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A Directly Cooled Grating Substrate for ALS Undulator Beam Lines

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Abstract

Design analyses using finite element methods are presented for thermal distortion of water-cooled diffraction grating substrates for a potential application at the LBL Advanced Light Source, demonstrating that refinements in cooling channel configuration and heat flux distribution can significantly reduce optical surface distortion with high heat loads. Using an existing grating substrate design, sensitivity of tangential slope errors due to thermal distortion is evaluated for a variety of thermal boundary conditions, including coolant flow rate and heat transfer film coefficients, surface illumination area and heat distribution profile, and location of the convection cooling surfaces adjacent to the heated region.

Water-cooled Diffraction Grating Substrates

Current plans for the initial ALS construction project include the installation of three undulator beam lines that will use a spherical grating monochromator design which was developed at LBL ("LBL-SGM") to accommodate water-cooled grating substrates. The substrate design was initially developed at the LBL Center for X-Ray Optics for use on Beam Line 6-1 at the Stanford Synchrotron Radiation Laboratory (SSRL), where thermal loads can be as high as 50 W of absorbed heat. More recently, finite element analyses have been performed to estimate thermal distortion of the grating substrate subjected to the direct beam from an undulator source at the ALS. Results of these design analyses are summarized below.

The brazed GlidCop,⁷ OFHC copper, and 304 stainless steel assembly for the LBL-SGM grating substrate is shown in Figures 1–3. It uses a single water circuit having 4 parallel cooling channels lengthwise below the optical surface. Surface figure distortion in the lengthwise direction (i.e., tangential slope errors) could limit the wavelength resolution that may be achieved with this monochromator. Optical performance is relatively insensitive to slope errors in the transverse, sagittal direction due to the grazing incidence arrangement. Preliminary calculations suggested that direct water cooling would be needed for acceptable performance with the anticipated heat loads, and a cooling channel configuration to reduce tangential errors was selected. The substrate design was initially proposed by T. Lauritzen of LBL, based primarily on mounting and fabrication requirements, and was then analyzed by the authors to determine whether slope errors due to thermal distortion would be acceptable. The only significant design change that resulted from finite element analyses was to establish an optimum wall thickness between the optical surface and the internal cooling channels.

With 3-d finite element analysis, one quarter of the substrate was modeled based on two planes of symmetry and heat loads centered on the optical surface, and was similar to the model shown in Figure 4. For the SSRL installation, maximum heating was assumed to be uniform along the full length of the grating, with a beam width of about 1.2 cm in the transverse direction. With a fully open entrance slit and maximum wiggler power, the peak absorbed power density may be as high as 7 W/cm² with 50 W of total absorbed heat. Normal operation with limited wiggler power output and with slit widths in the range of 10 to 300 µm for higher resolution reduces the total absorbed power to less than 20 W.

For the SSRL conditions of approximately uniform heating over the full length of the grating and constant beam width, tangential slope errors are directly proportional to total absorbed power; the estimated average slope error over 95% of the grating length is about $0.006 \,\mu\text{rad/W}$ of absorbed heat. The maximum slope error occurs at the ends, and is estimated to be less than $0.1 \,\mu\text{rad/W}$, with an average slope error of about $0.015 \,\mu\text{rad/W}$ for the entire length. For highest resolution with an entrance slit width of $10 \,\mu\text{m}$ and about $1 \,\text{W}$ of absorbed heat, performance is within the tolerance limit of $1 \,\mu\text{rad}$ maximum tangential slope error.

In the current design for the brazed substrate assembly, the 4 parallel cooling channels extend about 85% of the grating length. With full lengthwise heating, there is an optimum wall thickness for the cooling channels near the optical surface: below about 2 mm thickness, the surface distortion is "saddle-shaped" with convex distortion in the sagittal direction and concave distortion in the tangential direction. This results from higher temperatures at the grating ends, where heating occurs farthest from the cooling channels. However, with increasing wall thickness, the lengthwise concave shape disappears, and above about 3.5 mm thickness, the surface distortion is fully convex. Thus, a thickness of about 3 to 4 mm was chosen to minimize tangential slope errors. We also considered thickness requirements for polishing to prevent "print-through" effects. A 3 mm thickness over the D-shaped cooling channels is expected to be adequate for any polishing operation.

