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**Modeling of the Performance of a Liquid-Gallium-Cooled Silicon Monochromator
for a High-Energy-Resolution Scattering Beamline -
Comparison with Experimental Data***

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Modeling of the performance of a liquid-gallium-cooled silicon monochromator for a high-energy-resolution scattering beamline - Comparison with experimental data

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ABSTRACT

A finite element analysis method (FEA) was used to predict the performance of a silicon monochromator for a high-energy-resolution scattering beamline at sector 3 of the Advanced Photon Source (APS). The monochromator is internally cooled through 17 rectangular channels with liquid gallium and is designed to operate at photon energies near 14 keV, under beam from a 2.7 cm period undulator. The atomic planes of the monochromator have a (111) orientation with an asymmetric cut angle of 4.5° . The displacement profile calculated from the structural FEA was used to compute the double-crystal rocking curves at 14.41 keV. Both the simulations and the experiment show that this monochromator will operate at about 40 mA with rocking-curve broadening of only about 0.5 arsec. This corresponds to a surface heat flux of 1.2 W/mm^2 (i.e., 20 W/mm^2 at normal incidence) and a total absorbed power of about 86 watts. The monochromator was used for the commissioning of the beamline and to perform the first series of experiments up to 100 mA. In this paper, we give the results of the FEA calculations and diffraction simulations and compare these to the experimental data.

Keywords: Finite element analysis, liquid-gallium-cooled monochromator, synchrotron radiation optics, high heat load.

1. INTRODUCTION

The first optical component in the high-energy-resolution scattering beamline¹ at sector 3 of the Advanced Photon Source (APS) is a double-crystal silicon monochromator. This beamline uses a 2.5-m-long undulator with a 2.7 cm period and is designed to operate near 14 keV photon energy. When tuned

to the first harmonic at 14.41 keV, this undulator generates an x-ray beam with a total power of 470 W at 7 GeV energy and 100 mA ring current. In order to optimize thermally induced distortions and also to prevent breaking, the first crystal of the monochromator has to be cooled. For this purpose, a liquid-gallium alloy composed (by mass) of 61% gallium (Ga), 25% indium (In), 13% tin (Sn), and 1% zinc (Zn) was used.

Liquid gallium has relatively good physical properties compared to water, which makes it an attractive fluid as a coolant. Its thermal conductivity is 0.28 W/cm-K at 29.8 °C, its specific heat is 397.5 J/kg-K (in liquid state), and its vacuum pressure is low enough (10^{-12} Torr at 100 °C and 10^{-11} Torr at 300 °C) to make it relatively safer than water for use in high vacuum. In addition, gallium becomes liquid at 29.8 °C, and, when it is alloyed with indium to its eutectic form (76% Ga-24% In, by mass), the melting temperature is lowered to 16°C and it becomes liquid at room temperature. Further alloying of gallium with Sn and Zn (61% Ga, 25% In, 13% Sn, and 1% Zn, by mass) lowers the melting point to 10 °C.

It has been shown² that the rocking curve, at 5 keV, of a symmetric Si (111) double-crystal monochromator cooled with liquid gallium through rectangular channels, starts to broaden when was subjected to a surface heat flux of 4 W/mm² and a total power of about 80 W from an undulator beam. An asymmetric monochromator cut to an angle, α , will reduce the normal incidence heat flux by a factor of $1/\sin(\theta - \alpha)$ compared to a factor of $1/\sin\theta$ (where θ is the Bragg angle) for a symmetric one. The current design (see section 2) has an asymmetry angle of 4.5°. If set to diffract 14.41 keV from (111) planes (Bragg angle = 7.9°), the normal incidence heat flux (53 W/mm² at 100 mA) is reduced (by a factor of 16.86) to about 3.1 W/mm². This value of surface heat flux is less than the value used in reference 2. However, the rocking curve of an asymmetrically cut monochromator ($\alpha < 0$) is much narrower than that of a symmetric one. Therefore, we expect the thermal strain to have a higher impact in the studied monochromator at the nominal parameters of the ring (i.e., 100 mA current and 7 GeV energy). However, considering the fact that a gallium pump³ is available at the APS and a reliable pumping system requiring a low maintenance can be easily constructed, the expected performance of the monochromator was considered satisfactory as a first step for the commissioning of the sector 3 beamline.

2. THE MONOCHROMATOR DESIGN

The design of the first crystal of the monochromator is shown in Figure 1. It is made from a 38 mm x 45 mm x 70 mm silicon block and is cooled through seventeen rectangular channels, located 1 mm below the diffracting surface, perpendicular to the scattering planes. The fabrication and other aspects of the monochromator are detailed elsewhere.⁴ The crystal is asymmetrically cut to a 4.5° angle in order to spread the heat flux and at the same time increase the crystal's angular acceptance.

