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# A new monochromator with multiple offset cylindrical lenses 2: Aberration analysis and its applications

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ABSTRACT

In this article, we continue our investigation and offer a complementary discussion of our newly proposed monochromator (MC). It consists of multiple offset cylindrical lenses and achieves high performance with a simple structure. We simulate beam profiles in an extensive current range by means of a ray trace method. Through a multiple regression analysis, we derive the aberrations of the MC up to the third rank. The second-order aperture aberration and lateral energy dispersion are canceled on the exit image plane, which is a crucial condition when MCs are applied to electron microscopes. These aberrations enable the interpretation of the beam profiles for various currents and energy deviations. In addition, they provide the dependencies pertaining to the MC performance, such as the energy spread and brightness, of beam currents for various source conditions. This information is essential to implement the MC onto an electron microscope. By improved the spatial resolutions and energy resolutions, the microscope can reveal new information about various specimens. In addition, the simple and robust structure of the MC will satisfy the demand from industry. Additionally, this study contributes to charged particle optics theory in that it presents a practical example of aberration computation, of which the optics is too complicated to establish aberration integrals, through the ray trace method and regression analysis.

## 1. Introduction

Monochromators (MCs) are important optical components for advanced electron microscopes. MCs generate monochromatic beams, which improve spatial resolutions in (scanning) transmission electron microscopy ((S)TEM) and scanning electron microscopy (SEM). They also enhance the energy resolutions of electron energy loss spectroscopy (EELS) in microscopes with energy analyzers. Thus far, various types of MCs have been proposed, evaluated and commercialized.

Historically, MCs have frequently been used in high-resolution electron energy loss spectroscopy (HREELS) to analyze specimen surfaces in the reflection mode [1]. In an analysis of a thin specimen by transmitted electrons, Schröder et al. achieved 4–6 meV at 25 keV with an MC in conjunction with a retarding Wien filter [2]. Terauchi et al. integrated the same type of MC into a TEM optics [3,4]. Later, Mook et al. proposed MCs with thin Wien filters placed in the high-voltage region of an electron gun [5,6]. Batson achieved an energy resolution of 61 meV at 100 keV in STEM with the MC [7]. Similarly, various types of gun Wien filters have been proposed [8–13]. Rose proposed an electrostatic Ω-shaped MC in an electron gun. This MC consists of four toroidal deflectors [14]. A symmetric configuration and the curvatures of toroidal electrodes can cancel not only the energy dispersion but also all second-order geometric aberrations at the exit plane of the MC. An energy resolution of approximately 40 meV at 200 keV was confirmed by TEM with an imaging energy filter [15,16]. Krivanek et al. proposed an MC with an α-shaped configuration of three magnetic sectors in the ground potential, where numerous multipoles among these sectors increased the energy dispersion and canceled second-order aberrations [17,18]. Recently, they improved the energy resolution to 10 meV with a probe size of 1 nm at 60 keV, successfully revealing the phonon spectra of several materials, such as h-BN and $SiO_2$, with a high spatial resolution [19].

With regard to applications of MCs to SEM, Barth estimated an improvement in the probe size through reduced chromatic terms in ideal optics [20]. Afterward, an MC with a modified gun lens was commercialized [21,22]. The use of off-axial chromatic aberrations of the lens results in an energy spread of 0.15 eV for Schottky emitters and sub-nm image resolutions for the SEM at 1 keV. This MC is considered to be a modification of the Möllenstedt energy analyzer [23].

As described above, many varieties of MCs have been realized thus far. These MCs improve the spatial resolution by eliminating the contributions of the chromatic terms, specifically in the lower energy region, where the radiation damage to specimens can be reduced [24]. They also improve the energy resolution in EELS,

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revealing new information pertaining to the bandgaps, excitons, and dielectric properties of materials on the nanometer scale [25]. Therefore, the MC is regarded as an essential component in the latest electron microscopes. It is worthwhile to investigate new MCs to achieve further improvements for the next generations of these instruments. In addition, industry applications require simple and robust structures for MCs.

In a previous article, we proposed a novel MC with a high energy resolution and a simple structure [26]. It consists of two electrostatic cylindrical lenses (CLs) in a highly excited retarding mode, similar to a Möllenstedt energy analyzer [23]. There, we derived first-order matrix of offset CLs, showing that multiple CLs with a specified position can serve as MCs. In addition, we reported the beam profiles and energy resolutions of the MC by a ray trace method. This article will complement and advance the previous discussion. We will derive aberration coefficients up to the third rank, estimate fundamental performance of the MC, such as the brightness, and apply the results to various source conditions. These results are necessary to implement this MC in microscopes. In addition, the method of deriving the aberration coefficients has meaning in relation to charged particle optics theory. It enables to deal with optics in unified theory despite the fact that the aberration integrals of some of the components are unknown. We will discuss the MC and its optics in detail in the following sections.