Water-Cooled Gratings for ALS Undulator Beam Lines

The LBL-SGM with directly-cooled gratings was developed with applications for ALS beam lines in mind. Two of the proposed undulator beam lines use a condensing mirror system (similar to B.L. 6-1) which effectively filters much of the unwanted beam power. However, with grazing incidence angles of up to 10°, the peak power density at the grating is still likely to require water-cooled substrates in order to achieve acceptable surface figure distortions without compromising resolution. For the 3.9 cm period length undulator (previously 3.65 cm) current plans include a branch line in which the grating receives the x-ray beam directly from the undulator source, thereby exploiting the high brightness of the source and eliminating the condensing mirrors and entrance slit. We used finite element analysis to evaluate this application of the existing substrate design, and although many of the beam line parameters have since changed, the conclusions derived from the analyses are still relevant and are discussed below.

The main feature of synchrotron radiation from *undulator* sources that is significant with respect to thermal distortion of beam line optics is that much of the beam power lies outside the central cone, the solid angle containing sharp spectral peaks of radiation at harmonics of the fundamental.^{8,9} By passing the beam through an aperture, it is possible to limit the incident power on a mirror or grating without sacrificing any useful photon flux. Recognizing that surface figure errors due to thermal distortion are often most severe near changes or discontinuities in the absorbed heat distribution, we investigated the sensitivity of slope errors in the region illuminated by the central cone with respect to variations in aperture sizes.

Effect of Vertical and Horizontal Beam-Defining Apertures

The existing grating substrate was optimized for uniform, full-length heating. However, with a vertically deflecting grating, it is rarely possible to achieve a uniform heat distribution. The vertical power distribution in a synchrotron beam is approximately Gaussian, and the higher-energy x-rays, which are less easily reflected, are concentrated near the beam center. A condensing mirror system tends to flatten the vertical power distribution by filtering the hard x-rays. But on ALS undulator beam lines, only with small grazing incidence angles in which the grating is over-filled is it possible to approach uniform lengthwise heating. The effect of the natural variation in vertical power distribution is most severe when the grating receives a direct synchrotron beam and when the grating is not fully illuminated lengthwise due to large grazing incidence angles and proximity to the source. In this situation, although a vertical aperture that limits the beam height reduces the total absorbed power, the tangential slope errors in the region illuminated by the central cone can increase if the uniformity of the lengthwise heat distribution is further compromised by limiting the beam height to the size of the central cone.

Table 1 describes the thermal boundary conditions for finite element analysis of grating performance for the U3.65 beam line. The 1×1, 1×3, and 3×3 load cases represent actual thermal loads for varying horizontal and vertical rectangular aperture sizes, scaled from the smallest aperture (1×1) for the nominal full-width, half-maximum (FWHM) central cone size using the largest grazing incidence angle. The 1×Full (Gaussian) load case represents heat loads with no vertical aperture limits and the grazing angle matched to fully illuminate the grating length. The 1×Full (uniform) load case is a hypothetical comparison of performance with the same total power as the Gaussian case, but modified to uniformly distribute the heat load over the entire grating length. The 3×Full (uniform) load case demonstrates sensitivity of grating performance to an increase in the horizontal aperture size which increases the total power received by the grating.

The results of our analyses, summarized in Table 2, suggest that a vertical beam-defining aperture can produce, at best, only a small improvement in the tangential slope errors compared to a non-apertured beam, and then only when the aperture is large compared to the central cone size, as in the 1×3 and 1×Full (Gaussian) load cases. Performance is severely degraded if the beam is vertically apertured to match the central cone height (1×1 case). Thus, it appears that a vertical aperture that limits total absorbed power has no practical benefit for improving grating performance using the existing substrate cooling configuration. Figures 5a, 5b, and 5c show the calculated thermal distortion of the grating surface along the longitudinal grating axis and demonstrate that operating configurations which improve the lengthwise uniformity of the heat loads can significantly reduce the tangential slope errors in the region illuminated by the central cone.

Nevertheless, a horizontal beam-defining aperture can effectively reduce grating tangential slope errors with undulator sources. For any given lengthwise heat distribution, the tangential slope errors within the region illuminated by the central cone vary directly with the total absorbed power. Total power can change with electron beam current or with variations in the horizontal aperture size without changing the lengthwise heating profile. For undulator sources, tangential slope errors can be minimized without loss of flux by sizing the horizontal aperture to match the desired central cone.

