Simulation of electron mirrors by the differential algebraic method

Liping Wang*, Eric Munro, John Rouse and Haoning Liu

Munro’s Electron Beam Software Ltd., 14 Cornwall Gardens, London SW7 4AN, England

Abstract

A differential algebraic (DA) method has been developed for the aberration analysis of electron mirrors, and a software package MIRROR_DA has been developed. Time is used instead of axial position as our independent variable, and a reference ray is also employed. A single DA ray is traced in the fields of the mirror system, performed on a non-standard extension of real number space called \( \mathbb{D} \), and all aberrations coefficients can be obtained simultaneously, in principle up to arbitrary order and with extremely high accuracy. To demonstrate our software, an example of tetrode mirror is presented. From the results by MIRROR_DA, it is shown that when adjusting the voltages of two middle electrodes \( C_s \) and \( C_c \) change signs from positive to negative, and their values vary in a wide range: therefore this tetrode mirror can be used to cancel \( C_s \) and \( C_c \) of round lenses.

© 2008 Elsevier B.V. Open access under CC BY-NC-ND license.

PACS: 41.85.-p

Keywords: Differential algebra; Electron mirror; Aberration correction; Electron microscope

1. Introduction

The study and design of electron mirrors has become one of the hot topics in recent years for designers of modern charged particle optical systems in the quest for better performance [1-4]. As mirrors can generate aberrations of opposite sign to those of round lenses, they can be used - in combination with bending elements to separate the incident beam and the reflected beam - as aberration correctors in systems such as electron microscopes. For example, in SMART (Spectro-Microscope for All Relevant Techniques) for BESSY II in Germany [5], a mirror corrector has been used to correct the primary spherical and axial chromatic aberrations simultaneously to achieve ultra-high resolution. Another similar example is PEEM3, the third generation photoemission electron microscope developed at ALS, Lawrence Berkeley National Laboratory, USA [1], where an electron mirror is also an essential part.

* Corresponding author. Tel.: +44-20-7581-4479; fax: +44-20-7581-4479
E-mail address: mebs@compuserve.com

The concept of mirror correctors has a long history [6-7], however extensive studies followed up much later, performed by Kelman [8] in the 1970s, Rempfer [9-10], Shao [11-12], Rose [2-3] and coworkers in the 1990s. A simple two-electrode mirror with hyperbolic potential distribution was studied by Rempfer [9] and Shao [11]. Conventional aberration theories, which usually assume that the axial velocity is finite and the beam slopes are small and express the ray paths as functions of axial position, are not applicable to mirrors because, at the turning point of a mirror, the axial velocity goes to zero and the beam slopes can be infinite. Since the axial position is no longer a unique coordinate for the ray, it is essential to use time \( t \), or an equivalent length, as the independent variable. Shao and Wu developed a program to solve the equations of motion numerically to the third order for electron mirrors, and the spherical aberration coefficient was obtained by calculating several rays at different inclining angles, while the chromatic aberration coefficient was obtained by calculating several rays with different energy deviations [12]. However, the derivation of the explicit expressions for these coefficients is very arduous, and it is mandatory to employ an algebraic computer program [2]. During the development of PEEM3, both SIMION and COSY INFINITY are used to design its electron mirror by Wan et al. [4].

Following our previous work on the differential algebraic (DA) method [13] for the aberration computation of conventional systems [14], we have developed the DA method for the analysis of electron mirrors, and based on this a software package, called MIRROR_DA, has been developed. With the DA method, a single DA ray is traced in the fields of the mirror system and all aberrations coefficients can be obtained, in principle up to arbitrary order and with extremely high accuracy. There is no effort spent on deriving the formulae for the aberration coefficients of electron mirrors during this procedure. As a hyperbolic mirror is not adjustable for its aberration coefficients if the image and object positions are fixed, a four-electrode mirror was proposed by Shao and Wu [12] and their numerical analysis shows that its spherical and chromatic aberrations can be electrically varied. Tetrode mirrors are used in SMART [3] as well as PEEM3 [1]. In this paper, analysis of practical mirrors by our MIRROR_DA software is demonstrated by an example of a tetrode mirror.

