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On the utility of fluid flow models in the design of heat exchangers for cooling 4th generation X ray optics

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Abstract. As the Diamond Light source moves towards upgrading to a 4th generation source, increasing x-ray powers and reduced focal sizes will require improved cryogenic cooling to ensure that the projected new levels of brilliance are achieved. This will create a greater demand for LN₂, if current systems are maintained, laying a greater economic demand on the facility. As in most cases, new designs are tested using thermal-structural finite element simulation, neglecting the contribution of fluid flow. This leaves us without information about the effect of the fluid on the surface of the crystal, along with the efficiency of the flow itself. This results in under optimised cooling systems, leaving cooling capabilities of the system reduced, increasing the consumption of LN₂. This paper presents a full fluid-structure-thermal model, showing the full effects of the flow of liquid nitrogen on the system. This paper will discuss this model in comparison to a conventional thermal-structure model.

1. Introduction

The Diamond II upgrade at the Diamond Light Source is a coordinated programme of upgrades to the synchrotron, its beamlines and infrastructure [1]. This major machine upgrade will require commensurate improvements to the optics used in the beamlines, which will need to be more compact and able to withstand increased power densities. This will necessitate the development of novel approaches to the cryogenic cooling of the optics to enable them to cope with the higher heat loads and to ensure the projected new levels of brilliance predicted for the new light source are achieved.

Monochromators are used to select a particular wavelength from the broad-spectrum, high-intensity radiation generated by the synchrotron. In the case of monochromators, most of the light incident on the optical surface is absorbed as heat, resulting in thermal expansion which can be detrimental to its performance, necessitating cooling. Current cryogenic cooling systems rely primarily on increased LN₂ usage to address any increase in beam energy density [2]. This LN₂ is subsequently vented to the atmosphere, resulting in significant wastage and increasing the operation costs of the beamline. Furthermore, increased LN₂ flow rates can cause vibrations which reduces beam coherence [3–5].

The use of novel methodologies and design configurations for achieving cryogenic temperatures in monochromator assemblies has the potential to reduce the amount of LN₂ required to ensure their



satisfactory performance in the beamline. Wang *et al.* proposed an indirect cooling approach, in which multiple cooling channels were cut inside two copper heat exchangers on either side of the crystal to maximise the heat transfer area [6]. A novel side-cooling configuration which optimised the contact area between the heat sink and crystal was described by Jin *et al.* [7]. Thermal distortion in a multilayer mirror due to heat load in the ESRF-EBS upgrade beamline EBSL-2 was simulated by Brumund *et al.* [8]. The geometry of the multilayer substrate was optimized to minimize slope error on the reflecting surface. A novel indirectly cooled cantilevered silicon mirror was presented by Cutler *et al.* [9]. In this design, a cantilevered silicon crystal is end cooled through attachment to a nickel–iron Invar alloy manifold.

In this paper, the effect of LN2 flow on temperature distribution and distortion of the optical surface of the first crystal for the I20 monochromator at Diamond Light Source is investigated numerically. Comparison is made between a one-way coupled thermal-structural model and a one-way coupled fluid-thermal-structural model. The importance of considering fluid flow when predicting performance under beamline conditions is highlighted.

2. Model development

The numerical modelling work utilised simulations of the first crystal for the I20 monochromator at Diamond Light Source. Two models were created: a one-way coupled thermal-structural (no flow) and a one-way coupled fluid-thermal-structural (flow). The simulations were developed using COMSOL Multiphysics 6.0 [10], as detailed in the following subsections.

2.1. Geometry

The first crystal monochromator assembly used on the I20 beamline at the Diamond Light Source is shown in Figure 1. A copper heat exchanger surrounds a silicon crystal. The copper heat exchanger contains fluid channels in the side panels, through which LN2 flows. A layer of indium foil is placed between the copper and silicon to facilitate effective heat transfer.