Optimized Grating Substrate Design

It is likely that an optimal cooling channel configuration and substrate size could be found for any specific heat distribution pattern in order to achieve the lowest possible slope errors for a selected incidence angle and beam size. Typically, one would expect a mirror with a fixed deflection angle to be matched to a specific beam line application. However, the choices and compromises are more difficult for a grating monochromator designed for operation over a range of angles and central cone sizes. With the existing substrate design, tangential slope errors increase as the heat distribution departs from uniform, full-length heating. For ALS beam line applications, other optimal configurations might be more appropriate. We modeled one possible configuration in which the cooling channel length was shortened to match a vertically apertured beam (3×3 load case) covering about 1/3 of the grating length. With the shortened cooling channels, tangential slope errors in the central cone region are reduced by about 80% in comparison to the slope errors that occur in the existing, full-length cooling configuration. For best performance, whatever optimal configuration is selected for ALS applications, it should be well-matched to typical operating conditions.

Before pursuing any major design changes with the current grating configuration, we investigated other parameters and operating conditions in order to evaluate the achievable limits for minimizing thermal distortion for undulator beam line applications. Analyses show that a small but significant improvement can be made by locating the beam midway between the lengthwise cooling channels instead of directly over a cooling channel. With a vertically apertured beam (1×1 load case), tangential slope errors in the illuminated region are reduced by about 20%. Locating the beam between channels appears to exploit more effectively the convection cooling surfaces, thereby reducing overall temperature rise in the bulk volume of substrate material and also reducing the lengthwise temperature gradients that cause tangential slope errors. It is likely that there is some optimal cooling channel spacing that provides further improvement for a given beam footprint.

We analyzed the effect of changes in coolant flow parameters. Since flow-induced vibration is a common concern with the use of directly cooled optics, operation may be limited to laminar flow, in which the convective film coefficient is reduced to a fraction of the convective film coefficient for turbulent flow. This reduction causes an increase in the convection boundary layer and therefore an increase in the overall film temperature drop, which, in turn, increases the bulk temperatures in the substrate material. However, since temperature gradients in the substrate are more directly related to thermal conductivity, the tangential slope errors show only a weak sensitivity to changes in water flow rates. We used a nominal water flow rate of about 1.7 m/sec (5.5 ft/sec) with a Reynolds Number of 5000. This flow rate is just above the transition region to fully-developed turbulent flow, with a film coefficient of 0.77 W/cm²-K. For comparison, a 50% reduction in the film coefficient, corresponding to a flow rate of about 0.9 m/sec (3 ft/sec), resulted in only a 15% increase in the tangential slope errors in the 1×3 load case. Our conclusion is that only small improvements can be achieved with substrate and mounting configurations that are rigid and massive enough to allow much higher turbulent-flow rates without detrimental vibration effects. Careful design of water connections, bend radii, etc. can be beneficial, but our experience suggests that a practical design limit for water flow rates for optical components is around 3 m/sec (10 ft/sec). Higher flow rates produce only marginal gains.

Liquid Gallium vs. Water as Coolant

Finally, we evaluated the slope error reduction that may be possible using liquid gallium instead of water as the substrate coolant. Gallium offers up to 8 times the convective heat transfer rate of water. With the nominal grating configuration and an apertured beam (3×3 load case), the use of gallium produced a reduction of about 60% in the tangential slope errors in the central cone region. This improvement is significant, but considering the increased cost and difficulty of maintaining a liquid-gallium system instead of water, we expect that much greater gains would be needed in order to justify the added complexities. Since the total absorbed power on ALS gratings is relatively low, extreme measures such as the use of gallium or high water flow rates to improve the convective cooling are not likely to be cost-effective. The UHV requirements and the precision needed for high resolution monochromator performance already impose significant constraints on system design.

