Adaptive optics for high power beamlines using diamond crystal monochromators

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BNL--48490

DE93 009328

ABSTRACT

Preserving the high source brightness of the third generation of synchrotron radiation facilities will require that thermal and pressure deformations of the monochromator crystals be maintained within a few arc-seconds. Recent experiments at the National Synchrotron Light Source (NSLS) have demonstrated the potential of adaptive crystal optics to cope with high power densities. In this technique the crystals deformations are minimized both by an efficient water-jet cooling and by externally applied pressure loads. Thermal deformation can be reduced further with diamond crystals because of their high thermal conductivity and low coefficient of thermal expansion. In this paper we describe the results achieved by optimization of adaptive crystal optics for diamond crystals.

1. INTRODUCTION

A typical undulator beam of the third generation of synchrotron light sources will deposit highly concentrated heat flux at the first monochromator crystal. With power density exceeding 100 watt/mm^2 , and total power in a K watt range, the incident beam can result not only in unacceptably large thermal deformations, but also in crystal failure due to high thermal stresses. Several approaches are being pursued to solve this challenging problem. In one approach attention is focussed on improving the efficiency of cooling systems, e.g., by liquid gallium as the cooling medium¹, microchannel cooling², and cooling by jets^{3,4}. Another approach is to reduce the power density on the crystal by using an inclined geometry^{5,6}. Thermal deformations can also be reduced by using monochromator crystals with significantly higher thermal conductivity, e.g. silicon crystals at cryogenic temperatures⁷, or diamond crystals (natural Type IIa, or synthetic)⁸. Adaptive optics techniques^{9,10}, in which external pressure or bending moments are applied on the crystals to counteract the thermal deformations, have also been used with promising results.

A diamond crystal monochromator, designed to be cooled by an impinging water-jet and pressurized to adaptively correct for deformations, offers most of the advantages of different approaches mentioned above. In this paper we present analytical results that were obtained to optimize this design and to estimate the maximum slope errors.

2. DIAMOND TYPE IIa CRYSTAL MONOCHROMATOR

Diamond has the highest thermal conductivity of all known materials at room temperature. The thermal conductivity of high purity natural diamond, Type IIa (less than 300 ppm nitrogen, and effectively free of other impurities) is typically 20 watts/cm/K at room temperature. It increases with decreasing temperatures, reaching a peak value of approximately 120 watts/cm/K at 70 K , a cryogenic temperature that can be achieved with liquid nitrogen (LN2) cooling system. Fig. 1 shows thermal conductivity values for diamond Type IIa and silicon¹¹ in the temperature range 70 to 400 K . The thermal conductivity of diamond is one order of magnitude higher than that of silicon in this temperature range. Furthermore, diamond exhibits only a gradual decrease in

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*Work performed under the auspices of the U.S. Department of Energy, under contract DE-AC02-76CH00016.

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its thermal conductivity above room temperature. This ensures that run-away thermal condition, whereby increasing temperatures result in lower thermal conductivity which leads to even higher temperatures, is unlikely to occur with diamond crystals.

Thermal coefficient of expansion (α) for diamond is comparatively small. Fig. 2 compares α values for diamond and silicon¹¹. The figure of merit for thermal strains, k/α where k denotes thermal conductivity, for diamond Type IIa is $20 \times 10^6 \text{ watts/cm}$, compared to $0.6 \times 10^6 \text{ watts/cm}$ for silicon at room temperature. At cryogenic temperatures both material have practically zero thermal coefficient of expansion.

Diamond can also withstand high temperatures in an inert atmosphere without graphitization or loss of strength. Temperatures of up to 1800 K are achievable before these effects are detected¹². Consequently, high temperatures in localized regions, such as directly under the beam footprint, can be tolerated.

