA},
  fit = LinearModelFit[{
     $\frac{\text{set}[[2]]}{\text{set}[[4]]}$ , set[[8]]}, vARange[0,6], vA];
  {set[[1, 3]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVLs}];

CcpofvAconstVLfits = ParallelTable[Block[{set = VLsets[[i]], fit, vA},
  fit = LinearModelFit[{
     $\frac{\text{set}[[2]]}{\text{set}[[4]]}$ , set[[9]]}, vARange[0,6], vA];
  {set[[1, 3]] / set[[1, 4]], Normal[fit], fit["ParameterTableEntries"][[
    All, 1]], fit["FitResiduals"], fit}], {i, NVLs}];

dVAconstVL = ParallelTable[Block[{VA0 = Mean[VLsets[[i, All, 2]]],
  VC = -20 000, vA, vA0, dVMdVA,  $\delta$ CsdVA,  $\delta$ CcdVA},
  vA0 = VA0 / VC;
  dVMdVA =
    SeriesCoefficient[vMofvAconstVLfits[[i, 2]], {vA, vA0, 1}];
   $\delta$ CsdVA = SeriesCoefficient[
     $\frac{\text{CspofvAconstVLfits}[[i, 2]]}{\text{VC} (\text{CspofvAconstVLfits}[[i, 2]] /. \text{vA} \rightarrow \text{vA0})}$ , {vA, vA0, 1}];
   $\delta$ CcdVA = SeriesCoefficient[
     $\frac{\text{CcpofvAconstVLfits}[[i, 2]]}{\text{VC} (\text{CcpofvAconstVLfits}[[i, 2]] /. \text{vA} \rightarrow \text{vA0})}$ , {vA, vA0, 1}];
  {10-3 VLsets[[i, 1, 3]], 1 / dVMdVA // Abs,
    100  $\delta$ CsdVA / dVMdVA // Abs, 100  $\delta$ CcdVA / dVMdVA // Abs}
], {i, NVLs}];

```

```

dVMconstVA =
ParallelTable[Block[{v0 = Mean[ $\frac{VAsets[[i, All, 2]] - VAsets[[i, All, 4]]}{VAsets[[i, All, 2]] - VAsets[[i, All, 1]]}$ ],
  VA0 = Mean[VAsets[[i, All, 2]]], VM0 = Mean[VAsets[[i, All, 1]]],
  VC = -20 000, dVLdv,  $\delta Csdv$ ,  $\delta Ccdv$ , dVLdVM,  $\delta CsdVM$ ,  $\delta CcdVM$ },
  dVLdVM =  $\frac{v0 VC}{(VA0 - VM0)}$  SeriesCoefficient[
    vLofvfits[[i, 2]], {v, v0, 1}];
   $\delta CsdVM = \frac{v0}{(VA0 - VM0)}$  SeriesCoefficient[
     $\frac{Cspofvfits[[i, 2]]}{(Cspofvfits[[i, 2]] /. v \rightarrow v0)}$ , {v, v0, 1}];
   $\delta CcdVM = \frac{v0}{(VA0 - VM0)}$  SeriesCoefficient[
     $\frac{Ccpofvfits[[i, 2]]}{(Ccpofvfits[[i, 2]] /. v \rightarrow v0)}$ , {v, v0, 1}];
  { $10^{-3}$  VAsets[[i, 1, 2]], dVLdVM // Abs, 100  $\delta CsdVM$  // Abs,
    100  $\delta CcdVM$  // Abs}
], {i, NVAs}];

dVAconstVM =
ParallelTable[Block[{vA0 = Mean[VMsets[[i, All, 2]]] / -20 000,
  vA, dVLdVA,  $\delta CsdVA$ ,  $\delta CcdVA$ },
  dVLdVA = SeriesCoefficient[vLofvAfits[[i, 2]], {vA, vA0, 1}];
   $\delta CsdVA = \text{SeriesCoefficient}[\frac{CspofvAfits[[i, 2]]}{-20 000 (CspofvAfits[[i, 2]] /. vA \rightarrow vA0)}, \{vA, vA0, 1\}]$ ;
   $\delta CcdVA = \text{SeriesCoefficient}[\frac{CcpofvAfits[[i, 2]]}{-20 000 (CcpofvAfits[[i, 2]] /. vA \rightarrow vA0)}, \{vA, vA0, 1\}]$ ;
  { $10^{-3}$  VMsets[[i, 1, 1]], dVLdVA // Abs, 100  $\delta CsdVA$  // Abs,
    100  $\delta CcdVA$  // Abs}
], {i, NVMs}];

```