Acknowledgements

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Figure Captions

- Figure 1. LBL-SGM water cooled grating substrate details for Beam Line 6-1 at SSRL.
- Figure 2. LBL-SGM substrate parts prior to brazing, showing the internal cooling channels machined in the OFHC copper faceplate on the left, and the stainless steel water connections and welding stubs for conflat flanges.
- Figure 3. Final brazed assembly of the LBL-SGM substrate prior to electroless-nickel plating and polishing, attached to an aluminum plate for shipping and handling.
- Figure 4. Finite element model and heat loads for LBL-SGM grating thermal distortion analysis and isothermal contours for a selected load case (3×3). On the right, the quarter symmetry model shows contour lines (solid) and elements (dotted) for steady state heating. The zoomed region in the lower left illustrates tangential and sagittal surface slope errors caused by thermal distortion of the substrate.
- Figure 5. Estimated vertical (Y-axis) optical surface distortion with a water-cooled grating substrate using steady state finite element analyses for various apertures, heat flux distribution, and cooling channel configurations:
- Figure 5a. Illuminated area is limited by a rectangular aperture equal to the size of the central cone of the undulator radiation along the transverse (X-axis) and up to 3 times the central cone size along the Z-axis (1×1 and 1×3 thermal load cases).
- Figure 5b. Illuminated area is limited by a square aperture equal to 3 times the central cone size (3×3 thermal load case).
- Figure 5c. Illuminated area is limited by a transverse aperture up to 3 times the central cone size, and the grating is fully illuminated lengthwise with either a uniform or a Gaussian heat distribution (1×Full(uniform), 3×Full(uniform), and 1×Full(Gaussian) thermal load cases).
- Table 1. Summary of heat loads for finite element modelling to estimate thermal distortion of the LBL-SGM water-cooled diffraction grating substrates with various thermal boundary conditions.
- Table 2. Results of finite element analyses showing maximum slope errors and distorted radius of curvature in the central cone region for different illumination and cooling configurations. Tangential slope errors are lowest when the cooling channel length is equal to the illumination length, and when the undulator beam is apertured horizontally to the size of the central cone.