Additionally, diamond is one of the hardest materials having both high elastic moduli and a high fracture strength. The elastic moduli at room temperature, taken as averages of data reported in the literature^{12,13}, are

$$C_{11} = 10.60 \times 10^5 \text{ MPa}$$

$$C_{12} = 2.28 \times 10^5 \text{ MPa}$$

$$C_{44} = 5.20 \times 10^5 \text{ MPa}$$

These values result in a Young's modulus $E_{11} = 10.35 \times 10^5 \text{ MPa}$. The coefficient of anisotropy $2C_{44}/(C_{11} - C_{12})$ is 1.23, which means that Young's modulus is fairly constant in all orientations. In comparison, Young's modulus E_{11} and coefficient of anisotropy for silicon are $1.91 \times 10^5 \text{ MPa}$ and 1.44, respectively. The higher Young's modulus for diamond implies that the monochromator crystal would be less susceptible to deformations from external forces such as coolant pressure, vibration of drive mechanisms, and residual stresses due to fabrication. On the other hand, it also means that thermal stresses would be high since these are proportional to Young's modulus. However, because of its very high compressive strength, $\sigma_f \geq 8.6 \times 10^3 \text{ MPa}$, diamond is strong in resisting high thermal stresses. An important factor in comparing thermal resistance is the ratio $\sigma_f/E_{11}\alpha$. At room temperature this ratio for diamond is two order of magnitude higher than that for silicon.

Diamond Type IIa crystals of sizes up to 10 mm in diameter and 1 mm in thickness are readily available from commercial sources¹⁴. Specifications on parallelism and surface roughness for highly polished faces are less than 5 minutes of arc and 400 Å, respectively. Specific crystallographic orientations can be obtained within 3 degrees. Crystal edges may be metallized by RF sputtering for brazing to metallic substrates. The cost of a diamond Type IIa crystal is not prohibitively expensive when compared to the total cost of a typical high power undulator beamline. This is due to the small footprint of an undulator beam which allows the use of a small crystal, typically no larger than 10 mm in diameter. A crystal thickness of less than 0.5 mm is sufficient as discussed later in this paper.

3. IMPINGING WATER-JET COOLING

When a crystal wafer is cooled from the reverse side of its reflecting surface, its bending deformations are practically independent of the efficiency of the cooling scheme. This is the case even if the beam profile (assumed to be axisymmetric) is comparatively small resulting in a two dimensional heat transmission in the crystal⁹. Nevertheless, an efficient cooling scheme is necessary in order to remove the heat from the crystal and to ensure that the maximum heat flux at the crystal-coolant interface is below the critical heat flux (CHF).

It is impractical to fabricate complex cooling channels or manifolds within diamond platelets due to size limitations and extreme hardness of diamond. Impinging circular water jets provide highly efficient cooling with simple hardware that can be accommodated in a restricted space. The heat transfer mechanism in impinging jets has been studied extensively in the literature¹⁵, so that reasonably good estimates can be made for Nusselt number and critical heat flux for a given crystal-jet configuration. In the present analysis we use equations developed by Liu, Lienhard and Lombara¹⁶ for the Nusselt numbers, and by Monde and Inoue¹⁷ for CHF values. A jet with a nozzle diameter of 3 mm is assumed to which water is fed at constant pressure from a thermostatic reservoir. The water velocity and, therefore, the Reynolds number (Re) at the jet depend on the height of the reservoir above the crystal. Different Reynolds numbers were used in the analyses to investigate the effect of cooling efficiency.

4. SCHEMATIC DESIGN

Fig. 3 shows the schematic design of a water-jet cooled crystal monochromator. A diamond crystal (1), its diameter between 6 to 10 mm and thickness between 0.1 to 1 mm, is brazed to a copper frame (2). The diamond crystal is cooled by a water jet (3) which is placed co-axially within a connecting bar (4) holding the copper frame. The connecting bar is mounted on two cross-slides to provide high-precision angular adjustments to the diamond crystal with respect to the incident beam. This approach, that is using a connecting bar on cross-slides for precise angular motions, has been used successfully in some previous designs¹⁸. Bellows (5) allow for relative motion of the crystal while isolating the beam tube (6) from ambient air. The beam tube with beryllium windows on both sides can be pressurized with helium for compensating the crystal deformations adaptively.

