HIGH HEAT FLUX X-RAY MONOCHROMATORS: WHAT ARE THE LIMITS?

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ABSTRACT

First optical elements at third-generation, hard x-ray synchrotrons, such as the Advanced Photon Source (APS), are subjected to immense heat fluxes. The optical elements include crystal monochromators, multilayers and mirrors. This paper presents a mathematical model of the thermal strain of a three-layer (faceplate, heat exchanger, and baseplate), cylindrical optic subjected to a narrow beam of uniform heat flux. This model is used to calculate the strain gradient of a liquid-gallium-cooled x-ray monochromator previously tested on an undulator at the Cornell High Energy Synchrotron Source (CHESS). The resulting thermally broadened rocking curves are calculated and compared to experimental data. The calculated rocking curve widths agree to within a few percent of the measured values over the entire current range tested (0 to 60 mA). The thermal strain gradient under the beam footprint varies linearly with the heat flux and the ratio of the thermal expansion coefficient to the thermal conductivity. The strain gradient is insensitive to the heat exchanger properties and the optic geometry. This formulation provides direct insight into the governing parameters, greatly reduces the analysis time, and provides a measure of the ultimate performance of a given monochromator.

Keywords: x-ray monochromators, synchrotron radiation, undulators, high heat flux optics

1. INTRODUCTION

Insertion device beamlines at modern synchrotron sources produce narrow, highly collimated x-ray beams of unparalleled intensity. First optical elements, typically single-crystal silicon monochromators, are subjected to enormous heat fluxes. The challenge for optical designers is to develop monochromators that are not greatly thermally strained and thereby preserve the beam brilliance. The typical coolants that have been used to cool high heat load monochromators include, water, He gas, liquid metals, and liquid nitrogen. Monochromator crystals may be either directly or indirectly cooled. Numerous integral heat exchanger designs have been developed, including circular and rectangular cooling channels ranging in hydraulic diameter from several mm to about 50 μm. Other designs include jet cooling and numerous forms of porous matrices. A series of review papers on high heat load x-ray optics was included in a recent edition of *Optical Engineering.*[1]

To predict the performance of a particular monochromator design, the thermal strain gradient under the footprint of the beam and its impact on diffraction must be determined. The method most often used to calculate the thermal strain is finite element analysis (FEA). This technique can provide very accurate predictions of the temperature, stress and strain fields for complicated geometries and boundary conditions, which can then be used in a diffraction simulation to calculate the reflectivity of the monochromator crystal. The drawbacks to FEA are that it is very time consuming, computationally demanding, requires an expensive analysis program and a high degree of engineering expertise. Additionally, FEA does not readily provide a clear indication of the relative importance of the physical parameters.

In this paper, equations expressing the normal strain and strain gradient of the top surface of a cylindrical, three-layer monochromator crystal with a heat flux incident on the faceplate are presented. These equations are used to simulate the performance of a liquid-gallium-cooled silicon monochromator exposed to the beam from an undulator, and the results are compared to experimental data.

2. MATHEMATICAL MODEL

Many actively cooled x-ray monochromators consist of three layers: a faceplate, heat exchanger, and baseplate. For internally cooled monochromators, the heat exchanger may consist of a series a circular channels, rectangular slots, or some generalized porous matrix. Additionally, monochromator crystals are often indirectly cooled by placing them in contact with a cooled, usually copper, block. An In-Ga eutectic is often used to provide good thermal contact. The model presented here is applicable for any of these cases.