```

{{ListPlot[dVAconstVM[All, {1, 2}],
  FrameLabel → {"VM (kV)", "dVL/dVA"}, PlotLabel → "VM constant"},
ListPlot[dVAconstVM[All, {1, 3}],
  FrameLabel → {"VM (kV)", "(dCs/Cs)/dVA (%/V)"},
  PlotLabel → "VM constant"}, ListPlot[dVAconstVM[All, {1, 4}],
  FrameLabel → {"VM (kV)", "(dCc/Cc)/dVA (%/V)"},
  PlotLabel → "VM constant"}],
{ListPlot[dVMconstVA[All, {1, 2}],
  FrameLabel → {"VA (kV)", "dVM/dVL"}, PlotLabel → "VA constant"},
ListPlot[dVMconstVA[All, {1, 3}],
  FrameLabel → {"VA (kV)", "(dCs/Cs)/dVL (%/V)"},
  PlotLabel → "VA constant"}, ListPlot[dVMconstVA[All, {1, 4}],
  FrameLabel → {"VA (kV)", "(dCc/Cc)/dVL (%/V)"},
  PlotLabel → "VA constant"}],
{ListPlot[dVAconstVL[All, {1, 2}],
  FrameLabel → {"VL (kV)", "dVA/dVM"}, PlotLabel → "VL constant"},
ListPlot[dVAconstVL[All, {1, 3}],
  FrameLabel → {"VL (kV)", "(dCs/Cs)/dVM (%/V)"},
  PlotLabel → "VL constant"}, ListPlot[dVAconstVL[All, {1, 4}],
  FrameLabel → {"VL (kV)", "(dCc/Cc)/dVM (%/V)"},
  PlotLabel → "VL constant"}]} // TableForm

CsSensitivities =
ParallelTable[Block[{α, β, γ, dVLdVA, δCM, dVMdVL, δCA, dVAdVL, δCL},
  dVLdVA = Mean[dVAconstVM[All, 2]] +
    σ1 StandardDeviation[dVAconstVM[All, 2]];
  dVMdVL = Mean[dVMconstVA[All, 2]] +
    σ2 StandardDeviation[dVMconstVA[All, 2]];
  dVAdVL = Mean[dVAconstVL[All, 2]] +
    σ3 StandardDeviation[dVAconstVL[All, 2]];
  δCM = Mean[SortBy[dVAconstVM, Abs[#[[2]] - dVLdVA] &] [[1 ;; 4, 3]]];
  δCA = Mean[SortBy[dVMconstVA, Abs[#[[2]] - dVMdVL] &] [[1 ;; 4, 3]]];
  δCL = Mean[SortBy[dVAconstVL, Abs[#[[2]] - dVAdVL] &] [[1 ;; 4, 3]]];
  Abs[{σ1, σ2, σ3, α, β, γ}] /. NSolve[{α + β dVLdVA == δCM,
    β + γ dVMdVL == δCA, α dVAdVL + γ == δCL}, {α, β, γ}]
], {σ1, -2, 2}, {σ2, -2, 2}, {σ3, -2, 2}];

```

```

{ {ListPointPlot3D[Flatten[CcsSensitivities, 3][[All, 4 ;; 6]],
  AxesLabel → {"SA (%/V)", "SL (%/V)", "SM (%/V)"}],
  {TableForm[{"<SA> (%/V)", "<SL> (%/V)", "<SM> (%/V)"},
    Mean[Flatten[CcsSensitivities, 3][[All, 4 ;; 6]]],
    "", "(<SA>2+<SL>2+<SM>2)1/2",
    Total[Mean[Flatten[CcsSensitivities, 3][[All, 4 ;; 6]]2]1/2,
    √3 Mean[Flatten[
      Flatten[CcsSensitivities2, 3][[All, 4 ;; 6]]]1/2]}] // TableForm