5. ANALYTICAL RESULTS

(a) Finite Element Model

A two-dimensional axisymmetrical model of the diamond crystal was developed using the ANSYS finite element program. The copper frame to which the crystal is brazed was not included in the model for simplicity. This precludes transfer of heat from the diamond crystal to the copper frame. Additionally, the crystal edge was allowed to expand and rotate freely relative to the copper frame (i.e., simply supported edge). Both of these approximations are conservative in the sense that the crystal temperatures and deformations are over-estimated.

The power profile projected on the crystal was assumed to be Gaussian with circular symmetry, and full-width half-maximum (FWHM) of 1 mm. A peak power density of 100 watts/mm² was used resulting in a total incident power of 112 watts. Power absorbed in the crystal was calculated assuming an incident beam of 10 KeV. For crystal thickness values of 0.10 mm, 0.25 mm, 0.50 mm, 0.75 mm and 1.00 mm, the fraction of absorbed power¹⁹ was 0.07, 0.17, 0.30, 0.42 and 0.51, respectively. As an approximation the absorbed power was deposited at a plane quarter of the thickness away from the reflecting plane.

Several parametric analyses were performed to investigate the effects of crystal dimensions and cooling efficiency on the temperature and deformation fields in the crystals. In order to evaluate these effects we first describe the results for a representative case emphasizing features that are common for all the cases.

(b) Representative Results

A diamond crystal with 8 mm diameter and 0.5 mm thickness was selected for the representative case. The crystal was cooled by a 3 mm water jet with a jet velocity of 3.18 m/sec ($Re=10,000$). Fig. 4(a) shows the axisymmetric finite element model consisting of 306 nodes and 264 elements. The model represents one-half of a radial section through the crystal. Rotational axis of symmetry for both the crystal and the incident beam is Y-axis as shown in the figure.

Temperature rise contours in the crystal are plotted in Fig. 4(b). A maximum temperature rise of 30.4 K is obtained at the center on a crystal plane where the heat is deposited. Temperature drop across the crystal thickness is very small because of the high thermal conductivity of diamond. For instance, the maximum temperature drop is only 1.7 K at the center. Almost the entire temperature rise is, therefore, at the thermal boundary layer of the water jet. Radially (along X-axis), the temperature rise decreases gradually to a minimum of 21.6 K. The radial temperature rise is composed of two components: a constant temperature rise and an approximately Gaussian temperature rise. The first component is dominant due to a relatively high resistance to heat flow at the crystal-jet interface (thermal boundary layer) as compared to heat flow in the radial direction.

Thermal deformation of the crystal, magnified for clarity, is shown in Fig. 5(a). Since the temperature rise in the crystal is mostly uniform, the crystal deformation is characterized by thermal expansion with essentially no bending. The crystal expands radially and in thickness by approximately 0.10 and 0.02 microns, respectively. Similar to the temperature rise, the change in thickness has a very small Gaussian component along the radial direction. This thickness variation, known as the thermal bump, introduces thermal curvature to the reflecting plane. As shown in the figure, the thermal bump for the present case is small and results in a thermal curvature of only 0.9 arc-second.

Thermal stresses in the diamond crystal are low due to both a small temperature rise and simply supported boundary conditions assumed at the crystal edge. Fig. 5(b) shows effective (von Mises) thermal stress contours which basically follow the pattern of temperature contours in Fig. 4(b). The maximum stress is only 4.2 MPa for the radially unconstrained crystal. If the crystal is assumed to be radially constrained, the effective stress increases to 45 MPa. Even this higher value is, however, small compared to the fracture strength of diamond, approximately 10,000 MPa.