A closed-form algebraic solution for the thermal stress and strain in a finite cylinder of radius, b, exposed to a narrow cylindrical beam of radius, r_0, with uniform heat flux, q_0, at the center of the top face, was developed in Ref. 2. A schematic of the cooled monochromator is shown in Fig. 1. The cylinder is free from external loads. The lateral surface is thermally insulated, and the material is homogeneous and isotropic with no volume sources. The normal strain and the radial strain gradient of the top surface under the beam footprint are given by,

$$\delta z(r,0)\Big|_{r<r_0} = \frac{q_0 r_0^2(1+\nu)}{4}\frac{\alpha(T)}{k(T)}\left[\frac{1-\nu}{1+\nu}\left(1-\left(\frac{r}{b}\right)^2\right)-\left(\frac{r}{r_0}\right)^2+2\ln\left(\frac{b}{r_0}\right)+1\right], \tag{1}$$

$$\frac{\partial z}{\partial r}(r,0)\Big|_{r<r_0} = -\frac{q_0 r_0^2(1+\nu)}{2}\frac{\alpha(T)}{k(T)}\left[\frac{1-\nu}{1+\nu}\frac{r}{b^2}+\frac{r}{r_0^2}\right], \tag{2}$$

where ν is Poissons' ratio, the linear coefficient of thermal expansion is α, and k is the thermal conductivity. The strain under the beam footprint is parabolic and the strain gradient is linear. For completeness, the normal strain and the radial strain gradient of the top surface outside the beam footprint are given by the following equations,

$$\delta z(r,0)\Big|_{r\geq r_0} = \frac{q_0 r_0^2(1+\nu)}{4}\frac{\alpha(T)}{k(T)}\left[2\ln\frac{b}{r}+\frac{1-\nu}{1+\nu}\left(1-\left(\frac{r}{b}\right)^2\right)\right], \tag{3}$$

$$\frac{\partial z}{\partial r}(r,0)\Big|_{r\geq r_0} = -\frac{q_0 r_0^2(1+\nu)}{2}\frac{\alpha(T)}{k(T)}\left[\frac{1}{r}+\frac{1-\nu}{1+\nu}\frac{r}{b^2}\right]. \tag{4}$$

It should be noted that the strain and strain gradient are determined primarily by the magnitude of the absorbed heat flux and the crystal thermophysical properties (α/k) irrespective of the cooling boundary condition or the thickness of the faceplate. Hence, equations 1 - 4 may be used to determine the strain gradient of a cylindrical monochromator without solution of the heat equation. However, because the thermophysical properties are a function of temperature, it may be necessary to determine the temperature distribution if the temperature increase is significant.

There are essentially only three parameters that can be adjusted by the designer to reduce the strain gradient under the beam footprint: reduce the heat flux and/or the expansion coefficient, and/or increase the thermal conductivity. Various methods can be used to reduce the heat flux including using asymmetric[3] or inclined[4,5] crystals to decrease the incidence angle thereby spreading out the beam footprint. Also, a prefilter or mirror[6] can sometimes be used to reduce the heat flux on the monochromator. The thermophysical properties of monochromators can be enhanced by using either diamond and/or operating single-crystal monochromators at cryogenic temperatures.