CcSensitivities =
ParallelTable[Block[{α, β, γ, dVLdVA, δCM, dVMdVL, δCA, dVAdVL, δCL},
  dVLdVA = Mean[dVAconstVM[[All, 2]]] +
    σ1 StandardDeviation[dVAconstVM[[All, 2]]];
  dVMdVL = Mean[dVMconstVA[[All, 2]]] +
    σ2 StandardDeviation[dVMconstVA[[All, 2]]];
  dVAdVL = Mean[dVAconstVL[[All, 2]]] +
    σ3 StandardDeviation[dVAconstVL[[All, 2]]];
  δCM = Mean[SortBy[dVAconstVM, Abs[#[[2]] - dVLdVA] &][[1 ;; 4, 4]]];
  δCA = Mean[SortBy[dVMconstVA, Abs[#[[2]] - dVMdVL] &][[1 ;; 4, 4]]];
  δCL = Mean[SortBy[dVAconstVL, Abs[#[[2]] - dVAdVL] &][[1 ;; 4, 4]]];
  Abs[{σ1, σ2, σ3, α, β, γ}] /. NSolve[{α + β dVLdVA == δCM,
    β + γ dVMdVL == δCA, α dVAdVL + γ == δCL}, {α, β, γ}]
], {σ1, -2, 2}, {σ2, -2, 2}, {σ3, -2, 2}];

{ {ListPointPlot3D[Flatten[CcSensitivities, 3][[All, 4 ;; 6]],
  AxesLabel → {"SA (%/V)", "SL (%/V)", "SM (%/V)"}],
  {TableForm[{"<SA> (%/V)", "<SL> (%/V)", "<SM> (%/V)"},
    Mean[Flatten[CcSensitivities, 3][[All, 4 ;; 6]]],
    "", "(<SA>2+<SL>2+<SM>2)1/2",
    Total[Mean[Flatten[CcSensitivities, 3][[All, 4 ;; 6]]2]1/2,
    √3 Mean[Flatten[
      Flatten[CcSensitivities2, 3][[All, 4 ;; 6]]]1/2]}] // TableForm

```

Export tables, apply V_L voltage correction for different bore diameter

```
{δcsi, δcci} = {1, 1.5};
```

```

CsByVMsets0 = Select[
  ParallelTable[Block[{Cs = 2j/δcsi Cs0guess, vLf = vL200ofvL242},
    Quiet[Select[Select[
      Table[Block[{vAsol, vA, result, minVA, maxVA},
        vAsol = Quiet[FindMinimum[Abs[CspofvAfits[[i, 2]] - Cs],
          {vA, Mean[VMsets[[i, All, 2]] / (-20 000)}][[-1]]];
        {minVA, maxVA} = {Min[VMsets[[i, All, 2]]},
          Max[VMsets[[i, All, 2]]}];
        result = {VMsets[[i, 1, 1]], (-20 000) vA,
          (-20 000) (vLf /. vL242 → vLofvAfits[[i, 2]]),
          CspofvAfits[[i, 2]], CcpofvAfits[[i, 2]] /. vAsol};
        If[minVA < result[[2]] < maxVA, result, i]
      ], {i, NVMS}], # == Re[#] &],
    (-20 000) (vLf /. vL242 → Min[Zdata[[3]]] / (-20 000)) ≤ #[[3]] ≤
      (-20 000) (vLf /. vL242 → Max[Zdata[[3]]] / (-20 000)) &]]
  ], {j, -1, 1, .05}], Length[#] > 0 &];

