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Accelerator & Fusion Research Division

Presented at the Conference on Insertion Devices
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October 27-30, 1985

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W.R. Edwards, E.H. Hoyer, and A.C. Thompson

October 1985

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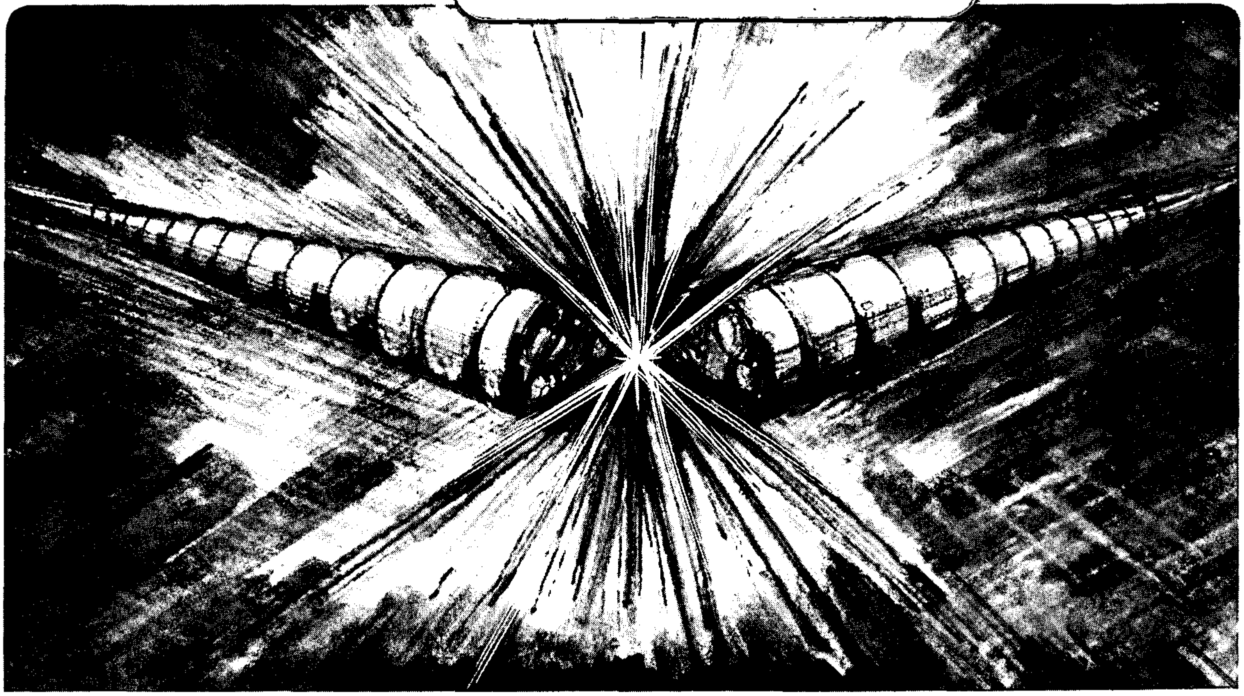

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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Finite Element Analysis of the Distortion of a Crystal Monochromator from Synchrotron Radiation Thermal Loading

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ABSTRACT

The first crystal of the Brown-Hower x-ray monochromator of the LBL-EXXON 54 pole wiggler beamline at Stanford Synchrotron Radiation Laboratory (SSRL) is subjected to intense synchrotron radiation. To provide an accurate thermal/structural analysis of the existing monochromator design, a finite element analysis (FEA) was performed. A very high and extremely localized heat flux is incident on the Si (220) crystal. The crystal, which possesses pronouncedly temperature-dependent orthotropic properties, in combination with the localized heat load, make the analysis ideally suited for finite element techniques.

Characterization of the incident synchrotron radiation is discussed, followed by a review of the techniques employed in modeling the monochromator and its thermal/structural boundary conditions. The results of the finite element analysis, three-dimensional temperature distributions, surface displacements and slopes, and stresses, in the area of interest, are presented. Lastly, the effects these results have on monochromator output flux and resolution are examined.

INTRODUCTION

The intense photon beams available from new insertion device synchrotron radiation beamlines will enable a new generation of experiments to be carried out. X-ray monochromators associated with these beamlines will be required to handle the high heat fluxes produced by these photon beams. The experiments that are planned for these beamlines may place extraordinary demands on the monochromator since they will be designed to fully utilize the high flux and brightness of these sources. Some of these experiments will use the high brilliance to study very small samples. Some will use the high intensity to study samples which are at very low concentration (i.e. monolayer coverage of a substrate) and others will use the high intensity to produce photon beams with very high energy resolution and low divergence. All these experiments require x-ray monochromators that produce output beams which are stable in both energy and position, as the total power input varies during a typical fill cycle.

The heat flux produced by the synchrotron beam may put especially demanding requirements on the first crystal of the x-ray monochromator. If an optical configuration is chosen in which the heat flux is very localized, high temperature gradients will result in the crystal. This will occur in the area that is used for monochromatization. The crystal is physically deformed by this temperature gradient: the crystal lattice spacing and the orientation of the crystal planes are changed non-uniformly. These distortions produce reduced throughput, distorted focus, and position and energy drifts of the monochromatized beam as the stored electron beam current changes.