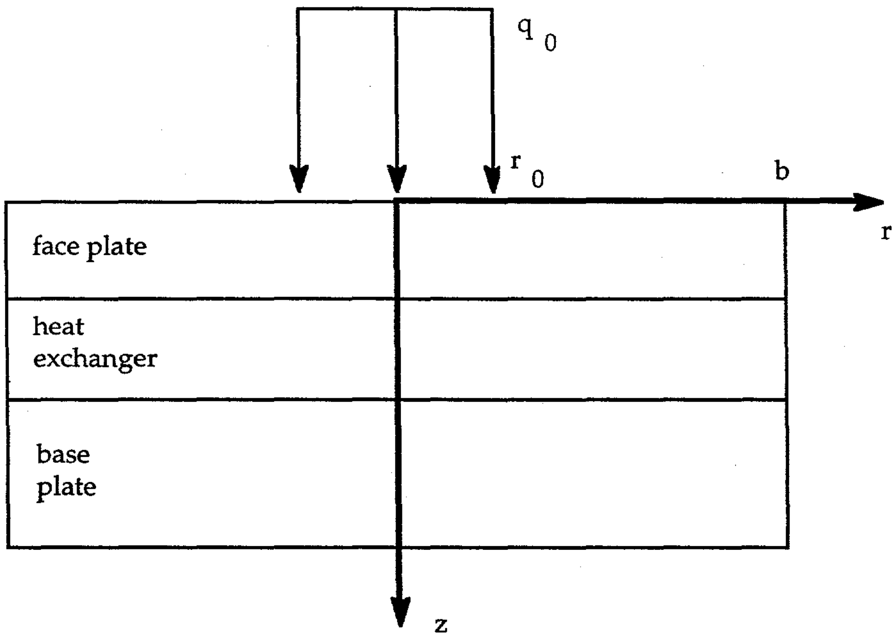

Fig. 1. Schematic of cooled monochromator consisting of a faceplate, heat exchanger, and base plate. A uniform cylindrical heat flux, q_0, with radius, r_0, is incident at the center of the faceplate surface.

The figure of merit, α/k of diamond is more than an order of magnitude better than that of silicon. Additionally, due to its smaller atomic number, it absorbs less of the incident x-ray power. Indirectly edge-cooled diamond monochromators have been tested using a focused undulator beam to a total power of 280 W (8.7 W absorbed) and incident peak power density of 3.5 kW/mm^2 (108 W/mm^2 absorbed) with no thermal degradation of the monochromatic beam.[7] However, diamond monochromators have found limited used so far due to the difficulty in obtaining diffraction-quality samples of useful size and orientation. The figure of merit of traditional silicon monochromators can be greatly improved by cooling them to cryogenic temperatures. The thermal conductivity of silicon increases by a factor of nine at liquid nitrogen temperature compared to room temperature. Also, the expansion coefficient decreases as the temperature is lowered going through zero at about 125 K and remaining slightly negative. Therefore, a silicon monochromator operated at 100 K can handle a heat flux about 40 times greater than the same crystal at room temperature due to the improved thermal properties.

The performance of a real monochromator crystal will depend on the effectiveness of its heat exchanger. It has been shown above that the strain gradient does not depend directly on the heat transfer coefficient or the thickness of the faceplate. However, the thermal design of the cooled monochromator should be such that the temperature rise is kept reasonably small because the ratio α/k increases with temperature. The temperature under the beam footprint of a poorly cooled crystal will be larger, thereby increasing the magnitude of the strain gradient via the influence of the material properties. Also, the coolant interface temperature must remain below the coolant saturation temperature to eliminate the possibility of boiling. The faceplate thickness is chosen so as to take advantage of the radial spreading of the heat, and this depends on the thermal conductivity of the faceplate and the heat transfer performance of the heat exchanger. Consequently, for cryogenic crystals, the optimum faceplate thickness is much larger than for a room temperature crystal. The two-dimensional, axisymmetric temperature field in a cylindrical, three-layer system has been solved and may be used in conjunction with the strain equations to optimize the monochromator crystal design.[8] The ultimate performance of the monochromator is determined by eq. 2 for α/k evaluated at the coolant temperature.

3. COMPARISON TO MEASUREMENTS

In order to determine the accuracy of the above model, a comparison to experimental data was made. An internally cooled, silicon monochromator crystal was previously tested using an undulator beam at CHESS.[9] The crystal was cooled with liquid gallium flowing through a series of rectangular channels just below the diffraction surface. The temperature field, normal strain, and strain gradient were calculated as a function of the storage ring current. The absorbed power was calculated to be 3.07 W/mA at 5 keV. The storage ring energy was 5.433 GeV, and the undulator gap was set at 17 mm corresponding to a first harmonic at 5.14 keV. The monochromator was 18 m from the source, and a total of 1 mm of Be attenuated the incident beam. The power distribution from an undulator is approximately Gaussian shaped. For the simulation, the beam size was cylindrical with a diameter given by the FWHM of the Gaussian power distribution. The magnitude of the uniform heat flux of the cylindrical distribution, q_0 was calculated so as to preserve the total absorbed power. The normal strain and radial strain gradient for the top surface of the gallium-cooled monochromator are shown in Fig. 2 for several values of the current.