3. ANALYSES AND RESULTS

3.1. The 3-D FEA model and results

Using ANSYS 5.1,⁵ a 3-D model was developed to predict the thermal and structural performance of the first crystal of the monochromator. The crystal is located at 29.5 m from the source. At a ring current of 100 mA and 7 GeV energy, the normal incidence heat flux at this location is about 53 W/mm². The total incident power is limited to 203 watts by a 4 mm x 2 mm slit opening. At 14.41 keV (i.e., the first harmonic of the undulator), the Bragg angle for Si(111) is 7.9° (thus, an incidence angle of 3.4 °). In this case, the surface heat flux is reduced to 3.2 W/mm².

Because of the low grazing incidence angle, the incident power profile was assumed to have been totally absorbed on the crystal surface. A heat transfer coefficient of 16 W/cm²-K was applied to the walls of the channels and was calculated for 1 gpm flow rate using the Lyon's correlation for liquid metals:⁶

$$Nu=7.0 + 0.025Re^{0.8} Pr^{0.8} ,$$

where Nu is Nusselt number, Re is the Reynolds number, and Pr is Prandlt number.

Temperature dependent properties of silicon were used. Temperature fields calculated with the finite element thermal analysis for several ring currents were used as an input to compute the crystal's distortion profile using the structural FEA model. The results are summarized in Table 1. For comparison, peak temperatures measured with an IR camera⁴ are also given

and agree well with the calculated values. Figure 2 shows the temperature profile calculated at 39 mA ring current. Figure 3 presents the distortion profile on the crystal surface, along the scattering plane, calculated at the same current. The slope error was found to vary quite linearly with the heat flux.

3.2. Effect of the thickness of the faceplate and the cooling channels

The distortion profile of the monochromator, presented in Figure 3, exhibits a waviness superimposed on the mapping distortion (thermal bump). This waviness, which has a peak-to-valley value of $1 \mu\text{rad}$ (0.2 arcsec.) at 39 mA current, is due to thermal effect of the channels located 1 mm below the diffracting surface. Its magnitude was not found to be critical for the rocking curves. However, flux measurements performed under the undulator beam showed that it was significant enough to alter the beam profile at the sample.⁴

To analyze this problem, a finite element analysis was conducted on a general case in which a channel's width is equal to the thickness of the wall between two consecutive channels. The results show that the smoothness of the slope error profile is always achieved when the ratio (faceplate-thickness/channel-width) is at least equal to a factor of two. It was also found that this ratio does not depend on the heat flux. Figure 4 shows the slope error profile of the monochromator with a 2-mm-thick faceplate (i.e., with a ratio of faceplate-thickness/channel-width = 2). The waviness has been dramatically reduced compared to the case with a 1-mm-thick faceplate presented in Figure 3. Note, however, that the peak slope error under the beam footprint has increased from $8 \mu\text{rad}$ for the 1 mm faceplate to $12 \mu\text{rad}$ for the 2-mm faceplate. Therefore, this study suggests that choosing narrower channels will lead to a smaller faceplate thickness, thus minimizing the crystal's temperature and the mapping distortion. Moreover, by doing so, a larger number of channels can be machined underneath the beam footprint, thus further improving the heat transfer.

4. ROCKING CURVES: SIMULATION AND EXPERIMENT

The main criterion that is used to measure the performance of an x-ray double-crystal monochromator is the value of the FWHM of its rocking curve (RC). A strained monochromator will have its rocking curve broadened compared to that of an unstrained one. A program⁷ has been developed to simulate the rocking curves of a distorted monochromator. It uses the dynamical diffraction theory, and the distortion profile, generated by a FEA code, is used as an input. Rocking curves for a double-crystal monochromator are obtained by convoluting the reflectivity profile of the distorted first crystal and that of an unstrained second crystal. Figures 5a and 5b compare calculated and measured RCs at 39 and 95 mA ring current. For reference, the rocking curve for an unstrained monochromator is also shown. Table 2 summarizes both simulated and experimental data. Note that the rocking curve at 39 mA shows only a slight broadening (0.5 arcsec.) compared to that of an unstrained monochromator, and the simulation is in excellent agreement with the experimental data obtained up to 50 mA current. At 95 mA, the simulated FWHM of the RC is 4.3 arc seconds, while the measured value was 6.3 arc seconds. The asymmetric shape of the experimental RC at 95 mA is due to the fact that the beam position was not centered relative to the vertical slits, thus leading to an asymmetric power load profile. The center of the beam was much closer to one of the edges of the vertical slits, as was revealed by the temperature profile recorded by an infrared camera placed on the top of the crystal to view the beam footprint.⁴ This results in an asymmetric slope error profile relative to the center of the beam, thus reflected in the shape of the rocking curve. The large discrepancy between the calculated and the measured FWHM of the RC at 95 mA, could be, therefore, partially explained by the fact that the central cone of the undulator radiation incident upon the crystal surface is experiencing a much sharper slope error than predicted for a symmetric power load. The location of the beam position relative to the slits was not known, and so the exact experimental conditions could not be accurately simulated. Among other contributing factors to this discrepancy could be the heating of the second crystal, but there were no measurements to ascertain this.