Since these new beamlines will require innovative monochromator designs and it is difficult to experimentally measure monochromator performance, a numerical procedure was developed to do design analysis. The procedure requires first that the crystal thermal loading be determined. The ANSYS[1] finite element program is then utilized to calculate the resulting temperatures and distortions of the monochromator crystal. The use of these two programs will enable the evaluation and optimization of current and new monochromator designs without the requirement of building and testing each new design.

In order to clearly understand the important parameters of a realistic monochromator design, the first case studied was the heating of the first crystal of the Brown-Hower x-ray monochromator (Figure 1) which is used on the LBL-EXXON 54 pole wiggler beamline at the Stanford Synchrotron Radiation Laboratory (SSRL). The power loading on this beamline is comparable to what will be produced by future insertion devices.

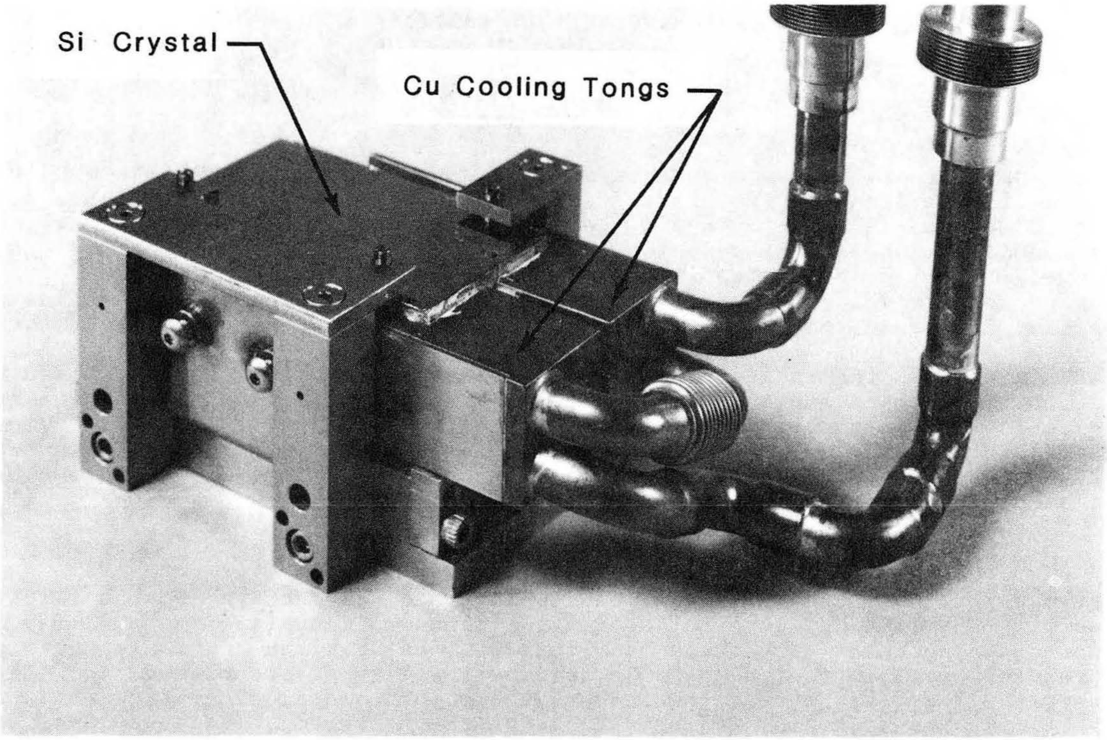

Figure 1. First Crystal of the Brown-Hower Monochromator

SYNCHROTRON RADIATION THERMAL LOADING

To analyze the distortion and stress distribution of the first crystal in the Brown-Hower monochromator, synchrotron radiation thermal loading profiles were developed. Computation of a profile was done starting with a set of source operation conditions (storage ring energy, current and wiggler field) and computing a source output power profile with the program SPECT[2]. The thermal loading profile is then computed, which is the power transmitted through the beam line which impinges on the monochromator. A simple model is used which takes into account loss of beam due to radiation absorption in the pyrolytic graphite filters, radiation not intercepting the toroidal mirror, radiation that is absorbed in the toroidal mirror (due to its cutoff energy) and radiation absorption in the beryllium windows. The model used in computing this power profile represents an upper limit on the transmitted power to the crystal. This is because wiggler output power is computed on the basis of a point source and other loss mechanisms are not accounted for (convective helium heat transfer in the monochromator, energy loss due to photo electric emission from the monochromator crystal, etc.).

The analysis reported here is based on SSRL operation at 3.0 GeV and 30 ma with the wiggler field at 1.0 Tesla. Wiggler output power is 342 watts with estimated power delivered to the crystal of 173 watts. The power distribution on the Si(220) crystal, set at a 32.5 degree incidence angle (6 KeV), is shown on Figure 2.