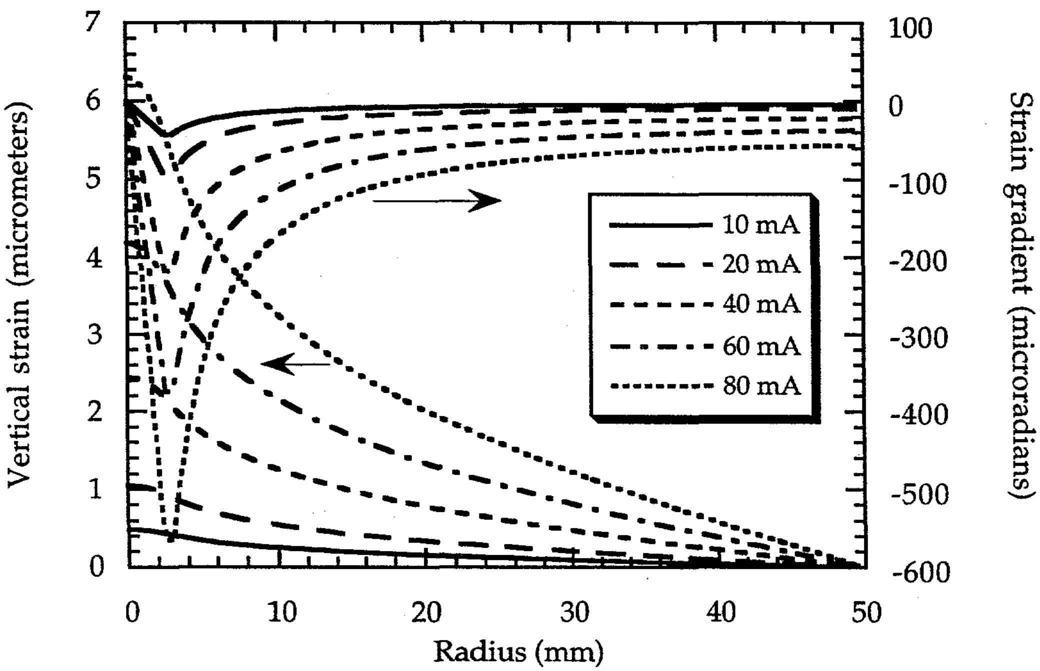

Fig. 2. Calculated normal strain and radial strain gradient of top surface as a function of radial position for several values of the stored current. The source was the CHESS/ANL undulator. The monochromator crystal was cooled by 1 gpm of liquid gallium at an inlet fluid temperature of 323 K. The Bragg angle was 23.3°.

A diffraction simulation program was developed using dynamical diffraction theory to calculate the reflectivity from the strained crystal and the resulting double-crystal rocking curve. The perfect crystal diffraction simulation program InPro, one of the programs bundled within XOP, was modified to calculate the reflectivity from the thermally strained crystals.[10] The methodology used was to assume that each part of the crystal diffracts as if it were perfect; however, the incidence angle is different at each radial position due to the strain gradient. This results in an angular shift of the peak of the reflectivity. The crystal under the beam footprint is segmented, and the reflectivity is calculated for each segment, multiplied by the normalized incident flux at that radial position and then summed over the rocking angle to find the integrated reflectivity. The resulting strained crystal reflectivity is normalized so that the integrated reflected power equals that from an undistorted crystal. The rocking curve is calculated by the convolution of the strained and perfect reflectivities. The measured and simulated rocking curve widths (FWHM) are shown in Fig. 3 for the first- and third-order reflections at 5 keV and 15 keV, respectively. The predicted values of the rocking curve width are in excellent agreement with the measured values over the entire range of currents.