DIFFRACTION GRATING SUBSTRATE BRAZE ASSEMBLY

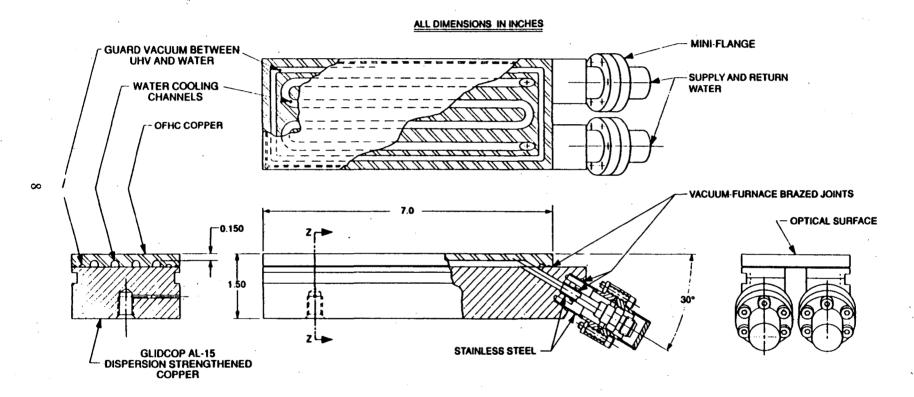


Figure 1

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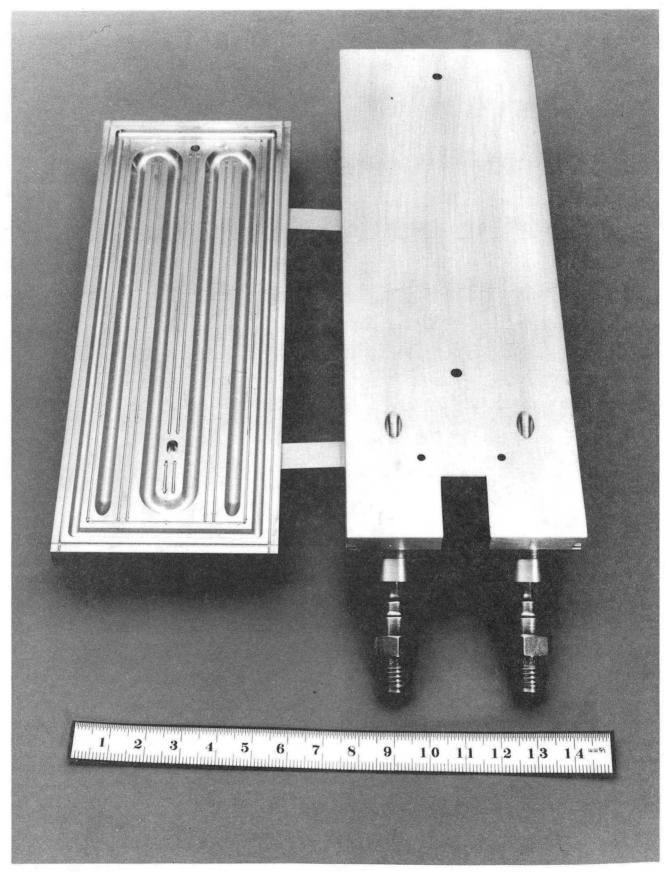
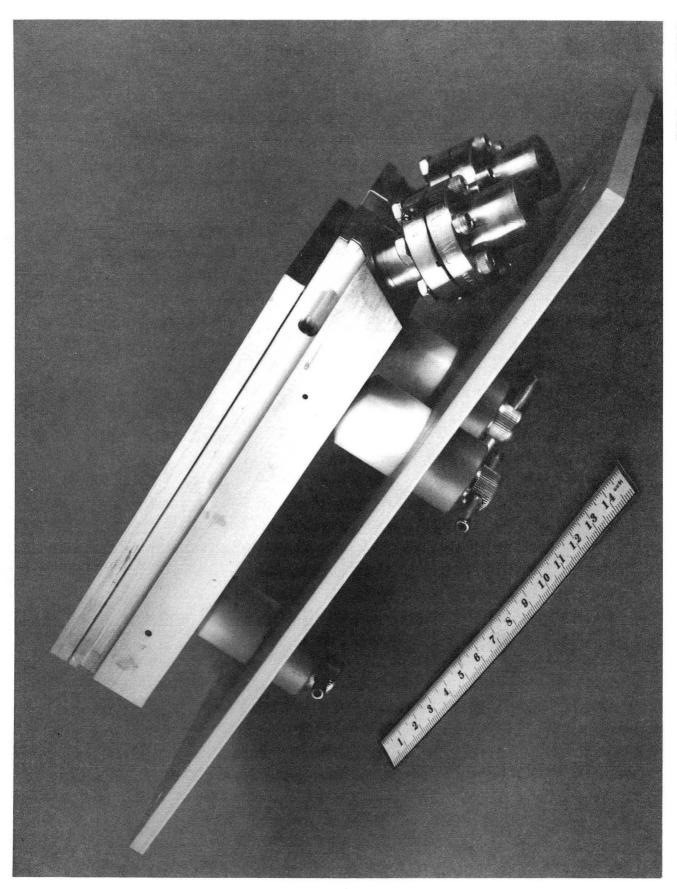
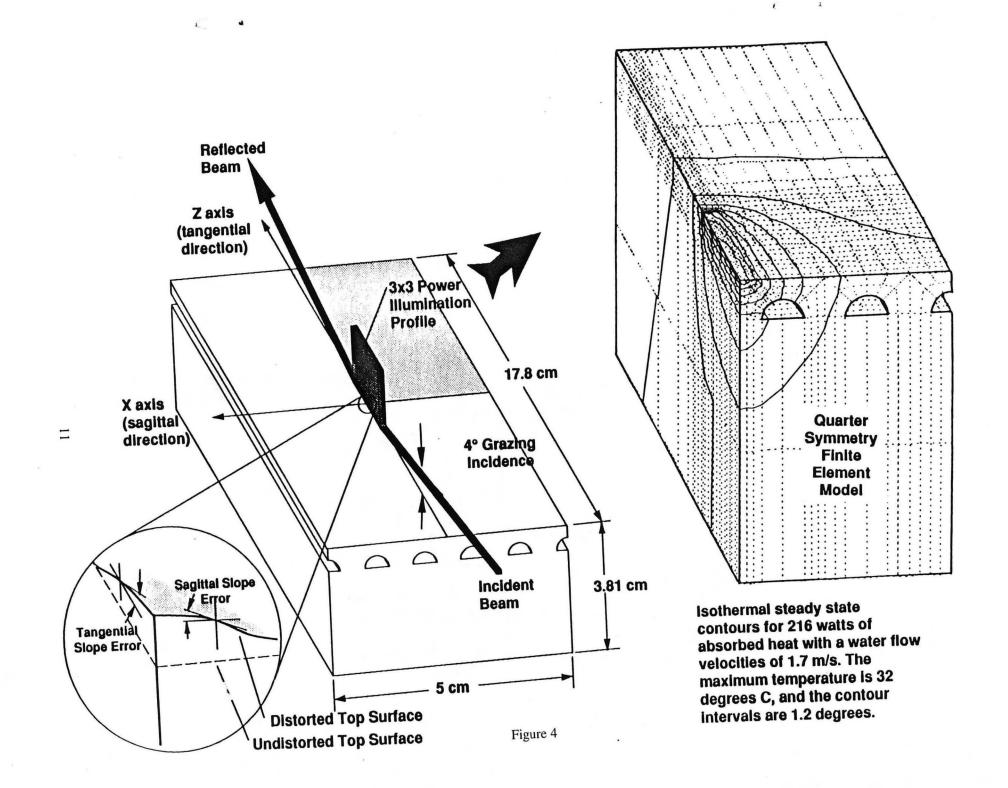