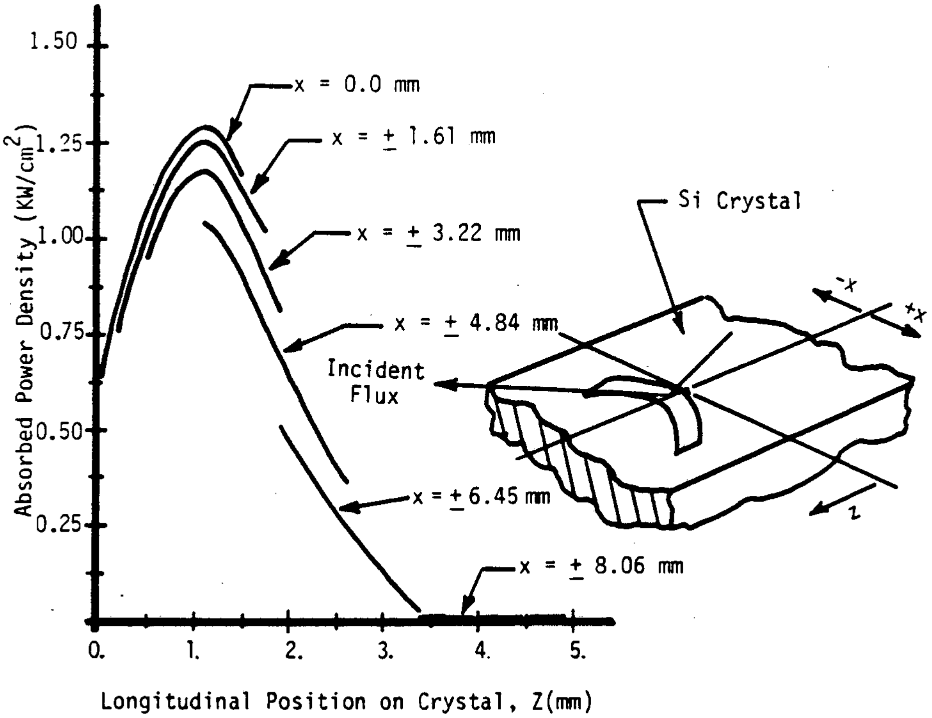

Figure 2. Power Distribution Incident on the Monochromator Crystal

FINITE ELEMENT ANALYSIS (FEA)

Thermal and Structural Boundary Conditions

The crystal in the Brown-Hower monochromator is placed in a mount which fixes its displacement at 3 points in the y coordinate direction (top surface) and one point in each of the x and z coordinate directions, see Figure 3. This optical mount allows free expansion to occur, yet fixes the orientation of the top (diffracting) surface of the crystal. These structural boundary conditions are easily converted to the finite element model by fixing the appropriate nodal displacement components at the corresponding nodal locations.

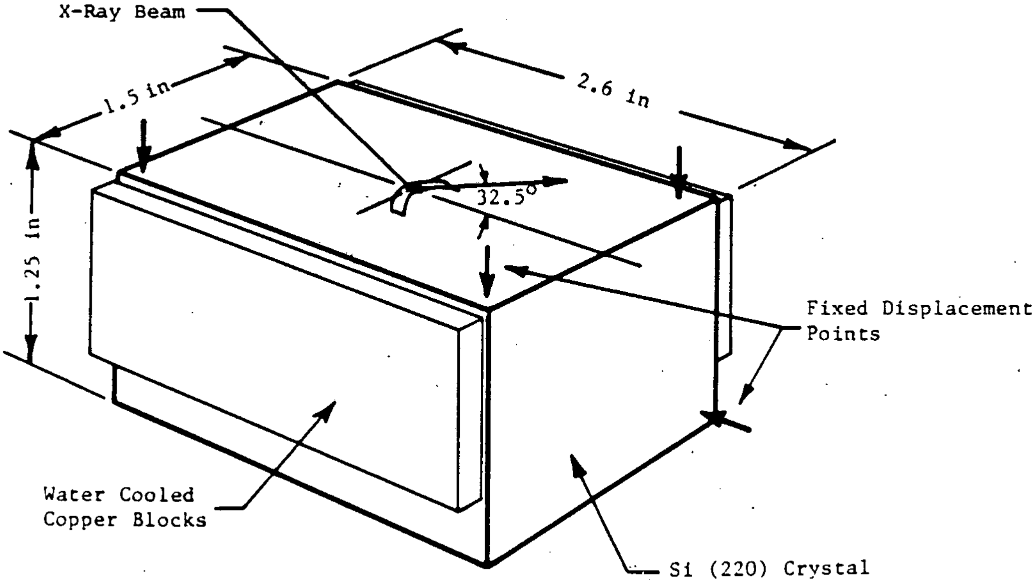

Figure 3. Schematic of Brown-Hower Monochromator First Crystal Showing FE Model Boundary Conditions

The process of determining the thermal boundary conditions is slightly more rigorous, however. The finite element model would simply be too large and require too much CPU time to run if the copper heat exchanger and conductive grease were included in the 3-d model. Because of this, a 2-d thermal model, illustrated in Figure 4, was constructed which included the silicon crystal, the copper heat exchanger, and 5 mils (0.005 inch) of conductive grease. Symmetry was utilized in modeling the crystal, and thus the heat load is reduced to 86 1/2 watts. Approximately one-half of this flux was applied in a similar distribution to the 2-d model. Heat was removed via convection by water (at 27°C) flowing through the 4-channel heat exchanger. The resulting temperature along the grease-crystal interface ranged from 120-125°C in the 2-d model. A constant 122°C value for fixed nodal temperature was assumed along the entire grease-crystal surface in the 3-d model. This assumption should yield conservative temperatures since conduction along the crystal length, and thus cooler surface temperatures, is ignored.