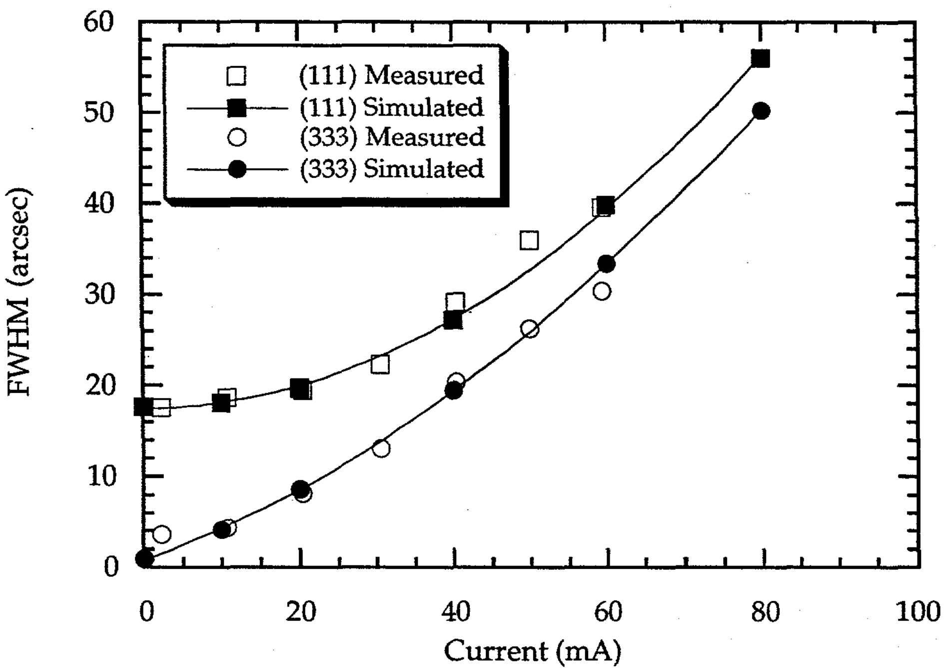

Fig. 3. Comparison of simulated and measured rocking curve widths (FWHM) for a Si(111) oriented monochromator as a function of machine current using the CHESS/ANL undulator. The crystal was cooled with liquid gallium flowing at 1 gpm. The crystal was set at a Bragg angle of 23.3° to diffract at 5 keV.

4. LIMITING HEAT LOAD

The above expressions, coupled with the solution of the heat equation and the diffraction simulation, provide the means to determine the performance for a given monochromator. However, eq. 2 can be used to estimate the ultimate performance for an infinitely cooled monochromator. This situation is approximated by a very thin faceplate and a highly effective heat exchanger (e.g., liquid metal cooling, microchannels, nucleate boiling). Assuming that the strain adds in quadrature with the Darwin width, one can choose an effective average strain, here taken to be the value computed at $r_0/3$, to determine the rocking curve width. If the strain gradient under the beam footprint is specified so that it should not exceed a certain fraction of the Darwin width, $x\omega_s$, then eq. 2 is solved for the maximum allowable current. A value of $x = 0.5$ results in the rocking curve being broadened by approximately 25%. For a silicon monochromator $(\nu \approx 0.2)$ where $r_0 << b$, the maximum allowable current is given by,

$$I_{\max} = \frac{5\pi\, FWHM_p\, x\, \omega_s}{2Q'\, sin\theta_B} \frac{k(T)}{\alpha(T)}, \tag{5}$$

where, $FWHM_p$ is the full width at half maximum of the beam power envelope, ω_s is the Darwin width, Q' is the power per mA, and θ_B is the Bragg angle. The material properties are evaluated at the fluid temperature.