(c) Effect of Cooling Efficiency

Bending deformations in small diameter silicon crystals have been shown to be essentially independent of the cooling efficiency⁹. As mentioned above, thermal curvature error in a diamond crystal is largely due to the thermal bump under the beam footprint. Since the temperature rise is directly related to the cooling efficiency, a closer look was taken on the relationship between the cooling efficiency and thermal curvature.

The cooling efficiency was varied by changing the Reynolds number of the water jet. Reynolds numbers of 5,000, 10,000, and 20,000 were used which are equivalent to water velocities of 1.59, 3.18 and 6.36 m/sec, respectively, for a jet of 3 mm nominal diameter. The corresponding film coefficients in the stagnation region of the jet¹⁶ are 0.027, 0.039 and 0.055 watts/mm².K. Calculated values for the critical heat¹⁷ flux are 8.7, 10.8 and 12.3 watts/mm², respectively.

Fig. 6 shows maximum temperature rise in the crystals for the three Reynolds numbers. Results are plotted for crystal thickness values in the range 0.1 mm to 1.0 mm. The figure shows that for a crystal of specific thickness, the temperature rise increases with decreasing Reynolds number. Since the temperature rise occurs mainly across the thermal boundary layer, it decreases almost linearly with respect to the film coefficient values. For all Reynolds numbers, maximum temperature rise increases with increasing thickness. Even though thicker crystals facilitate radial flow of heat, they also intercept higher percentages of the incident beam power. In diamond crystals the latter effect dominates the temperature rise.

Temperature rise at the boundary layer (not shown in Fig. 6) is also higher for thicker crystals. For 1 mm crystal the calculated values at the center of beam footprint are 50.7 K, 42.6 K and 31.1 K, respectively, for Reynolds numbers of 5,000, 10,000 and 20,000. Heat flux values across the boundary layer are 1.38, 1.64 and 1.69 watts/mm².K for the three cases. These are considerably lower than the corresponding critical heat flux values given above.

Thermally induced curvature is plotted in Fig. 7 as a function of the crystal thickness. The

curvature grows with increasing thickness and is essentially proportional to the absorbed power in the crystals. Curvature errors of less than an arc-second are obtained for crystal thickness of less than 0.5 mm. As shown in the figure, the thermal curvature is practically independent of Reynolds numbers, i.e. the cooling efficiency. Because of the high thermal conductivity of diamond Type IIa, a change in cooling efficiency results in a basically uniform temperature change across the thermal boundary layer and in the crystal. Thermal gradients in the crystal are, therefore, not changed appreciably. Since the thermal curvature is directly related to the thermal gradients, it also shows little variation with changing Reynolds numbers.

(d) Effect of Crystal Diameter

The cost of a diamond crystal rises exponentially with its size. The thermal performance of the crystal was, therefore, evaluated as a function of its diameter. The diameter of the crystal was varied from 6 to 10 mm while its thickness was kept constant, 0.5 mm. Reynolds number of 10,000 was assumed for the water-jet velocity.

Fig. 8 depicts maximum temperature rise in the crystal versus its diameter. The temperature rise decreases from 43.5 K to 23.8 K as the diameter increases from 6 mm to 10 mm. This decrease is due to the larger surface area of the boundary layer through which the absorbed heat flux is removed. The effect of increasing the crystal diameter is more prominent for smaller crystals since the absorbed power as well as the heat flux through the boundary layer are concentrated at the center.

In spite of a substantial reduction in the maximum temperature, the thermal curvature does not change appreciably with increasing crystal diameter. The curvature decreases from 0.92 arc-second for 6 mm crystal to 0.89 arc-second for 10 mm crystal. These results indicate no significant advantage in using larger crystals when considering only the thermal curvature errors. The size may be governed by other criteria such as the beam size, critical heat flux, surface strains from the boundary constraints, and space requirements for the water jet.