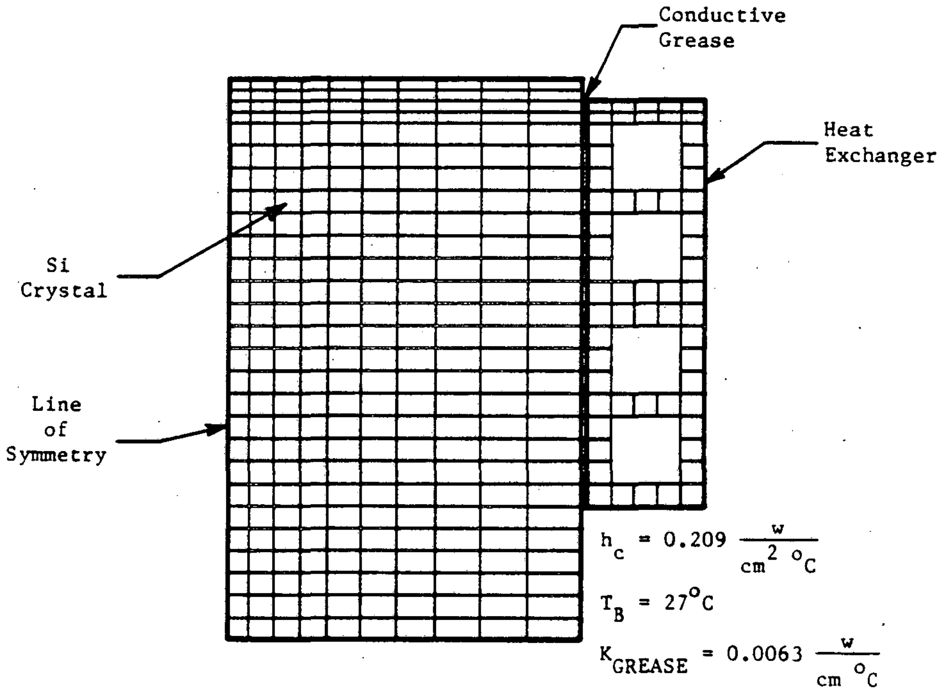

Figure 4. Monochromator 2-d Finite Element Model

Modeling

The ANSYS finite element program allows convenient transformation of coarse model displacement and temperature results to a locally refined model for further processing. This feature may be visualized in an example such as a complicated structural component in which the only results of interest are in a local area, such as at a stress concentration. In this case, the entire structure need not be modeled so as to get very accurate displacement and stress results throughout. Instead, a coarse-mesh model can be analyzed, from which the displacement results can then be transposed to a local-refined model. When this model is analyzed, relatively accurate stress results are computed. This feature within ANSYS enabled the monochromator crystal to be analyzed conveniently using two relatively small mesh-models (see Figure 5).

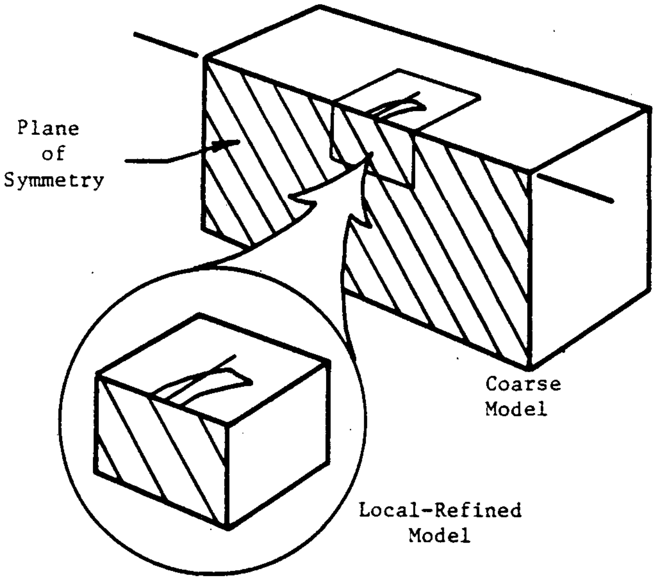

Figure 5. Transition from Coarse to Local-Refined Model

The analysis proceeded in the following manner:

1) A coarse mesh model of the entire monochromator crystal was developed. (utilizing symmetry, 3042 nodes, 2304 brick elements)
2) From this a coarse thermal analysis was performed using the entire crystal's thermal boundary conditions and a coarse representation of the synchrotron radiation heat flux.
3) A coarse structural analysis was performed utilizing the crystal's structural boundary conditions and the temperature distribution from the coarse thermal run.
4) Next, a local-refined mesh model was constructed of the monochromator crystal in the area of the steepest thermal gradients. This was done to get a better representation of both thermal and structural results. (2178 nodes, 1600 brick elements)
5) A local-refined thermal analysis was completed using coarse model temperature results as cut boundary conditions, and a more refined representation of the incident thermal load.
6) Utilizing the refined and improved temperature results from above, a refined structural analysis was done. In this analysis, the local displacement boundary conditions from the coarse structural run were utilized. This resulted in a better representation of displacement and slope results.

