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Calculation of the performance of magnetic lenses with limited machining precision

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1. Introduction

High resolution scanning transmission electron microscopy requires very accurate shaping of the objective lens pole pieces in order to produce a focused round spot on the sample. The objective lens pole pieces are typically made with tolerances of 1 μ m on the crucial regions of the design, which is at the edge of current machining technology. Even with such an extreme mechanical precision, parasitic aberrations are generated, deforming the beam shape. To minimize the influence of these aberrations, correcting elements are used.

The beam shape and the errors due to different pole piece mechanical imperfections can be calculated in order to understand which correction is needed and under which conditions it will be possible to reach an ultimate HR-STEM resolution. In today's best microscopes the resolution is in the order of magnitude of Ångstroms.

2. Theory

The standard treatment of the electron optics assumes an ideal optical system free of mechanical imperfections. Such an ideal form cannot be realized using current manufacturing techniques. The

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ABSTRACT

To meet a required STEM resolution, the mechanical precision of the pole pieces of a magnetic lens needs to be determined. A tolerancing plugin in the EOD software is used to determine a configuration which both meets the optical specifications and is cost effective under the constraints of current manufacturing technologies together with a suitable combination of correction elements.

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highest mechanical precision which is reproducible and costeffective is in the order of magnitude of micrometers, and only high-end machining tools can produce parts with a precision up to a half of micrometer. This requires a sophisticated equipment with a tightly controlled environment, operated by appropriately trained personnel. Additionally, strict final inspection of the machined parts is necessary to select those fulfilling the requirements.

An overview of methods for calculation of parasitic aberrations and their influence can be found in [1,2]. However published papers deal with electrostatic lenses. To determine the minimum precision of a pole piece for a given purpose, one needs to model the perturbations of the field, resulting from mechanical imperfections, acting on the electrons. That has been published by Munro for electrostatic lenses [3]. Using the same technique for magnetic lenses published by Sturrock [4], boundary conditions of the reduced magnetic potential on pole pieces, $\Psi_m = \Phi_m/r^m$, where Φ_m is the scalar magnetic potential, can be defined [5].

The boundary conditions caused by an ellipticity are

$$P_2 = -H_r E$$
,

where $E = e \exp(i2\theta)$ is a complex parameter characterizing the size of the ellipticity and its rotation (see Fig. 1). On material surfaces without ellipticity, $\Psi_2 = 0$.

The boundary conditions caused by a misalignment are

 $\Psi_1 = -H_r S$,

where $S = s \exp(i\theta)$ is a complex parameter characterizing a misalignment shift in the plane perpendicular to the axis (see Fig. 1).





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For a tilt of a pole piece around the point z_c , the following boundary condition holds:

$$\Psi_1 = [rH_z - (z - z_c)H_r]T,$$

where $T = t \exp(i\theta)$ is a complex parameter characterizing the tilt and its rotation around the *z*-axis (see Fig. 1) and $\vec{H}(r, \varphi, z) = (H_r, 0, H_z)$ is the magnetic field of the lens.

On the axis of symmetry and outer boundaries of the calculation region, $\Phi_m = 0$. Reduced potential is then calculated using the first order Finite Element Method for the Laplace equation for the *m*-th multipole component [6]:

$$\frac{\partial^2 \Psi_m}{\partial r^2} + \frac{2m+1}{r} \frac{\partial \Psi_m}{\partial r} + \frac{\partial^2 \Psi_m}{\partial z^2} = 0.$$

3. Influence of mechanical imperfections of $0.25~\mu m$ and $0.5~\mu m$ on lens performance

As an example of the procedure for calculating the influence of mechanical imperfections on the spot size, consider the 200 kV objective lens presented by Tsuno [7] in 1986. This lens was also studied by Lencová and Wisselink [8] and it is a standard example part used in Electron Optical Design (EOD) software [5]. (The full geometry and the magnetization curves used are available as supplementary data.) A graded mesh with 100 000 mesh points was used to calculate the magnetic flux density. Double deflectors

and stigmators were added to simulate a standard STEM configuration (Fig. 2). These calculations were made in EOD 3.155 with the tolerancing plug-in [5]. Excitation of the lens was decreased from 16 000 A-turns to approximately 10 500 A-turns in our case for HR-STEM.

The spatial arrangement of the lens, stigmators and deflectors is shown in Fig. 2 with a detailed view on the pole pieces. Parameters of the saddle coils of stigmators and deflectors are described in detail in Table 1. Axial field functions are shown in Fig. 3.

The equation of motion for electrons was solved using the Runge–Kutta–Fehlberg method of the 7th–8th order, with a relative accuracy of 10^{-14} . The EOD uses quadrupole-precision arithmetic to improve the solution accuracy. The field was interpolated using the radial series expansion about the axis using the axial field data, which gives correct field values near the axis and enables a fast computation with the precision of the particle position in the image plane of about 1 pm.

The object position was put to $z_0 = -130$ mm and the Gaussian image plane was set to z=0 mm. The spot was observed and optimized at the Scherzer defocus plane $z_i = -45.8$ nm. The spherical aberration of the objective lens in this configuration was $C_S=0.59$ mm and the angular magnification is $M_a = 69.95$. The optimal semi-angle of the beam limited by the spherical aberration and the diffraction in the image plane is $\alpha = 10$ mrad.



Fig. 1. Definition of mechanical imperfections - (a) ellipticity, (b) misalignment and (c) tilt.



Fig. 2. Setup of the objective lens, the stigmators and the deflectors. Details of the pole pieces and the tolerance regions A and B. Left-slanted hatching – general iron, rightslanted hatching – permendur, cross-hatching – coil. Left solid rectangle – region A, right solid rectangle – region B, vertical lines – Y deflectors, horizontal line – X deflectors, crossed lines – stigmators.

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