2. DA method and software MIRROR_DA

The mathematical foundation of the DA method is Non-Standard Analysis developed by Robinson [15]. It was introduced into accelerator physics by Berz [13] with great success. In the DA method, the analysis is carried out on a non-standard extension of the real space \( R \), called \( {}_n D_r \). \( {}_n D_r \) is the collection of DA-quantities \( q \) - special vectors relating to the partial derivatives up to \( n \) degree of any continuously differentiable function \( f \) of \( v \) variables. \( {}_n D_r \) has many properties that are remarkably similar to real space \( R \), such as arithmetic operations and their laws, “zero” and “unit”, ordering, “positive” and “negative”, etc. However, \( {}_n D_r \) has some extraordinary features. For example, in \( {}_n D_r \), there are infinitesimals, \( \delta \):

\[
0 < \text{abs}(\delta) < \tilde{r} ,
\]

for any positive real number \( r \) \( \quad (1) \)

where \( \tilde{r} \) is the counterpart of \( r \) in \( {}_n D_r \). An important property of infinitesimals is that they are nilpotent, that is, in \( {}_n D_r \),

\[
\delta^m = 0 , \quad \text{for} \ m > n
\]

Any DA-quantity can be expressed as the sum of a real and an infinitesimal. Furthermore, we can introduce series in \( {}_n D_r \). Fundamental functions in \( R \) can always be extended into \( {}_n D_r \), and many properties of these functions remain while extended.
For an electron mirror system, we use time instead of axial position as our independent variable, and following other researchers [2,3], we also use a reference ray. The reference ray enters the mirror travelling along the optical axis with nominal kinetic energy, while the position of an arbitrary ray is measured with respect to the reference ray. Using \( \zeta(t) \) to denote the axial position of the reference ray at time \( t \) and \( h(t) \) to represent the axial separation of the arbitrary ray from the reference ray, the position of reference ray in Cartesian coordinates is \( (0,0,\zeta(t)) \) while the position of the arbitrary ray is \( (x(t), y(t), \zeta(t) + h(t)) \).

Starting from the Lorentz equation, the equations of motion for the reference ray are:

\[
\frac{d\zeta}{dt} = \zeta, \quad \frac{d\zeta}{dt} = \frac{q}{m} E_z(0,0,\zeta)
\]  

(3)

For an arbitrary ray, the Lorentz equation can be transformed into a set of equations in \( x, y \) and \( h \) thus:

\[
\begin{align*}
\frac{dx}{dt} &= \dot{x}, \quad \frac{dx}{dt} = \frac{q}{m} \left( E_x + \dot{y}B_z - \dot{z}B_y \right) \\
\frac{dy}{dt} &= \dot{y}, \quad \frac{dy}{dt} = \frac{q}{m} \left( E_y + \dot{z}B_x - \dot{x}B_z \right) \\
\frac{dh}{dt} &= \dot{h}, \quad \frac{dh}{dt} = \frac{q}{m} \left( E_z + \dot{x}B_y - \dot{y}B_x \right) - \zeta
\end{align*}
\]

(4)

where \( \dot{x}, \dot{y}, \dot{z} \) as well as \( \zeta \) are components of velocities (i.e. derivatives with respect to time), \( \dot{h} = \dot{\zeta} - \zeta \), and \( m \) and \( q \) are the mass and charge of the particle, respectively.

At the object plane \( z = z_o \), for the reference ray with nominal potential \( \Phi_0 \) (measured relative to where the electron is at rest), its initial position and velocity are

\[
\zeta_0 = z_o, \quad \dot{\zeta}_0 = -\frac{2q\Phi_0}{m}
\]  

(5)

As for an arbitrary ray with deviation \( \Delta\Phi \) from the nominal potential, suppose its position at the object plane is \( (x_o, y_o, z_o) \), then the components of its initial velocity are

\[
\begin{align*}
\dot{h}_0 &= \dot{z}_0 - \zeta_0 = \dot{\zeta}_0 \left( \frac{(1 + \Delta\Phi/\Phi_0)}{1 + (x_o^2 + y_o^2)/\Phi_0^2} - 1 \right) \\
\dot{x}_0 &= x'_0 \dot{z}_0, \quad \dot{y}_0 = y'_0 \dot{z}_0
\end{align*}
\]

(6)

where \( x'_0 \) and \( y'_0 \) are the initial slope components of the ray. At time \( t_f \) when the reference ray reaches the image plane \( z = z_i \), the off-axial position of the arbitrary ray \( (x_f, y_f) \) is not at the image plane \( z = z_i \). The final position of the arbitrary ray \( (x, y) \) at the image plane can be obtained by linear extrapolation in the case of a “field-free” region near the image plane, or more generally, quadratic extrapolation.

For aberrations of a mirror system, the equations of motion are solved by DA method, wherein a single DA ray trace is performed on \( \gamma D \). All variables for the arbitrary ray, as well as the potentials and fields, are transformed into DA quantities. In the DA ray trace, the same numerical techniques used in traditional ray tracing can be employed, but all steps are transferred from the real space \( R \) to \( \gamma D \). After the DA ray trace, the aberrations of the mirror system are obtained, in principle up to arbitrary order \( n \), and with very high accuracy, due to the remarkable algebraic properties of \( \gamma D \). Obtaining aberration coefficients of electron mirrors by DA method looks somewhat “automatic” since the enormous effort to derive explicit formulae for the aberration coefficients is avoided.
A software package MIRROR_DA has been developed for the aberration analysis of electron mirrors, based on the DA method. This software is written in ANSI Standard C++, where DA quantities can be represented by a C++ Class. The MIRROR_DA package includes a main program MIRDA for computing optical properties in the mirror by DA method, and a post-processing program DASP for plotting spot diagrams of the aberrations at the mirror screen plane. The program handles electron mirrors containing any combination of rotationally symmetric electrostatic and magnetic fields. The program can also handle combinations of electron mirrors and electron lenses.