CRYSTAL BEHAVIOR

Thermal/Structure Behavior

The results of the finite element analysis, temperatures, displacements and stresses are shown in Table 1 for $Q = 173$ watts. Plots of iso-thermal contours and deflected shape for both the coarse and locally-refined mesh models are shown in Figure 6, a through d. As can be seen in Figures 6a and 6c, there is a rapid 200°C temperature drop within a highly localized volume centered about the incident synchrotron beam. It is this steep thermal gradient which causes the relatively steep sided bump in the crystal shown in Figures 6b and 6d. (This localized vertical displacement is emphasized in the figures by multiplying the displacements by a scale factor of 1100 and 900 respectively.)

Table 1. Thermal/Structural Results of Finite Element Analysis for 173 Watts Incident Power

	Refined Model	Coarse Model
Maximum Temperature: (T_{Max}) (initial temperature = 27°C)	367°C	362°C
Maximum Vertical Growth of Refracting Surface (δy_{Max})	3.42μm	3.39μm
Maximum Principle Stress:		
σ_1	16.7 psi	-104 psi
σ_2	-1911	-1644
σ_3	-5366	-4611

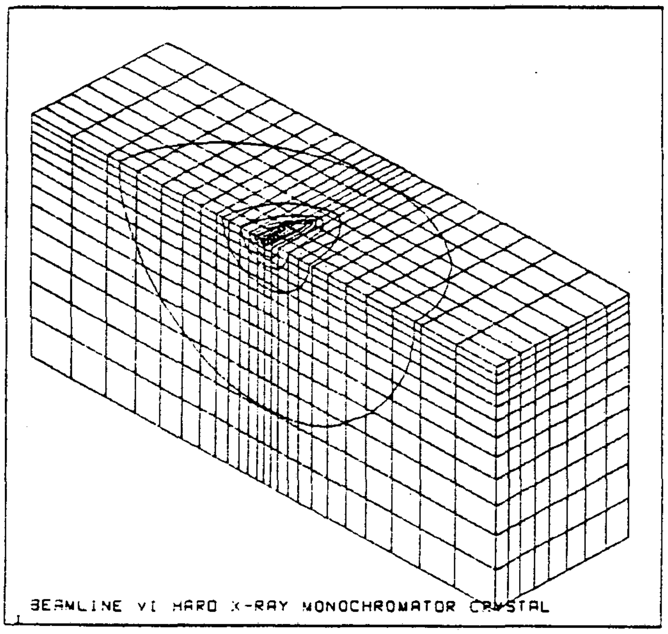

Figure 6a. Iso-Thermal Contour Plot of Coarse Model (25°C per increment)

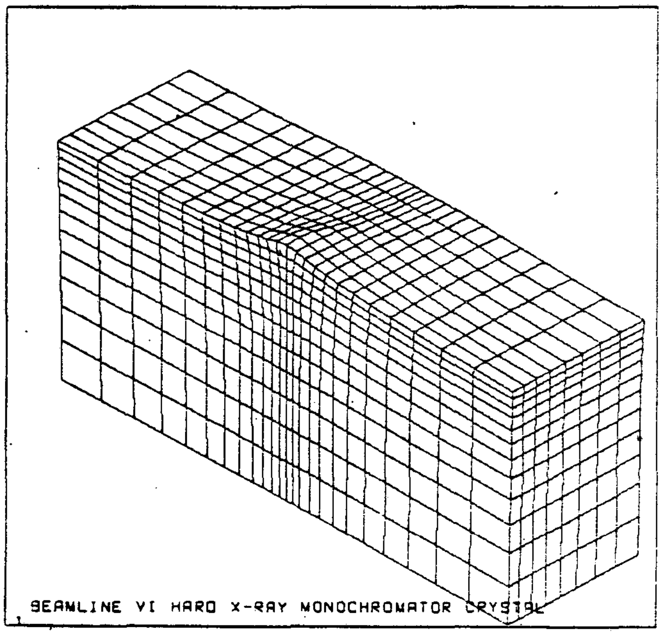

Figure 6b. Deflected Shape Plot of Coarse Model (Displacement scale =1100)

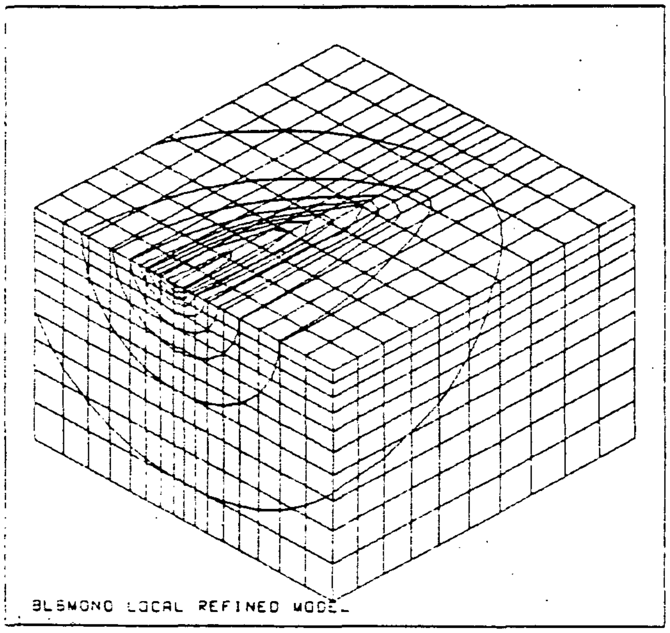

Figure 6c. Iso-Thermal Contour Plot of Local-Refined Model (25°C per increment)

