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Aberration Analysis Calculations for Synchrotron Radiation Beamline Design

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ABSTRACT

The application of ray deviation calculations based on aberration coefficients for a single optical surface for the design of beamline optical systems is reviewed. A systematic development is presented which allows insight into which aberration may be causing the rays to deviate from perfect focus. A new development allowing analytical calculation of lineshape is presented.

Keywords: beamline design, aberrations, ray tracing

1. INTRODUCTION

Is intuition is needed for the complicated task of beamline design? The number of surfaces, apertures, gratings, and other components provide so many parameters that the designer does not really know if the best system has been reached by ray tracing without supplementary information which provides insight. In addition, the recent high-resolution spectra which have been obtained with grazing incidence systems require that the focusing properties of spherical grating monochromators (SGMs) be understood in more detail. Figure 1 shows such a spectrum where it is not clear without careful analysis how much of the width of the absorption features is due to the inherent aberrations of the optical system or how much is due to figure errors on the grating in the SGM.1

2. ADVANTAGES OF ABERRATION ANALYSIS

Terms like defocus, coma, and astigmatism have definite hooks into the intuition of the designer. The aberration analysis method allows the effects of individual terms in the wave front curvature to be seen. Calculation for a single surface is fast, and is easily done by a simple computer program. Aberration balancing, or cancellation, can be achieved by developing experience about what types of surface produces what type of aberration.

3. DISADVANTAGES OF ABERRATION ANALYSIS

The major drawback of the aberration term method is that only one surface can be treated accurately. Because the field terms from both the object and the image appear in the coefficients, it has not been possible to uniquely propagate ray deviations between separate elements. Koike et al.2 have given a method in which nine rays are traced through a complete multi-element system, and the shape of the wavefront is inferred by fitting polynomials to the optical path difference at
Figure 1. High Resolution Absorption Spectrum of Helium taken at the Advanced Light Source with a Spherical Grating Monochromator
each ray. This gives the coefficients for the entire system, and provides numerical, but not analytic expressions for the aberration coefficients. Bahrdt\textsuperscript{3} laboriously solves the implicit ray deviation equations numerically, obtaining numerical results which allow the definition of matrices which can represent each surface and be multiplied together for an entire system. These complications may remove much of the calculation beyond the intuition of the designer.

Furthermore, the coefficients may not mean exactly the same thing to each designer, because of the ambiguity in the naming of the aberrations in the grazing incidence case. In the case of coma, which is a third-order aberration including a field variable in the axially symmetric Seidel aberration set, there is disagreement on what to call what. Howells has proposed the name "aperture defect" for the third-order tangential term for the non-axially symmetric extreme off-axis case in order to remedy the situation.\textsuperscript{4}

4. Equations

We first write down the familiar optical path equation for a single mirror/grating. AP and PB are the geometrical distances from the source point to the optical surface, and from the optical surface to the image point. Nmλ allows for the fact that, for a grating different pieces of the converging wavefront at the image point leave the source at different times. (A grating is a wave front slicer/recombiner.)

\[ F = AP + PB + Nmλ. \]

The first term of this may be written as\textsuperscript{5}

\[ F = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} F_{ijk} y^i z^j z^k. \]

The \( F_{ijk} \) s are the aberration coefficients, \( y \) and \( z \), the aperture variables, and \( z_a \) is the out-of-plane height at the object point. The second term is similar, with substitution of image angle and distance for those of the object point, and the corresponding out-of-plane height at the image. When Fermat's principle is applied, the first-order terms of the complete expansion give the grating equation which incorporates the Nmλ, and move the image point out of the principal plane in case of a finite field coordinate. Terms of interest to the construction of spot diagrams begin with the second order which is defocus. or, "the image is focused but not where you want it." The aberration coefficients are functions of the conjugate distances, angles, shape of the optical surface, and field heights.

The shape of the surface enters through the "sag" of the optical surface in question, expressed through the "\( a_{ij} \)" coefficients. These can be readily derived from geometry or looked up in the literature. They allow the sag to be expanded in the two aperture variables, \( y \) in the tangential direction, and \( z \) in the sagittal direction on the optical surface. The table below gives \( a_{ij} \) coefficients for "bicycle tire" toroids. R and \( \rho \) are the major and minor radii, respectively.\textsuperscript{6,7}
Finally, the individual ray deviations which are caused by each term in the aberration expansion are found by applying Fermat's principle—taking the derivative of the optical path function with respect to the two aperture variables and multiplying by the distance from the pole of the mirror/grating to the image point. In the cases most interesting to the synchrotron community, the tangential ray deviation must be divided by the cosine of the reflection/diffraction angle. This comes from the coordinate transformation to the image plane, and is a direct consequence of the grazing incidence.