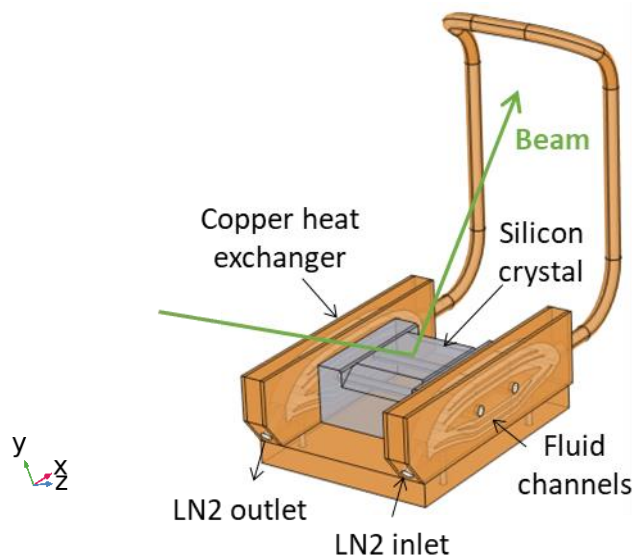


Figure 1. Schematic diagram of first crystal for the I20 monochromator at Diamond Light Source.

2.2. Meshing

The geometry was meshed using an in-built algorithm in COMSOL. A tetrahedral mesh was specified, with the global mesh set to extremely fine. A face sizing of 0.01 mm was applied to optical surface. The fluid-structure interactions were handled through a boundary layer mesh in the fluid-thermal-structural model.

2.3. Material properties

Material properties for copper and silicon were taken from the NIST database, with the temperature dependence of values for thermal conductivity (W/(m.K)), thermal expansion coefficient (1/K) and specific heat capacity ((J/K)/kg) over a temperature range of 70 K to 200 K considered [11,12].

2.4. Boundary conditions

Fixed supports were applied to four mounting holes in the base of the copper heat exchanger, visible in Figure 1. The thermal boundaries between the copper and silicon were modelled as thermally conductive boundaries with a thermal contact conductance of 1000 W/m² and 200 W/m² for the side interfaces and base interface, respectively. The side contact interface is representative of the conductance of a silicon-indium-copper boundary under full contact pressures, with the base value being representative of a boundary with low contact pressure [13]. To simulate the thermal loading, a heat flow of 600 W was applied uniformly over the projected beam footprint of 14.17 mm x 21.5 mm, which is representative of one of the multiple incident beam footprints which can be created on the first crystal as it moves through its rocking curve. For the no flow model, the temperature of all inner faces of the cooling channels in the copper heat exchanger was set to 70 K. For the flow model, fan conditions were used to define the LN2 flow direction at the inlets and outlets shown in Figure 1. Normal flow is applied, with an input pressure 1 MPa.

3. Results and discussion

The numerical modelling work focused on a comparison of predictions for i) temperature profile of reflecting surface and ii) the flatness of the reflecting surface for the no flow and flow models.

3.1. Effect of flow rate on peak temperature of reflecting surface

Simulations were conducted in which inlet flow rate was varied between 1 and 6 L/min, and the inlet temperature was set to 70 K, 77 K and 80 K, representative of assumed fluid temperature, the temperature of phase change at standard pressure and the temperature of phase change at working pressures, respectively. Peak surface temperature as a function of LN2 flow rate is shown in Figure 2 for both the no flow and flow models.