CcByVMsets0 = Select[
  ParallelTable[Block[{Cc = 2j/δcci Cc0guess, vLf = vL200ofvL242},
    Quiet[Select[Select[
      Table[Block[{vAsol, vA, result, minVA, maxVA},
        vAsol = Quiet[FindMinimum[Abs[CcpofvAfits[[i, 2]] - Cc],
          {vA, Mean[VMsets[[i, All, 2]] / (-20 000)}][[-1]]];
        {minVA, maxVA} = {Min[VMsets[[i, All, 2]]},
          Max[VMsets[[i, All, 2]]}];
        result = {VMsets[[i, 1, 1]], (-20 000) vA,
          (-20 000) (vLf /. vL242 → vLofvAfits[[i, 2]]),
          CspofvAfits[[i, 2]], CcpofvAfits[[i, 2]] /. vAsol};
        If[minVA < result[[2]] < maxVA, result, i]
      ], {i, NVMS}], # == Re[#] &],
    (-20 000) (vLf /. vL242 → Min[Zdata[[3]]] / (-20 000)) ≤ #[[3]] ≤
      (-20 000) (vLf /. vL242 → Max[Zdata[[3]]] / (-20 000)) &]]
  ], {j, -1, 1, .05}], Length[#] > 0 &];

{"VM (V)", "VA (V)", "VL (V)", "Cs (mm)",
  "Cc (mm)", "Intended Cs/Cs0-1", "Intended Cc/Cc0-1"};
CsCcsets = Flatten[Join[CsByVMsets0, CcByVMsets0], 1];
CsCcsets =
  ParallelTable[Block[{Cs = 2i/δcsi Cs0guess, Cc = 2j/δcci Cc0guess},
    Join[SortBy[Ccsets, Norm[#[[4 ;; 5]] / {Cs, Cc} - 1] &][[1, 1 ;; 5]],
      {Cs / Cs0guess, Cc / Cc0guess} - 1]
  ], {i, -1, 1, .05}, {j, -1, 1, .05}];

```

```

tablesgraphic =
  ListPlot[(Flatten[CSCsets, 1]<[[4 ;; 5]] / {Cs0guess, Cc0guess} - 1)<,
    PlotStyle → Black, FrameLabel → {" $\delta C_s$ ", " $\delta C_c$ "},
    GridLines → {2Range[-1,1,.05]/ $\delta c_{si}$ }, 2Range[-1,1,.05]/ $\delta c_{ci}$ } - 1, PlotRange →
      1.3 {{2-1/ $\delta c_{si}$ , 21/ $\delta c_{si}$ } - 1, {2-1/ $\delta c_{ci}$ , 21/ $\delta c_{ci}$ } - 1}, ImageSize → 450]
SetDirectory[$HomeDirectory<>
  "/Dropbox/Electron optics/Simion/triode mirror and lens"];
Export["dCc vs dCs.png", tablesgraphic]
Export["triode primary range Cc vs Cs, mm.wdx",
  Flatten[CSCsets, 1]<[[4 ;; 5]]]