6. ADAPTIVE COMPENSATION FOR CRYSTAL DEFORMATIONS

The total force exerted by an impinging jet is equal to $A_j \rho v^2$, where A_j is the jet area, ρ is the coolant density, and v is the jet velocity. A diamond crystal cooled by a water jet of 3 mm diameter and 3.18 m/sec jet velocity ($Re = 10,000$) will experience a force of 0.007 Kg. Maximum pressure at the center of the jet impingement area will be 5 KPa. The jet pressure will cause significant crystal deformation which, for thinner crystals, may even exceed the thermal deformation. Maximum pressure and thermal deformations at the center of the crystal are compared in Fig. 9 for crystal thickness in the range 0.1 mm to 1.0 mm. As shown in the figure, for thickness of less than 0.2 mm, the deformation due to the jet pressure is more than a magnitude higher than that due to the absorbed power. The two deformations are comparable for crystal thickness of 0.35 mm. In the proposed design, both the pressure and thermal deformations in the crystals may be compensated by adaptively increasing the helium pressure in the monochromator chamber. The chamber is nominally pressurized to 101 KPa to balance the atmospheric pressure on the coolant side of the crystal. The success of this technique has been demonstrated previously for thin silicon crystals⁹.

7. CONCLUSIONS

Analytical results discussed above verify the superior thermal performance of diamond Type IIa crystal monochromators. Thermal curvature errors of less than one arc-second can be achieved with diamond crystals approximately 8 mm in diameter and less than 0.5 mm in thickness. Thinner crystals are shown to have better performance primarily because they absorb lesser amount of the incident power.

The conceptual design presented in the paper is based on a highly efficient impinging water jet cooling. Although the cooling efficiency has been demonstrated to have little effect on thermal

curvature errors, it can be an important consideration at higher incident power because of the critical heat flux limitations. Impinging jet cooling is also amenable to simple and compact design for the crystal monochromator.

Pressure deformations in thin diamond crystals (less than 0.35 mm in thickness) have been shown to be greater than the thermal deformations. Both pressure and thermal deformations can be adaptively corrected by pressurization of the monochromator chamber.

8. ACKNOWLEDGMENTS

One of the authors (S. Sharma) gratefully acknowledges discussions on jet cooling with Dr. D.T. Vader of the IBM corporation, and technical assistance provided by Dr. Al Sheng and Mr. E. Rotela of the Argonne National Laboratory. This work was supported by the US Department of Energy under Contract No. DE-AC02-76CH00016.

9. REFERENCES

1. R.K. Smither, G.A. Forster, D.H. Bilderback, M. Bedzyk, K. Finkelstein, J. White, L.E. Berman, P. Stefan, and T. Oversluizen, "Liquid gallium cooling of silicon crystal in high intensity photon beams," *Rev. Sci. Instrum.*, Vol. 60, pp. 1486-1492, 1989.
2. J. Arthur, W.H. Tompkins, C. Troxel, Jr., R.J. Contolini, E. Schmitt, D.H. Bilderback, C. Henderson, J. White, and T. Settersten, "Microchannel water cooling of silicon x-ray monochromator crystals," *Rev. Sci. Instrum.*, Vol. 63, pp. 433-436, 1992.
3. P. Van Zuylen, A.D. Lemaire and A.J.Th.M.A. Wijsman, "Cooling of crystals for x-ray monochromators," report to European Synchrotron Radiation Facility, Grenoble, France, 1988.
4. L.E. Berman and M. Hart, "Adaptive crystal optics for high-power synchrotron sources," *Nucl. Instrum. Methods Phys. Res., Sect. A*, Vol. 302, pp. 558-562, 1991.
5. J. Hrdy, "Double crystal monochromator for synchrotron radiation with decreased radiation power density," *Rev. Sci. Instrum.*, Vol. 63, pp. 459-460, 1992.
6. A. M. Khounsary, "A novel monochromator for high heat load synchrotron x-ray radiation," *Rev. Sci. Instrum.*, Vol. 63, pp. 461-464, 1992.
7. G. Marot, M. Rossat, A. Freund, S. Joks, H. Kawata, L. Zhang, E. Ziegler, L. Berman, D. Chapman, J.B. Hastings, and M. Iarocci, "Cryogenic cooling of monochromators," *Rev. Sci. Instrum.*, Vol. 63, pp. 477-480, 1992.
8. J. Als-Nielsen and A.K. Freund, "Diamond single crystals as x-ray monochromators for synchrotron radiation," *ESRF newsletter*, No. 13, PP. 4-5, 1992.
9. L.E. Berman, M. Hart and S. Sharma, "Adaptive crystal optics for undulator beamlines," *Nucl. Instrum. Methods Phys. Res., Sect. A* 321, pp. 617-628, 1992.
10. L.E. Berman and J.B. Hastings, "An adaptive crystal bender for high power synchrotron radiation beams," these proceedings.
11. Y.S. Touloukian, R.W. Powell, C.Y. Ho and P.G. Klemens, Thermophysical Properties of Matter, Vol. 2 and 13, IFI/Plenum, New York, 1970.
12. Dubbeldee Harris Diamond Corporation, Properties of Diamond, product literature, Mount Arlington, New Jersey.
13. J.E. Field, The Properties of Diamond, Academic Press, 1979.