Calculated using eq. 5, the maximum allowable current as a function of energy for a room temperature silicon monochromator at the APS using undulator A is shown in Fig. 4. The Si(111) monochromator is positioned at 29 m from the source. The beam size at normal incidence at the crystal was 2.0 x 2.5 (V x H) mm^2, and the allowable broadening of the reflectivity was taken to be one-half of the Darwin width. Prefilters consisting of 170 μm of diamond, 300 μm of graphite, and 500 μm of Be attenuated the white beam removing about 12% of the emitted power. What is shown is the first-order reflection from the (111) planes while tracking the first and third harmonic. At 3.28 keV (gap = 11.0 mm), the current should not exceed 20 mA. Not until about 11.5 keV (gap = 23.4 mm) can the monochromator handle 100 mA.

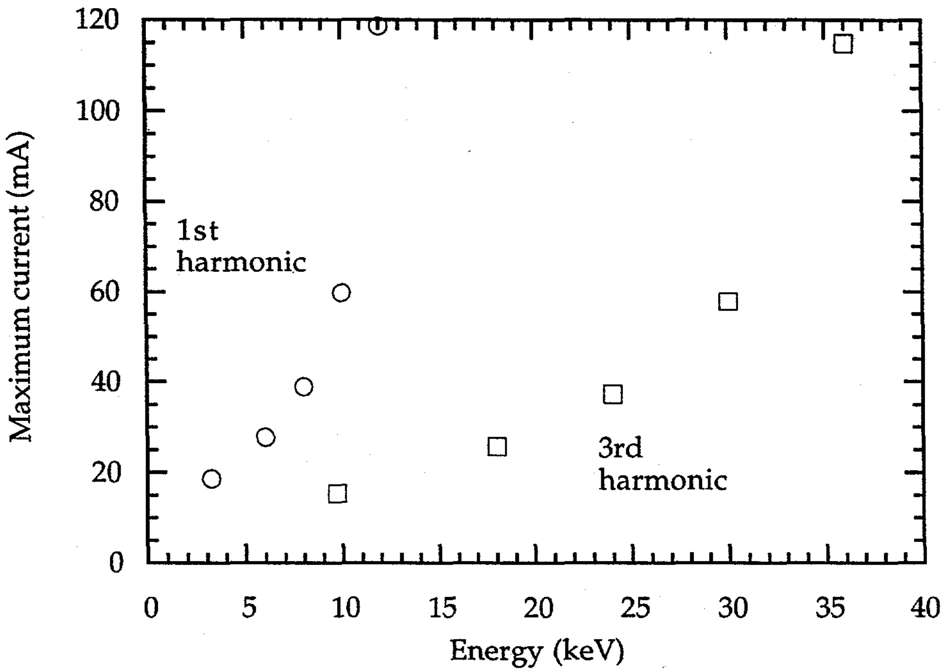

Fig. 4. Maximum allowable current calculated using eq. 5 for a room temperature Si(111) monochromator diffracting from the (111) planes using APS undulator A. The beam size was 2.0 x 2.5 (V x H) mm^2 at the crystal position of 29 m from the source. The allowable reflectivity broadening was one-half of the Darwin width.

5. CONCLUSIONS

It has been shown that the solution presented for the thermal strain gradient accurately predicts the performance of an internally cooled x-ray monochromator exposed to an undulator beam. The calculated rocking curve widths agree extremely well with the measured values over a wide current range. Coupled with the solution of the heat equation, the equations given in this paper may be used to predict the performance of a large class of high heat flux x-ray optics. This set of equations allows the optimization of a monochromator design that is not readily achievable with FEA. In addition, it provides a clear indication of the fundamental limits of high heat flux monochromators. It is shown that it is not possible for a room temperature silicon monochromator operated in the standard Bragg reflection geometry, regardless of how well it is cooled, to function adequately with an unattenuated undulator beam at the APS.

Future work will include an extension of the model to rectangular systems and the modeling of x-ray mirrors. The thermal performance limits and optimized designs of high heat flux x-ray optical components will be determined for various coolant and heat exchanger systems. The optimized geometry of room temperature and cryogenic optics can be quite different due the much greater radial expansion of heat in the cryogenic system and the poorer heat transfer properties of liquid nitrogen.

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