SetDirectory[$HomeDirectory<>
  "/Dropbox/Electron optics/Simion/triode mirror and lens"];
Array[Export[{"VM, V.txt", "VA, V.txt", "VL, V.txt",
  "Cs, mm.txt", "Cc, mm.txt", "Intended dCs over Cc0.txt",
  "Intended dCc over Cc0.txt"}][#],
  CSCsets[[All, All, #]], "TSV"] &, 7]

```

Appendix J PEEM control: triode mirror branch tables

The results of characterizing the triode mirror branch in SIMION, containing the triode mirror and lens as pictured in Fig. 5.2b. The aberration values here cover the center of the triode corrector range, and vary logarithmically away from the central value. There are approximately 5×5 values in each quadrant, one-sixteenth of the number of points in Figs. 5.4 and 5.5 but with similar extent. Each pair of aberration correction values is accompanied by the mirror column potentials that create that condition. These are evaluated for an interface lens with bore diameter of 6.15 mm (0.242 in). The columns here have units of mm (C_s , C_c) and V (V_M , V_A , $V_I = V_L$).

C_s (mm)	C_c (mm)	V_M (V)	V_A (V)	V_L (V)
-1989304	-30505.0	-22000	-9306.9	-21134.2
-1989304	-21267.8	-23100	-3462.2	-21356.5
-1989304	-36870.1	-21600	-11548.1	-21098.9
-1989304	-33342.3	-21800	-10416.4	-21110.2
-1989304	-19207.5	-23500	-1396.2	-21435.3
-1989304	-23073.3	-22800	-5024.2	-21290.4
-1989304	-25355.3	-22510	-6558.2	-21233.4
-1989304	-27856.6	-22240	-8003.6	-21179.6
-1953159	-18350.8	-23600	-857.3	-21430.9
-1921541	-18275.4	-23600	-844.1	-21418.9
-1731789	-18982.3	-23300	-2305.3	-21280.9
-1731789	-17686.2	-23600	-758.4	-21342.6
-1731789	-23150.7	-22610	-5924.6	-21137.5
-1731789	-25427.2	-22340	-7370.6	-21083.3
-1731789	-27783.6	-22100	-8673.3	-21037.2
-1731789	-21258.0	-22900	-4392.2	-21198.1
-1731789	-33440.9	-21680	-11013.3	-20980.8
-1731789	-36809.9	-21500	-12049.6	-20977.3
-1731789	-30468.0	-21880	-9887.8	-21002.2
-1672798	-17409.8	-23600	-726.3	-21314.5
-1609364	-17121.9	-23600	-691.0	-21283.9
-1507611	-19042.0	-23100	-3233.8	-21132.6

C_s (mm)	C_c (mm)	V_M (V)	V_A (V)	V_L (V)
-1507610	-23105.3	-22460	-6629.3	-20998.4
-1507610	-27739.0	-21980	-9250.9	-20909.0
-1507610	-17600.3	-23400	-1672.0	-21197.0
-1507610	-21373.9	-22710	-5294.6	-21053.3
-1507610	-30559.2	-21760	-10481.6	-20875.7
-1507610	-25411.3	-22200	-8040.4	-20948.6
-1507610	-33141.6	-21600	-11397.5	-20865.8
-1507610	-37139.1	-21400	-12571.3	-20875.3
-1504621	-16730.8	-23600	-633.7	-21234.9
-1406650	-16350.1	-23600	-577.1	-21187.3
-1312451	-37859.1	-21300	-13110.2	-20786.8
-1312451	-30466.1	-21670	-10923.0	-20766.6
-1312451	-27836.8	-21860	-9842.8	-20788.5
-1312451	-15921.3	-23600	-517.4	-21137.9
-1312451	-21007.8	-22600	-5785.3	-20929.6
-1312451	-19158.6	-22900	-4186.7	-20994.5
-1312451	-17668.8	-23200	-2606.7	-21059.1
-1312451	-23113.2	-22320	-7298.7	-20871.3
-1312451	-25356.9	-22080	-8615.1	-20824.3
-1312451	-33348.0	-21500	-11909.1	-20758.5
-1142555	-33866.8	-21400	-12440.1	-20668.1
-1142555	-19413.3	-22710	-5104.7	-20862.6
-1142555	-21051.9	-22460	-6453.0	-20809.1
-1142555	-30243.2	-21600	-11259.2	-20666.1
-1142555	-15983.9	-23400	-1452.6	-21009.3
-1142555	-25470.3	-21960	-9207.6	-20711.6
-1142555	-17309.0	-23100	-3028.4	-20945.1
-1142555	-27875.4	-21760	-10337.7	-20681.0
-1142555	-36199.2	-21300	-13048.0	-20685.5
-1142555	-23107.2	-22200	-7874.3	-20755.9
-1103635	-15404.0	-23500	-904.2	-21009.0
-994652	-32501.1	-21400	-12379.2	-20576.5
-994652	-27815.1	-21680	-10729.9	-20583.9