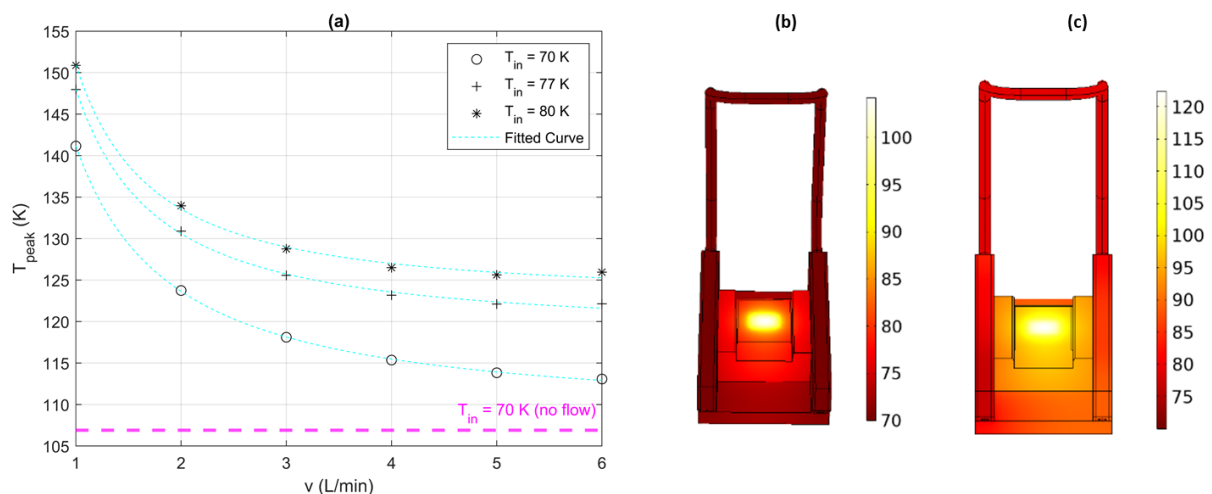


Figure 2. Temperature distribution in the assembly with (a) peak surface temperature (T_{peak}) as a function of LN2 flow rate, (b) temperature distribution for the no flow model and (c) temperature distribution for the flow model ($v = 3$ L/min, $T_{in} = 70$ K).

Figure 2 (a) shows that the variation in peak surface temperature with LN2 flow rate can accurately be described using a two-term power series model. These results highlight the importance of specifying an accurate inlet temperature in terms of the accuracy of prediction. As can be seen, an

approximate drop of 25 K occurs between 1 L/min and 6 L/min. Figure 2 (a) also reveals a significant underestimation of peak surface temperature in the absence of flow (e.g., approximately 20% at 3 L/min where $T_{in} = 80$ K). Figures 2 (b-c) reveal the influence of considering fluid flow on the temperature distribution in the assembly, with the temperature difference at the inlet and outlet clearly visible in Figure 2 (c).

3.2. Flatness of reflecting surface

The total deformation of the optical surfaces for both the no flow and flow models are shown in Figure 3.

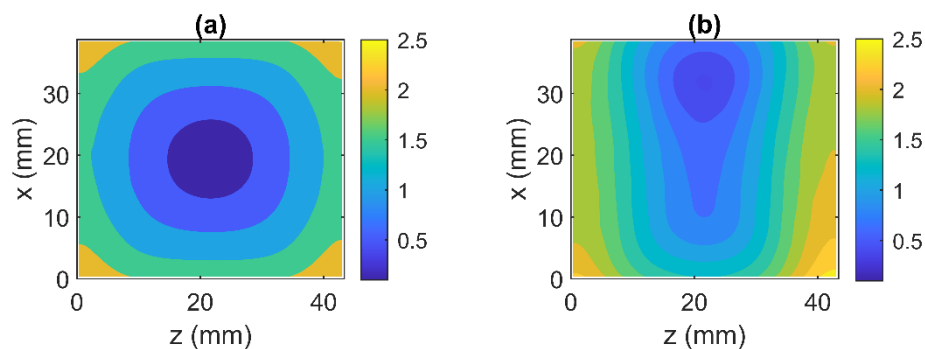


Figure 3. Distortion of the optical surface (μm) for (a) no flow model and (b) flow model ($v = 3$ L/min, $T_{in} = 70$ K).

Figure 3 shows the large disparity between the distortion profiles predicted by the no flow and flow models. The no flow model in Figure 3 (a) predicts a largely symmetrical deformation under load. When flow is considered however, a significant asymmetry is observed, with the point of largest deformation moving from the center of the crystal to nearer the edge, as shown in Figure 3 (b). This can be attributed to asymmetry in the temperature distribution in the flow model. The asymmetry in distortion of the optical surface in Figure 3 (b) is most prominent in the meridional direction, which will have a comparatively greater magnitude of influence on angular distortion of the diffracted beam [8].

4. Conclusions

In this paper, the effect of considering fluid flow on the temperature distribution and distortion of the optical surface of the first crystal for the I20 monochromator at Diamond Light Source was investigated using numerical simulation. Predictions from two models were compared: a one-way coupled thermal-structural (no flow) model and a one-way coupled fluid-thermal-structural (flow) model. It was found that peak surface temperature was underestimated by approximately 20% for models which do not consider fluid flow. It was also shown that asymmetry in the temperature distribution in models considering fluid flow leads to asymmetry in distortion of the optical surface, which has the potential to impact on angular distortion of the diffracted beam. Accurate modelling of heat load management in X-ray optics is essential in the design of next generation optics. Explicitly modelling fluid flow allows for more accurate prediction of performance under beamline conditions.

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