Figure 2

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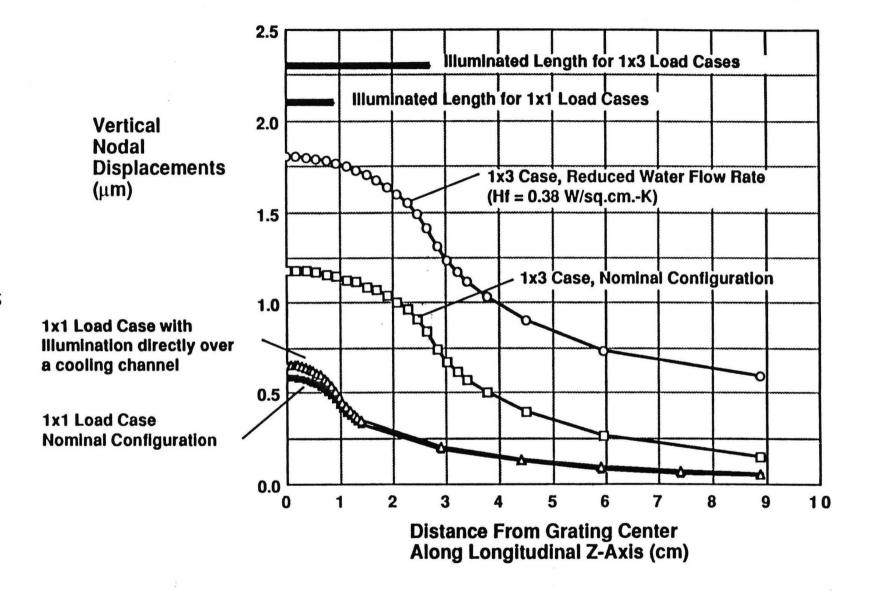