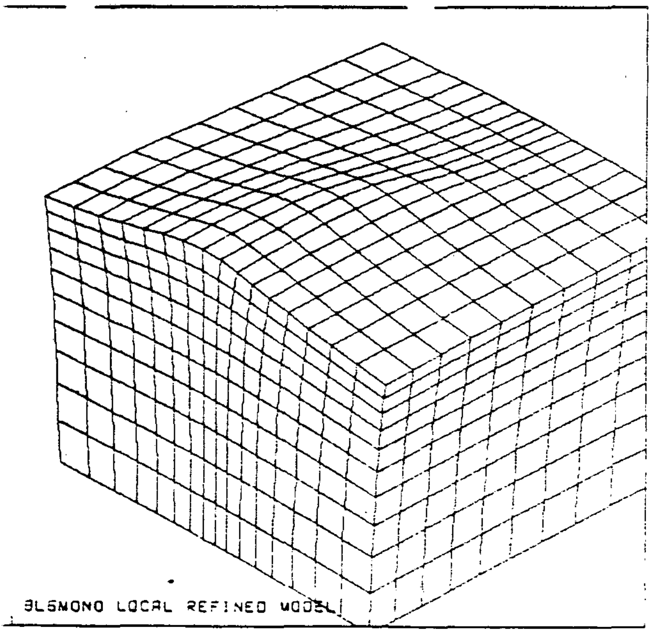

Figure 6d. Deflected Shape Plot of Local-Refined Model (Displacement scale =900)

The stress results from the local refined analysis are used to determine if the monochromator crystal will survive the heat load.

Stress Results and Failure Theories

Experiments have shown that in silicon, appreciable plastic deformation starts at about 600°C.[3] Below 600°C, silicon deflects elastically until fracture stress is reached. Thus, silicon is classified as a brittle material in the temperature range the monochromator experiences under the current heat loads.

The Coulomb-Mohr Theory of brittle failure was used in determining if the monochromator crystal would survive the thermal gradient.[4] The Coulomb-Mohr theory is analogous to the Maximum Shear Stress theory in failure of ductile materials. Both of these theories are generally accepted as always being conservative.

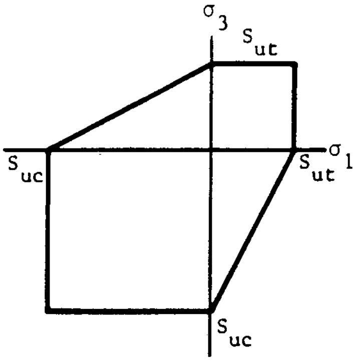

Figure 7. Graph of Coulomb-Mohr Theory of Brittle Failure

The Coulomb-Mohr theory states that when the principle stresses are arranged such that $\sigma_1 > \sigma_2 > \sigma_3$ (tensile and compressive), failure is predicted when Equation (1) holds true.

$$\frac{\sigma_1}{S_{ut}} + \frac{\sigma_3}{S_{uc}} > 1.0 \qquad (1)$$

S_{ut} and S_{uc} represent the ultimate tensile and compressive strengths respectively. Equation (1) would be represented by a point lying outside the boundary shown in Figure 7.

For semiconductor grade silicon, large samples with relatively little surface preparation other than sawing and a light etch give breaking strength values in the range of 10,000 to 20,000 psi. In small samples prepared with etched surfaces, a range from 25,000 to 60,000 psi is observed. In choosing a single value of tensile breaking strength for the monochromator crystal, a value of 15,000 psi for large polished single crystal would seem appropriate.

From the results of the refined structural model, the three principle stresses in the location of maximum stress are:

$$\sigma_1 = 16.7 \text{ psi} \qquad \sigma_2 = -1911 \text{ psi} \qquad \sigma_3 = -5366 \text{ psi}$$

From Equation (1):

$$\frac{\sigma_1}{S_{ut}} + \frac{\sigma_3}{S_{uc}} = 0.36 \qquad (2)$$

In the calculation of Equation (2), the value of ultimate tensile strength was used for both tension and compression. Since compressive strength in brittle materials is usually many times greater than tensile strength, we are adding conservatism to our calculation.

A "factor of safety" is calculated in Equation (3):

$$\frac{1}{0.36} = 2.8 \qquad (3)$$

Therefore, the monochromator crystal design under the 173 watt synchrotron crystal radiation thermal loading will not fail due to insufficient strength.

D-Spacing and Slope Errors

Crystal diffraction can be characterized by Bragg's Law where the output monochromatic beam is defined by Equation (4).

$$n\lambda = 2 D \sin \Theta \qquad (4)$$

Considering just the fundamental and differentiating, a two-term relationship can be derived as in Equation (5) for wavelength resolution in terms of D-spacing and angular changes.

$$\frac{d\lambda}{\lambda} = \frac{dD}{D} + \frac{d\theta}{\tan\theta} \qquad (5)$$

dD/D or change in D-spacing, is the same as the strain at the surface in the vertical (out-of-plane) direction.

dθ/tanθ is the slope change of the distorted crystal at any point divided by the tangent of the incidence angle.