14. Dubbeldee Harris Diamond Corporation, private communication, June 1992.
15. H. Martin, "Heat and mass transfer between impinging jets and solid surfaces," *Advances in Heat Transfer*, Academic Press, Vol. 13, pp. 1-60, 1977.
16. X. Liu, J.H. Lienhard V and J.S. Lombara, "Convective heat transfer by impingement of circular liquid jets," *Journal of Heat Transfer*, Vol. 113, pp. 571-582, 1991.
17. M. Monde and T. Inoue, "Critical heat flux in saturated forced convective boiling on a heated disk with multiple impinging jets," *Journal of Heat Transfer*, Vol. 113, pp. 722-727, 1991.
18. M. Shleifer, S. Sharma, E. Rotela and C. Brite, "Design of a high- precision tunable double crystal monochromator," BNL-47194, Informal report, National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York, 1992.
19. D. Chapman, N. Gmur, N. Lazarz and W. Thomlinson, "Photon: A program for the synchrotron radiation dose calculations," *Nu. Instrum. and Meth.*, Vol. A226, pp. 191-194, 1988.

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Figure Captions

Fig. 1. Thermal conductivity versus temperature for diamond Type IIa and silicon¹¹.

Fig. 2. Thermal coefficient of expansion versus temperature for diamond Type IIa and silicon¹¹.

Fig. 3. Schematic of a jet-cooled diamond crystal: (1) diamond crystal, (2) copper frame, (3) water jet, (4) connecting bar, (5) bellows, and (6) beam tube.

Fig. 4. Finite element model of a diamond crystal: (a) Two-dimensional axisymmetric model, (b) Temperature rise contours.

Fig. 5. Finite element results: (a) Crystal deformation, (b) Thermal stress contours.

Fig. 6. Effect of cooling efficiency on the maximum temperature rise in diamond crystals. Cooling efficiency is represented by the Reynolds number of the water jet.

Fig. 7. Effect of cooling efficiency on the thermal curvature in diamond crystals. The curves for the three Reynolds numbers are practically identical.

Fig. 8. Maximum temperature rise versus crystal diameter (thickness = 0.5 mm).

Fig. 9. Maximum pressure and thermal deformations at the center of a diamond crystal (diameter = 8 mm).

Fig. 1

FIG. 7

Fig 3

(a) Finite element model

A=22, B=23, C=24, E=25, F=26, G=27, H=28, I=29, J=30

(b) Temperature rise contours ($^{\circ}$ K)

(a) Crystal deformation

A=1.2, B=1.6, C=2.0, D=2.3, E=2.7, F=3.1, G=3.4, H=3.9, I=4.2

(b) Thermal stress contours (MPa)

FIG. 5

Fig. 9

Fig. 9

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