Figure 5a

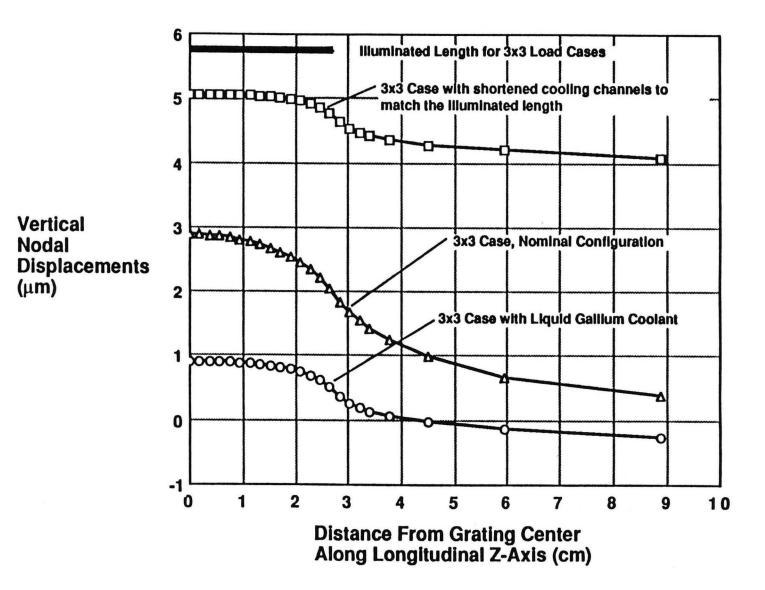


Figure 5b

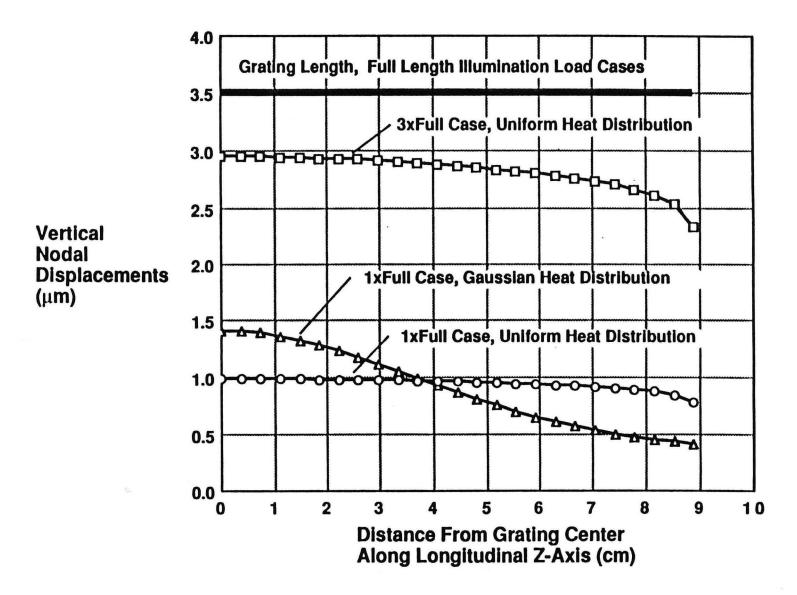


Figure 5c

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Diffraction Grating Thermal Models for Finite Element Analysis for ALS Undulator Beam Line U3.65

Load Case (Illuminated Area Normalized to Central Cone size Horiz. x Vert. FWHM)*	Illuminated Area Horiz. [cm] x Vert. [cm]	Total Absorbed Power [W]	Peak Power Density [W/sq.cm.]	Peak Lineal Power Density along the Tangential Axis) [W/cm]
1 x 1	0.13 x 1.8	24	84	12.8
1 x 3	0.13 x 5.3	72	84	12.8
3 x 3	0.38 x 5.3	216	84	38.4
1 x Full (Gaussian)**	0.13 x 17.8	116	84	13.6
1 x Full (Uniform)	0.13 x 17.8	117	40	6.6
3 x Full (Uniform)	0.38 x 17.8	350	40	19.8

^{*} FWHM central cone size is 0.11 mrad with 4 deg. grazing incidence at 12 meters from the source, with a rectangular (horizontal and vertical) beam defining aperture.

^{**} FWHM for the vertical (tangential) Gaussian heat distribution is 6.8 cm. 1xFull and 3xFull load cases have uniform lengthwise heat distribution.

Diffraction Grating Thermal Distortion Calculations

Load Case (Illuminated Area Normalized to Central Cone size: Horiz. x Vert. FWHM)	Convection Film Coefficient and Coolant [W/sq.cmK]	Cooling Channel Length [cm]	Distorted Tangential Radius of Curvature at the Central Cone ** [m]	Maximum Tangential Slope Error Within the the Central Cone [μrad]
1 x 1	0.77 (Water)	17.8	350	35
1 x 1 *	0.77 (Water)	17.8	270	41
1 x 3	0.77 (Water)	17.8	1360	6
1 x 3	0.38 (Water)	17.8	1100	8
3 x 3	0.77 (Water)	17.8	440	19
3 x 3	0.77 (Water)	5.3	2270	3.6
3 x 3	6.1 (Gallium)	17.8	1380	6
1 x Full (Gaussian)	0.77 (Water)	17.8	1480	8
1 x Full (Uniform)	0.77 (Water)	17.8	24,500	0.2
3 x Full (Uniform)	0.77 (Water)	17.8	10,700	8.0

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^{*} Illuminated area is directly over a cooling channel. For all other cases, heating is midway between 2 channels.

^{**} Tangential thermal distortion within the central cone region is approximately circular for all cases. Undistorted surface figure is modeled as flat.

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