To evaluate changes in resolution and loss of diffracted beam, temperature and displacement results were further processed to obtain D-spacing and slope changes as shown in Table 2.

Table 2. D-Spacing and Slope Errors
for 173 Watts Incident Power

Refined Model

Maximum D-Spacing Change $\frac{dD}{D}$ Max (from zero-strain):	1.272×10^{-4}
Maximum Relative Variation in D-Spacing $\frac{dD}{D}$ in centrally illuminated area:	-5.31×10^{-5}
Absolute Value of Maximum Slope within Irradiated Area:	4.725×10^{-4} radians
Maximum Relative Slope Change $\frac{d\theta}{\tan\theta}$	7.45×10^{-4}

Shown in Figures 8a and 8b are plots of D-spacing and slope superimposed on the local-refined model. Figure 8a shows lines of constant D-spacing relative to the maximum value of D-spacing. Figure 8b shows lines of constant slope change relative to the highest point on the deformed crystal. Here positive slope is defined as that which increases the angle of incidence of the beam.

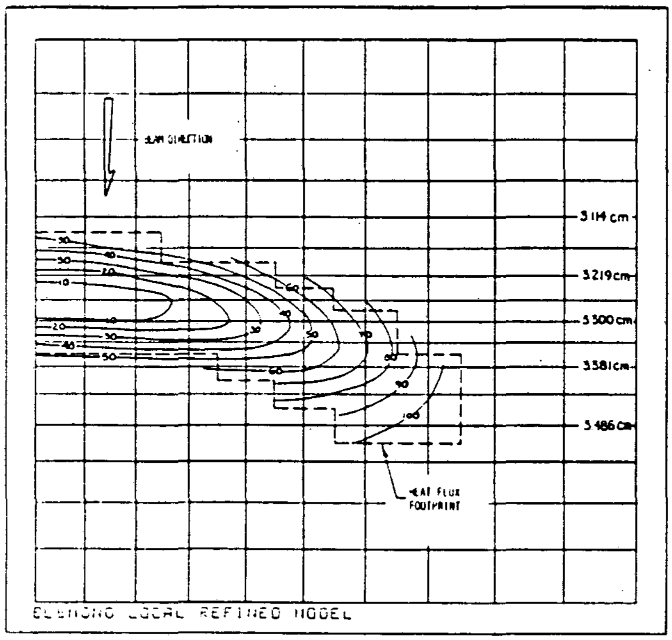

Figure 8a. D-Spacing Error $\frac{dD}{D} \times 10^{6}$ Superimposed on Local-Refined Model

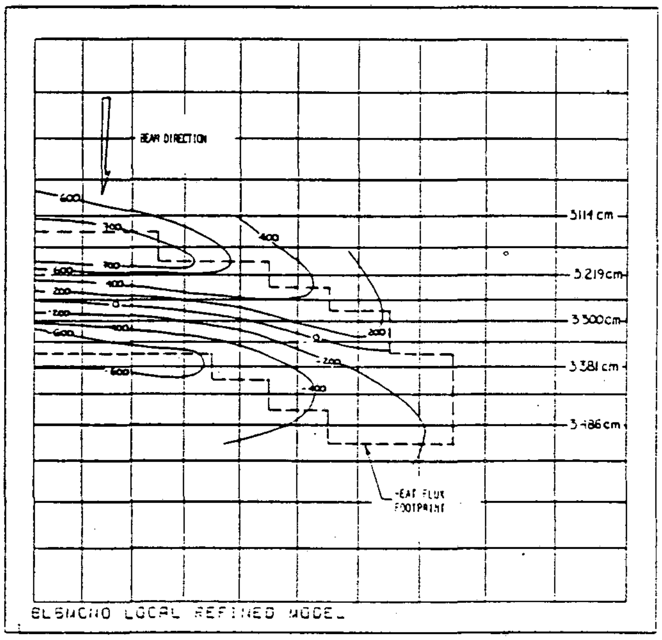

Figure 8b. Slope Error $\frac{d\theta}{\tan\theta} \times 10^{6}$ Superimposed on Local-Refined Model

In Figure 9 it is easy to see the slope change at the crystal center line relative to the heat flux profile. The steepest slopes occur within the footprint of the flux.