5. CONCLUSION AND SUGGESTIONS

The FEA calculations and diffraction simulations have been used to predict the performance of a gallium-cooled monochromator with internal rectangular cooling channels. The results were compared with the experimental data. Both the simulation and experiment agree that the monochromator will operate up to about 40 mA ring current, with a RC broadening of only about 0.5 arsec. This corresponds to 1.2 W/mm^2 surface heat flux (i.e., a normal incidence peak heat flux of 20 W/mm^2), and a total absorbed power of 86 watts. The FEA calculations show that, in order to avoid the thermal effect of the cooling channels, the thickness of the faceplate should be at least twice the width of a channel.

For future development, narrower channels should be considered because they will allow a thinner faceplate, and in addition a larger number of channels can be machined under the heated surface, thus improving the heat transfer. However, due to the finite size of the footprint, the mapping distortion will still be a limiting factor at higher heat flux. Note also, that because liquid gallium is a relatively dense fluid ($\rho=6 \text{ g/cm}^3$), the difficulty of it flowing through a cooling channel increases as the channel's size becomes smaller, and the pressure-induced deformation might not be negligible.

Other alternatives consist of use of a diamond monochromator⁸ or cryogenically cooled silicon.⁹⁻¹⁰ At room temperature, single crystal diamond has a figure-of-merit (k/α) (where k is the thermal conductivity and α is the expansion coefficient) similar to that of a single silicon crystal at liquid-nitrogen temperature. Therefore, a diamond monochromator can be operated near room temperature with less sophisticated cooling equipment (water pumping instead of liquid-nitrogen pumping). In addition, a diamond monochromator has a narrower synchrotron radiation bandpass and thus is suitable for a high-energy-resolution synchrotron beamline.

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Table 1. Results of the FEA thermal and structural analyses at 14.41 keV: I is the ring current, F is the normal incidence peak heat flux, Tcal-mx and Texp-mx are the calculated and measured peak temperatures, respectively, ΔT_1 is the calculated maximum temperature difference across the crystal surface in the tangential (or beam) direction, ΔT_2 is the calculated maximum temperature across the thickness of the face plate, Ψ_1 and Ψ_2 are the calculated tangential and sagittal peak slope errors on the crystal surface, respectively. Here, Texp-mx was measured using an infrared camera.

I (mA)	Power (W)	F (W/mm ²)	Tcal-mx (°C)	Texp-mx (°C)	ΔT_1 (°C)	ΔT_2 (°C)	Ψ_1 (μ rad)	Ψ_2 (μ rad)
39	82	20.4	39.3	-	9.3	5.7	8.4	16.9
50	102	25.5	41.5	35.0	11.6	7.1	10.4	21.1
95	194	49.5	54.1	47.5	23.2	15.2	20.8	43.7

Table 2. Simulated and measured rocking curve (RC) widths at 14.41 keV for several ring currents. I is the ring current, F is the normal incidence peak heat flux. The FWHM for an unstrained asymmetric-cut Si(111) double-crystal monochromator is 2.83 arcsec.

I (mA)	Power (W)	F (W/mm ²)	FWHM of RC, simulated (arc sec.)	FWHM of RC, measured (arc sec.)	Broadening of RC (arcsec.)
39	82	20.4	3.2	3.3	0.5
50	102	25.5	3.4	3.6	0.8
95	194	49.5	4.3	6.3	3.5

Figure 1: Design of the first crystal. Seventeen $0.472'' \times 0.1181''$ ($1.2 \text{ mm} \times 3 \text{ mm}$) channel were ultrasonically machined $0.039''$ (1 mm) below the diffracting surface, perpendicular to the scattering plane.

Figure 2. Temperature profile calculated, using ANSYS, for 39 mA ring current (i.e., for 86 watts and 1.2 W/mm^2 absorbed power and surface peak heat flux, respectively) for 1/4 of the crystal.

Figure 3. Displacement and slope error profiles along the crystal center line, calculated at 39 mA (i.e., corresponding to 86 watts power and 1.2 W/mm^2 surface heat flux). The faceplate is 1 mm thick. The waviness of the slope error is due to the thermal effect of the cooling channels.

Figure 4. Displacement and slope error profiles along the crystal center line, calculated at 39 mA (i.e., corresponding to 86 watts power and 1.2 W/mm^2 surface heat flux). Here the faceplate is 2 mm thick. Note that the magnitude of the waviness of the slope error due the cooling channels is dramatically reduced compared to the 1 mm faceplate case.

a)

b)

Figure 5. a) Simulated and b) measured rocking curves versus current at 14.41 keV (Si(111), with an asymmetric-cut angle of 4.5°). They both show very little broadening (0.5 arcsec.) at 39 mA, which corresponds to a surface peak heat flux of 1.2 W/mm^2 and a total absorbed power of about 86 watts. The rocking curve for an unstrained silicon double-crystal monochromator is shown for reference. The gallium alloy flow rate was 1 gpm, and the undulator was tuned the first harmonic at 14.41 keV.