-994652	-17538.0	-22900	-3997.3	-20818.9
-994652	-21052.3	-22340	-7027.1	-20700.1
-994652	-23141.5	-22090	-8407.6	-20648.9
-994652	-16130.7	-23200	-2404.3	-20883.9
-994652	-14901.3	-23500	-826.1	-20946.7
-994652	-37435.2	-21200	-13617.1	-20628.6
-994652	-25269.3	-21880	-9585.8	-20610.4
-994652	-19190.8	-22610	-5557.7	-20758.1

C_s (mm)	C_c (mm)	V_M (V)	V_A (V)	V_L (V)
-994652	-30629.2	-21500	-11781.8	-20572.5
-865895	-36018.3	-21200	-13562.2	-20539.4
-865895	-25459.0	-21780	-10090.0	-20514.9
-865895	-23100.1	-22000	-8842.5	-20554.0
-865895	-27921.2	-21600	-11134.1	-20496.2
-865895	-15937.2	-23100	-2842.1	-20785.1
-865895	-14686.6	-23400	-1251.5	-20847.4
-865895	-21041.7	-22240	-7503.4	-20601.3
-865895	-17387.5	-22800	-4447.8	-20720.4
-865895	-19268.3	-22480	-6182.6	-20650.8
-865895	-33391.0	-21300	-12932.8	-20505.6
-859008	-31220.8	-21400	-12318.6	-20487.9
-753806	-37720.3	-21100	-14160.9	-20511.3
-753805	-32220.3	-21300	-12880.1	-20426.7
-753805	-15781.8	-23000	-3291.4	-20693.0
-753805	-17505.1	-22660	-5125.8	-20618.5
-753805	-19242.8	-22380	-6658.8	-20558.7
-753805	-30202.9	-21400	-12268.0	-20415.7
-753805	-14535.6	-23300	-1688.5	-20754.7
-753805	-21058.8	-22140	-7990.7	-20508.5
-753805	-25282.7	-21720	-10375.7	-20433.1
-753805	-23072.2	-21920	-9229.7	-20465.7
-753805	-28455.4	-21500	-11667.1	-20414.4
-656859	-36502.6	-21100	-14114.0	-20434.7
-656226	-14411.0	-23200	-2136.8	-20668.2
-656226	-16207.1	-22800	-4291.2	-20583.6
-656226	-27534.0	-21500	-11614.6	-20344.8
-656225	-19155.5	-22300	-7033.1	-20474.8
-656225	-17775.6	-22510	-5873.8	-20520.6
-656225	-25372.6	-21650	-10729.3	-20358.4
-656225	-23104.4	-21840	-9627.6	-20384.8
-656225	-33575.0	-21200	-13460.2	-20380.0
-656225	-21036.2	-22060	-8376.6	-20425.9
-656225	-31184.8	-21300	-12830.8	-20354.6
-583773	-32697.3	-21200	-13420.9	-20320.7
-571278	-30266.6	-21300	-12784.7	-20288.7
-571278	-16155.5	-22710	-4711.6	-20505.0
-571278	-35399.5	-21100	-14069.5	-20363.5
-571277	-14359.0	-23100	-2596.4	-20587.6
-571277	-23111.2	-21780	-9920.5	-20314.7
-571277	-17528.0	-22460	-6083.6	-20449.7

C_s (mm)	C_c (mm)	V_M (V)	V_A (V)	V_L (V)
-571277	-21070.4	-21980	-8773.3	-20350.6
-571277	-28359.9	-21400	-12170.1	-20281.1
-571277	-19307.7	-22200	-7531.3	-20395.2
-571277	-25249.8	-21600	-10971.7	-20289.7
-497406	-34417.3	-21100	-14028.0	-20298.4
-497326	-19184.2	-22140	-7810.5	-20325.4
-497326	-27574.7	-21400	-12125.6	-20222.0
-497326	-15991.8	-22650	-4975.2	-20436.8
-497326	-29448.9	-21300	-12741.7	-20228.5
-497326	-23115.4	-21720	-10219.4	-20248.4
-497326	-21062.9	-21920	-9063.5	-20283.6
-497326	-14355.4	-23000	-3066.0	-20511.7
-497326	-17523.4	-22380	-6467.5	-20377.9
-497205	-37993.5	-21000	-14717.6	-20392.0
-495151	-25951.9	-21500	-11518.0	-20220.9

Appendix K PEEM control: objective branch tables

The objective branch is composed of the cathode, objective, and auxiliary lenses. The distance from the cathode to the objective varies slightly with sample, so the objective must be able to change focal distance to bring the virtual specimen into focus. The auxiliary lens ensures that the image has a consistent position in magnetic deflector A, as illustrated in Fig. 3.1 and App. Appendix A. As such, the objective and auxiliary lens must vary continuously with variations in sample height δz_C . The two lenses work together as a zoom pair, giving the freedom to choose image magnification over the range $3.5\text{--}7.5\times$. The quoted magnification includes the demagnification of the first objective aperture. To give continuous focusing at constant magnification, the lens potentials are modeled as polynomials of sample height δz_C , which can vary over several hundred microns. The aberration of the pair can similarly be calculated. The total aberration of the objective branch in transfer space, including the cathode, can be estimated from a sum of the objective-auxiliary aberration and the cathode aberration multiplied by the magnification, as given by Eqs. (3.26) and (3.27). Presented here are the polynomial coefficients of the fits of V_O , V_X , C'_s , and C'_c as functions of δz_C for discrete magnifications. The potentials are given in units of V_C , the aberration coefficients are given in mm, and the variable δz_C is given in microns.

Appendix K.1 Objective lens potential

Objective lens potential V_O in units of V_C can be expressed as a polynomial of sample height δz_C in microns. The polynomial coefficients, noted here, change with magnification. Additional magnifications are possible.

Mag	$(dz_C)^0$	$(dz_C)^1$	$(dz_C)^2$
3.50	9.652E-01	2.126E-05	1.063E-09
4.00	9.685E-01	2.135E-05	1.026E-09
4.50	9.710E-01	2.140E-05	1.012E-09
5.00	9.730E-01	2.143E-05	9.972E-10
5.50	9.746E-01	2.146E-05	9.902E-10
6.00	9.759E-01	2.149E-05	9.824E-10
6.50	9.771E-01	2.150E-05	9.739E-10
7.00	9.781E-01	2.151E-05	9.728E-10

Appendix K.2 Auxiliary lens potential

Auxiliary lens potential V_X in units of V_C can be expressed as a polynomial of sample height dz_C in microns. The polynomial coefficients, noted here, change with magnification. Additional magnifications are possible.

Mag	$(dz_C)^0$	$(dz_C)^1$	$(dz_C)^2$
3.50	4.15E-01	7.59E-06	-1.61E-10
4.00	4.00E-01	9.19E-06	-1.64E-10
4.50	3.84E-01	1.11E-05	-2.54E-10
5.00	3.66E-01	1.34E-05	-3.72E-10
5.50	3.48E-01	1.60E-05	-5.70E-10
6.00	3.27E-01	1.91E-05	-8.30E-10
6.50	3.05E-01	2.30E-05	-1.21E-09
7.00	2.79E-01	2.83E-05	-1.99E-09

Appendix K.3 Spherical aberration

Transfer space spherical aberration C'_s without the cathode in units of mm expressed as a polynomial of sample height dz_C in microns. The polynomial coefficients, noted here, change with magnification. Additional magnifications are possible.

Mag.	$(dz_C)^0$	$(dz_C)^1$	$(dz_C)^2$	$(dz_C)^3$
3.50	3.560E+05	-6.139E+01	3.537E-03	0.000E+00
4.00	5.728E+05	-1.015E+02	5.748E-03	0.000E+00
4.50	8.875E+05	-1.670E+02	1.187E-02	0.000E+00
5.00	1.340E+06	-2.775E+02	2.589E-02	0.000E+00
5.50	1.996E+06	-4.716E+02	6.079E-02	0.000E+00
6.00	2.989E+06	-8.617E+02	1.547E-01	0.000E+00
6.50	4.595E+06	-1.719E+03	5.808E-01	-1.405E-04
7.00	7.618E+06	-4.177E+03	2.160E+00	-6.689E-04

Appendix K.4 Chromatic aberration

Transfer space chromatic aberration C'_c without the cathode in units of mm can be expressed as a polynomial of sample height dz_C in microns. The polynomial coefficients, noted here, change with magnification. Additional magnifications are possible.

Mag.	$(dz_C)^0$	$(dz_C)^1$	$(dz_C)^2$	$(dz_C)^3$
3.50	1.301E+03	-6.558E-02	9.133E-07	0.000E+00
4.00	1.645E+03	-8.480E-02	1.630E-07	0.000E+00
4.50	2.038E+03	-1.114E-01	1.579E-06	0.000E+00
5.00	2.484E+03	-1.473E-01	3.719E-06	0.000E+00
5.50	2.989E+03	-1.934E-01	8.990E-06	0.000E+00
6.00	3.567E+03	-2.591E-01	1.791E-05	0.000E+00
6.50	4.239E+03	-3.573E-01	4.125E-05	-6.740E-09
7.00	5.039E+03	-5.267E-01	9.457E-05	-1.882E-08