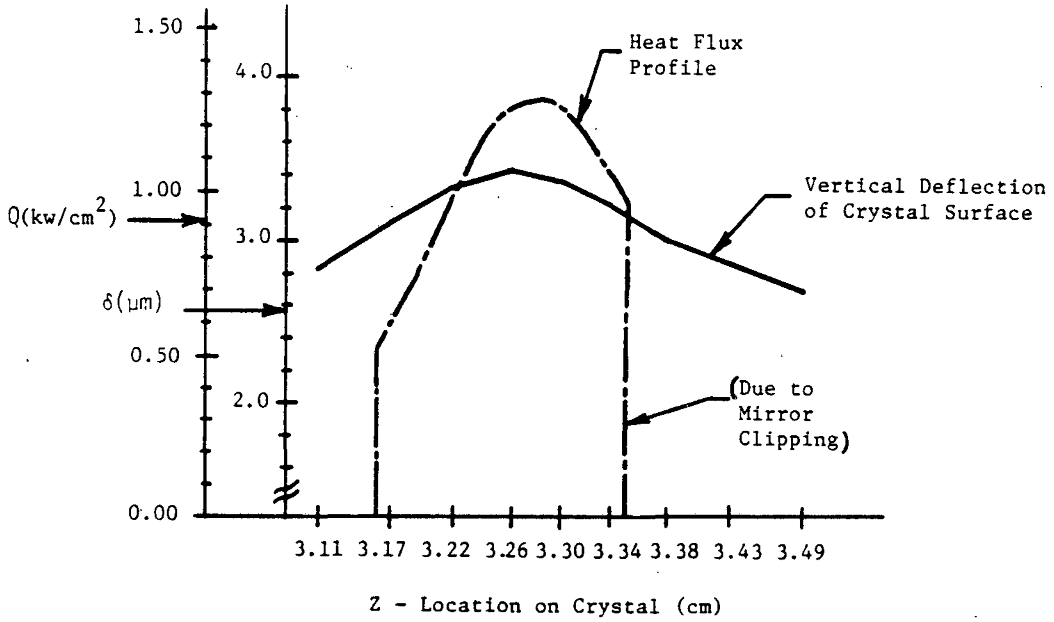

Figure 9. Heating Profile at Crystal Center Line Superimposed on Slope at Crystal Surface

Typically, for a specific wave length at low thermal loading, crystal diffraction shows a lowering of the peak intensity and broadening of the monochromatized spectrum dλ/λ from what would be expected from a Darwin type crystal rocking curve. With increased thermal load, crystal curvature increases with the crystal rocking curves following this curvature. When a portion of the crystal is sufficiently curved, with respect to the beam envelope of beam impinging on the crystal, some of the incoming beam cannot be diffracted. At still greater thermal loading there will be further rocking curve rotation until finally no beam will be diffracted from a portion of the crystal.

In summary, with 173 watts of x-ray power (with a profile shown in Figure 2) incident on a Si(220) crystal and the Brown-Hower monochromator set at 6 keV, we calculate that:

a) The slope error is much more important than the d-spacing change in decreasing the monochromator performance.

b) The Darwin rocking curve width, dλ/λ, for a Si(220) crystal is 1×10^{-4} and the effective bandwidth of the converging synchrotron beam is about 2×10^{-4} while the maximum slope error, $d\theta/\tan\theta$ is 7.4×10^{-4}. Therefore, much of the beam striking the first crystal will experience slopes greater than the combined Bragg and converging beam width and will not be diffracted within the acceptance cone of the second monochromator crystal.

c) Since the stored electron beam current changes by a factor of about 2 during a typical fill cycle, the incident power and therefore the slope error will fluctuate considerably. Because of this, it is anticipated that the performance of the monochromator will be very dependent on machine operation. Changes in beam profile and energy calibration during a fill cycle should therefore be expected since the slope error and d-space changes are greater than the Darwin rocking curve width.

SUGGESTIONS FOR FUTURE WORK

The results of this work suggest a need for improvement in two areas when discussing monochromators for high-flux beam lines. The first is the subject of this paper, analytical techniques. The use of FEA brings the detailed analysis of these optical elements a significant step forward. However, there is still room for improvement in the current FE model. To improve the accuracy of slope estimates in the diffracting portion of the crystal, the mesh refinement in the local model should be increased in the direction of the beam. Better material property data could be included in the model. For instance, adding temperature dependency to Youngs Modulus (E) and coefficient of thermal expansion (α) (conductivity (k) has already been made temperature dependent), could improve both slope and D-spacing values. The theoretically calculated loads need verification and therefore, the need for experimental measurements of absorbed heat flux in the monochromator and other important optical elements is obvious.

Another area for improvement is in monochromator crystal design. Alternate cooling geometries, such as cooling flow channels integral to the crystal or thin crystals cooled from the bottom, need to be investigated. Crystal operation at cryogenic temperatures and alternate monochromator materials or composites should also be considered. Distortion is reduced when materials exhibiting a low thermal expansion/thermal conductivity α/K ratio, at the operating temperature, are utilized.[3,6]

CONCLUSIONS

The thermal distortion of the x-ray monochromator on the LBL-EXXON beamline at SSRL has been calculated using the ANSYS finite element computer program. A focussed beam with a total power of 173 watts was assumed to be incident on a Si(220) monochromator set at 6 keV. The distortion calculated is nearly an order of magnitude larger than the normal Darwin rocking curve width and therefore the performance of the monochromator will be seriously affected. The analysis also indicates that the change in the monochromator resolution due to slope error outweighs the d-spacing error by an order of magnitude. Therefore, to improve the current monochromator design, the magnitude of the slope change must be reduced. Some improvement in slope error might be accomplished with improved heat exchanger design. Large reduction in slope might be achieved for silicon crystals if they were cooled to cryogenic temperatures, for example, where the thermal coefficient of expansion is considerably smaller and the thermal conductivity is higher.

The application of finite element analysis to the thermal loading of x-ray mirrors and monochromators will enable the design of x-ray optical elements with the assurance that performance specifications will be met.

ACKNOWLEDGEMENTS

This work was supported by the Office of Energy Research, U. S. Department of Energy, contract number DE-AC03-76SF00098.

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This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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