## 2. Methods

In charged particle optics, aberration coefficients can be derived by the following methods: aberration integrals, differential algebra, and ray tracing. The use of aberration integrals is a traditional and common method, where aberration coefficients are derived by solving aberration integrals with paraxial rays and axial potentials [27]. Berz introduced differential algebra in charged particle optics [28]. Recently, this method has been applied to calculate aberrations in various areas of optics, such as a mirror corrector [29]. Compared with the two methods above, there has been little research on the ray trace method, although Hawkes noted that it can be useful for systems for which the aberration integrals are numerous or very complicated or even unknown [30]. Kasper applied least squares fitting to compute the aberration coefficients by means of a ray trace simulation [31]. Martínez et al. showed that this method has sufficient accuracy on third- and fifth-order aberrations by comparing its results to those of analytical solutions [32]. Van der Stam et al. described a generalized method that can be used in various optical components, including sector magnets [33]. Recently, Lencová et al. developed commercial software which includes the functions of the method [34], and Oral et al. examined its accuracy on the fifth-order aberrations of a two-tube lens [35]. This method became practical only recently because thousands of rays can be calculated in much less time (measured in minutes or even seconds) due to increases in the computation speeds of PCs.

In this study, we adopt the ray trace method, as the optical axis of the MC passes through a complicated electric field distribution with steep changes in the off-axis region of the CLs. We utilize EO-3D software by MEBS Ltd. [36]. This software can compute 3D electrostatic potential distributions for any electrode shapes by the finite difference method. The accuracy of the potential distributions was confirmed to be 1% or better. The software can derive electron trajectories in the potential distributions by solving the equation of motion directly:

$$\frac{d}{dt}(m\boldsymbol{v}) = -e\boldsymbol{E}\,. \tag{1}$$

where $m$ is the mass of electron, $\boldsymbol{v}$ is the velocity of electron, $e$ is the elementary charge, and $\boldsymbol{E}$ is the electrostatic field. With parameters of position ($x$, $y$, $z$) and velocity ($v_x$, $v_y$, $v_z$) of the electron, Eq. (1) is considered as six first-order ordinary differential equations. The software solves them with a standard fourth-order Runge–Kutta formula, and the solution algorithm was confirmed to be stable, accurate and reliable.

Our simulation method can be described as follows. Initially, the initial conditions of the positions, angles, and energies are randomly generated within specified ranges. For each initial condition, the ray of an electron beam is simulated by the ray trace method. From the trajectories, a number of positions ($x$ and $y$) of particles are read out at specified $Z$ positions as outputs. As a result, the relationships between the initial conditions and the outputs are acquired. Considering geometric symmetry of the optics, the types of aberrations are determined. This is done because some coefficients are canceled due to the symmetry. In this study, we adopt the definition of aberrations by Wollnik [37]. By submitting the initial conditions into functions of these aberrations, explanatory variables are calculated. The outputs are considered as response variables. By applying a multiple regression analysis to these variables, the aberration coefficients of the MC are obtained. Here, we use the statistics tools available in Microsoft Excel. Based on statistical significance levels and contribution amounts, the dominant aberration coefficients are selected. This is a brief outline on the method used to calculate the aberrations of the MC.

## 3. Results

### 3.1. MC with multiple offset CLs

In the previous article, we proposed a new MC with multiple offset CLs [26]. A CL consists of three electrodes with rectangular openings in the center. This offers a stronger focusing effect in the $X$ direction of the shorter side of the openings and a weaker one in the $Y$ direction of the longer side. Here, electrons travel in the $Z$ direction. The detailed dimensions of the CLs are as follows: the thickness of the electrodes, the gap between the electrodes, and the shorter side of the opening are 10 mm, and the longer side of the opening is 100 mm. Fig. 1 shows schematics of this MC, including two cylindrical lenses (CL$_1$, CL$_2$), two round transfer lenses (TL$_1$, TL$_2$), two apertures, and an electron emitter. Simplified rays ($x_\alpha$, $y_\beta$, $x_\gamma$, $y_\delta$, $x_\kappa$), the incident angles ($\alpha$, $\beta$, $\gamma$, $\delta$), the optical planes ($Z_0$–$Z_4$), and the focal lengths ($f_c$, $f_1$, $f_2$) are also shown. These optical components are located at specified distances, as shown in Fig. 1. Two CLs are arranged in mid-plane symmetry with $Z_2$. They are offset by $X_d$ from the optical axis of a microscope in the $X$ direction. Subsequent discussions adopt the following values: $f_c = 40$ mm and $X_d = 0.407$ mm, where the excitation voltages of the CLs ($V_{CL}$) are $-0.248$ kV from the emitter in the case of incident energy of 4 keV. TL$_1$ collimates the beams from the emitter, and TL$_2$ focuses the beams on exit plane $Z_4$. The focal lengths of the TLs, $f_1$ and $f_2$, are 10 mm. The entrance aperture limits the angles ($\alpha$, $\beta$) from the emitter, which define incident currents $I_{in}$ into the MC. The energy selection aperture filters energy-dispersive rays out of zero-loss rays at $Z_2$. The total optics of the MC becomes symmetrical with middle plane $Z_2$.

The schematics in Fig. 1 show that the trajectories are identical in the $X$ and $Y$ directions on the regions of $Z_0$–$Z_1$ and $Z_3$–$Z_4$, but they take different optical paths in the region of $Z_1$–$Z_3$ due to the astigmatic focusing power of the CLs. In the $X$ direction, the $x_\alpha$ ray is asymmetric, and $x_\gamma$ ray is symmetric with middle plane $Z_2$. In a similar way to our previous article, we adopt the ray-tracing method for the CLs in the region of $Z_1$–$Z_3$, which are difficult to be treated in a conventional manner, and utilize first-order matrices for the TLs in the regions of $Z_0$–$Z_1$ and $Z_3$–$Z_4$ [26]. For the simulations, the following initial parameters are adopted: incident energy $E_0$, incident currents $I_{in}$, and number of trajectories $n$. In the