Firstly, the electrostatic and magnetic fields can be computed with our numerical field calculation software SOFEM [16], which uses second-order finite element method. After the electrostatic and magnetic potentials over the whole FEM mesh are obtained, the axial potential or flux density distribution can be extracted. Then these functions are fitted with Hermite series using our HERM1 program [17]. These Hermite coefficients are then fed into MIRDA to reconstruct the axial functions. This is very accurate because series of Hermite functions are continuously differentiable and are especially suitable for field functions that tend to zero at faraway axial distances [18]. From these axial functions, the potential and fields at any off axis point can be obtained. For a rotationally symmetric mirror, the potential at any off axis point can be written as:

\[
\Phi_0(z,r) = f_0(z) - \frac{1}{4} f_0''(z)r^2 + \frac{1}{64} f_0'''(z)r^4 + \ldots
\]  

(12)

where \( f_0(z) \) is its axial function, while by \( \mathbf{E} = -\nabla \Phi \) the electrostatic field components are

\[
E_x(x,y,z) = \frac{1}{2} f_0'(z)x - \frac{1}{16} f_0''(z)(x^2 + y^2)x + \frac{1}{384} f_0'''(z)(x^2 + y^2)^2 x + \ldots
\]

\[
E_y(x,y,z) = \frac{1}{2} f_0'(z)y - \frac{1}{16} f_0''(z)(x^2 + y^2)y + \frac{1}{384} f_0'''(z)(x^2 + y^2)^2 y + \ldots
\]

\[
E_z(x,y,z) = -f_0(z) + \frac{1}{4} f_0''(z)(x^2 + y^2) - \frac{1}{64} f_0'''(z)(x^2 + y^2)^2 - \ldots
\]

(13)

The DA ray trace is performed in MIRDA by a fifth-order Runge-Kutta technique, with adaptive step size [19].

From the DA quantities obtained from MIRDA, the spot diagram at the mirror image plane can be easily plotted. The post-processing program DASP is written for this purpose, by which ideal Gaussian image, beam blur, image distortion and chromatic aberration can be viewed for specified shaped beam and chosen aberration order.

This software has been tested against analytical models whose electrostatic and magnetic fields can be expressed by Fourier Bessel series. By direct ray tracing in the analytical fields, the primary aberration coefficients can be extracted. These are compared with the results from MIRROR_DA, and they agree well [20].

3. Example

The software MIRROR_DA can be used to simulate and design practical mirrors, for example, tetrode mirrors, where the image position, spherical aberration coefficient and chromatic aberration coefficient can be adjusted independently. One example of tetrode mirror we calculated is shown in Fig. 1. The object and image planes are fixed at a distance of 200 mm from the mirror electrode. The incident beam energy is 10keV. Electrode voltages \( V_2 \) and \( V_3 \) are adjustable, while mirror electrode voltage \( V_1 \) is varied for focusing.
The electrostatic fields of the mirror are computed by SOFEM. The equipotential lines as well as axial potential distribution in the case of $V_1 = -286.24$ volts, $V_2 = 50$ volts, $V_3 = 3$ kV and $V_4 = 10$ kV, are shown in Fig. 1. Then axial potential functions are extracted for each electrode, and fitted by 100 terms of a Hermite series using our program HERM1. Fig. 2 shows the fitting of the axial potential functions for each electrode. The upper plots show the Hermite fits superimposed on the numerically computed axial potential functions generated by SOFEM (they are indistinguishable on the plots). The lower plots show a very highly magnified view of the deviation of the Hermite fits from the numerical SOFEM data. In this example, the maximum deviations of the fitting were found to be 0.00267%, 0.003322%, 0.000052 and 0.000028% respectively.

Fig. 2. Hermite fitting of the unit axial potential functions for each electrode.

These Hermite fitted functions are then used by MIRROR_DA to calculate the optical properties of this tetrode mirror. The primary focusing ray and field ray calculated from MIRROR_DA are plotted in Fig. 3. In this example, the mirror is operating in unity magnification mode with unity angular magnification.

Fig. 3. Primary rays for the tetrode mirror in the case of $V_1 = -286.24$ volts, $V_2 = 50$ volts, $V_3 = 3$ kV, $V_4 = 10$ kV calculated by MIRROR_DA.