5. THEY ADD!

Figure 2 shows the main point of this review. For the high f/# grazing incidence systems used most often for synchrotron radiation applications, the final ray-traced spot's position is the simple sum of all of the individual ray deviation terms with a one-to-one correspondence with the aberration coefficients. Figure 2a shows all that can be garnered from a ray trace: that the ray got there. In Figure 2, y prime and z prime are coordinates in the image plane of the surface. Figure 2b, on the other hand, shows that for the fictional single element system in question, the ray arrived off the perfect focus in the tangential direction because of $F_{20}$, which is defocus, and $F_{30}$, which is "coma/aperture defect." It arrived in the image plane off the perfect focus in the sagittal direction by $F_{20}$, which is astigmatism, and $F_{40}$, which many call higher order astigmatism. Knowing this, the designer can have at least a beginning idea of how to combat the aberrated performance. Over time, the designer can develop an expert-knowledge base, which we call intuition.

6. ADDING IN THE OTHER EFFECTS

Other effects must be added to model the complete shape of a spectral feature. Figure 3 shows the fundamental difference between what we have discussed so far and the next effect to be
Figure 2 Comparison of ray trace and aberration-based calculations

Figure 3 Finite image size from aberrations (A), and finite image size from source size (B)
considered, which is the contribution of finite slit size. The light from the point source is imaged with defects to a blurred spot in the figure, (point A). Each point on the grating/mirror sends the ray from the object point to a slightly different place in the image plane. On the other hand, if the source has a finite width, each point on the grating/mirror will receive light over a small spread in incidence angles, and even with zero aberration, the image will have a finite width (B). At large enough slit widths this effect will dominate, and so it is generally not included in the "quick and dirty" style aberration calculator which we are reviewing here. It is readily calculated by multiplying the entrance slit width by the grating magnification in the tangential direction, and converting to wavelength or energy units with the dispersion relation, if the optic is a grating.

Of more importance to the modeling of high resolution measurements such as those in Figure 1 are the effects of diffraction and the distribution in angle of the radiation from the source. For narrow slits, the amount of light which reaches the grating along the tangential direction is often to a great extent determined by the diffraction from the entrance slit. This may be modeled accurately enough for our purposes by using a Gaussian shape. It is important to do this, because coma/aperture defect, for example, varies as the square of the tangential field coordinate on the grating. A ray from the edge of the grating will miss the center of the image by a much greater distance than a ray which hits the middle of the grating. If the distribution of light is considered to be constant across the grating, the calculated point-source response image will be much too large.

Of equal importance for synchrotron-related applications, the distribution of the light from the source in the tangential direction has the same effect. If the source of illumination is an undulator, the light may be concentrated in the center of the grating, where aberrations are much smaller. A wiggler or bending magnet source, depending on the magnetic parameters, may fill the entire grating much more fully, resulting in a much larger aberrated point-source response. These two effects, which spread the beam onto places on the optic which map the ray farther from the ideal image point, diffraction and source distribution, are very profitably convoluted together into the point-source-response in a quick aberration-based single-surface calculator.

7. LINESHAPE CALCULATIONS

These two important effects may be added together analytically. Hettrick and Underwood² show lineshapes for three lower-order aberrations, although a systematic procedure was not given. Padmore has recently contributed a scheme where the shape of the intensity distribution across the exit slit may be analytically calculated.² This is shown in Figure 4. The top graph plots the ray deviation calculated from the point-source response as a function of the grating field coordinate in the tangential direction. It is labeled in energy units. The vertical bar near the vertical axis represents the width in volts of a narrow slit which is to be analytically scanned over the exit image. As we move the bar up, we first contact the ray intercept curve along tangent line A. The fact that this tangent line is horizontal translates into a very high intensity at that point in the slit. The concept is fully illustrated at point C, where the horizontal lines at each edge of the narrow energy range intercept the curve and "collect" only a small amount of the intensity at that point in the slit. The ray deviation curve was deliberately chosen to be multi-valued for this figure.
Figure 4 Inference of exit image distribution from aberrations and intensity distribution in angle
(coma/aperture defect combined with another aberration, for example), to illustrate what occurs at point B. Here rays from both sides of the center of the optic are deviated in the same direction at the slit, and a jump in the slit-scan distribution can occur at this point of transition. Below B, light arrives with the same ray deviation from two points on the grating, and above B, light arrives from only one point on the grating. The full interpretation of high-resolution spectra as shown in Figure 1 requires the inclusion of these effects.

8. SUMMARY

We have briefly reviewed the advantages and disadvantages of the simple calculation of ray deviation distances from individual aberrations terms in the light path function expansion for a single reflecting mirror or grating. These individual ray deviations add together, for the grazing incidence region, to give insight into the focusing behavior of these optics. Recent analytical results should allow the approximate de-convolution of instrumental broadening from the natural shape of high-resolution spectral features.

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