The computation results by MIRROR_DA for some voltage settings are given in Table 1, where $C_s$ and $C_c$ are the primary spherical aberration and chromatic aberration coefficients, referred to the image side.
Table 1
Computed results (in S.I units) by MIRROR_DA for the mirror of Fig. 2.

<table>
<thead>
<tr>
<th>$V_1$ (Volts)</th>
<th>$V_2$ (Volts)</th>
<th>$V_3$ (Volts)</th>
<th>$V_4$ (Volts)</th>
<th>$C_s$ (m)</th>
<th>$C_c$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-287.331</td>
<td>80</td>
<td>3000</td>
<td>10000</td>
<td>47.59</td>
<td>29.05</td>
</tr>
<tr>
<td>-287.096</td>
<td>60</td>
<td>3000</td>
<td>10000</td>
<td>22.02</td>
<td>32.74</td>
</tr>
<tr>
<td>-286.242</td>
<td>50</td>
<td>3000</td>
<td>10000</td>
<td>6.12</td>
<td>34.80</td>
</tr>
<tr>
<td>-280.416</td>
<td>20</td>
<td>3000</td>
<td>10000</td>
<td>-56.45</td>
<td>41.93</td>
</tr>
<tr>
<td>-333.498</td>
<td>50</td>
<td>6000</td>
<td>10000</td>
<td>35.32</td>
<td>45.26</td>
</tr>
<tr>
<td>-306.056</td>
<td>50</td>
<td>5000</td>
<td>10000</td>
<td>27.92</td>
<td>45.04</td>
</tr>
<tr>
<td>-1020.966</td>
<td>50</td>
<td>1000</td>
<td>10000</td>
<td>173.46</td>
<td>1.33</td>
</tr>
<tr>
<td>-4049.778</td>
<td>50</td>
<td>500</td>
<td>10000</td>
<td>385.72</td>
<td>-6.67</td>
</tr>
</tbody>
</table>

The variation of $C_s$ and $C_c$ with respect to $V_2$ and $V_3$ are plotted in Fig. 4(a) and (b) respectively, while the mirror voltage $V_1$ for different $V_2$ and $V_3$ values to reflect and focus the beam to the object plane are plotted in Fig. 4(c). It is shown that when adjusting $V_2$ and $V_3$, $C_s$ and $C_c$ change sign from positive to negative, and their values vary over a wide range, therefore this mirror can be used to cancel the $C_s$ and $C_c$ of round lenses.

(a) Spherical aberration coefficient $C_s$

(b) Chromatic aberration coefficient $C_c$

(c) Mirror voltage $V_m$ as a function of electrode voltages $V_2$ and $V_3$. 
Using the DASP program, the spot diagram at the image plane can be plotted from the obtained DA quantities. Only as a demonstration, Fig. 5 shows the spot diagram at the image plane in the case of \( V_1 = -297.917 \) Volts, \( V_2 = 0 \) Volts, \( V_3 = 5 \) kV and \( V_4 = 10 \) kV as calculated by MIRROR_DA. It is for a 0.1x0.1 mm\(^2\) square shaped beam with 2 mrad beam angle.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{spot_diagram.png}
\caption{Spot diagram at the image plane in the case of \( V_1 = -297.917 \) volts, \( V_2 = 0 \) volts, \( V_3 = 5 \) kV and \( V_4 = 10 \) kV as calculated by MIRROR_DA.}
\end{figure}

4. Conclusions

We have developed the DA method for the simulation of mirror systems, and based on this a software package MIRROR_DA was developed. For electron mirror systems, because there is a reflection in the electron path and large ray slopes occur near the turning point, the axial position is no longer suitable as the independent variable and the electron trajectory equation used in conventional lens theory is no longer feasible. We use time instead of axial position as our independent variable, and a reference ray is also employed. A single DA ray is traced in the fields of the mirror system, performed on non-standard number space \( nD \), and all aberrations coefficients can be obtained to arbitrary order and with extremely high accuracy. This looks somewhat "automatic", since with the DA method the enormous effort to derive explicit formulae for the aberration coefficients of electron mirrors is avoided. The MIRROR_DA package includes a main program MIRDA for computing optical properties in the mirror system by DA method, and a post-processing program DASP for plotting spot diagrams of the aberrations at the mirror screen plane.

An example of tetrode mirror has been presented to demonstrate our software MIRROR_DA. The electrostatic fields of the mirror are computed by SOFEM, and the axial potential functions are fitted by HERM1. \( C_s \) and \( C_c \) of this mirror are calculated for a fixed image and object position and various settings of two middle electrode voltages. From the results of MIRROR_DA, it has been shown that when adjusting these voltages, \( C_s \) and \( C_c \) change signs from positive to negative, and their values vary in a wide range, therefore this mirror can be used to cancel \( C_s \) and \( C_c \) of round lenses.
References