A Thermal Exploration of Different Monochromator Crystal Designs

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Abstract

Eight potential monochromator crystal designs were subjected to a combination of three different beam powers on two different footprints. The temperature and thermal deformation were determined for each. It was found that thermal deformation of the lattice is negligible compared to the surface curvature, and that while the thinnest crystal wafer showed the smallest temperature increase, crystals cooled from the bottom alone demonstrated a far more uniform thermal deformation and a larger radius of curvature.

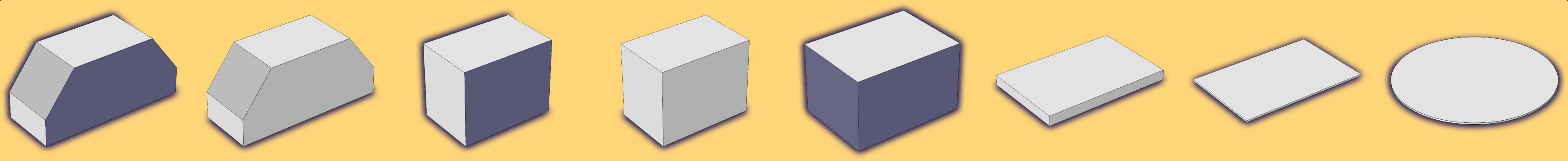
Monochromator crystals are used to select a single X-ray energy from a synchrotron's broad spectrum emission. However, the excess power from the other energies is absorbed into the crystal, causing significant heating and thermal deformations. In order to attempt to reduce or even eliminate this thermal deformation it must be understood how different parameters affect the system. To this end we have modelled several different designs of monochromator crystal to see what effect changing the geometry has on the thermal deformation.

As we were concerned primarily with thermal behaviours, we have made a number of approximations. The cooled surfaces remain at 80K throughout; this is to approximate the flow of liquid nitrogen with an ideal thermal contact. It is also assumed that each crystal is initially thermalized at a uniform temperature of 80K.

Despite varying designs between the different crystals, the boundary conditions used stay the same; each crystal is anchored by a single fixed point in the centre of its base, with a line extending from this point to the diffracting surface prescribed movement in the x- and y-directions. The entire crystal is also mounted to a spring foundation of ten Newtons per metre; this allowed the crystal much freedom of movement without being able to translate unrealistically. This combination of boundary conditions enables us to model free thermal expansion, giving an accurate image of how each crystal would behave.

There are two possible causes for concern here; the deformation of the diffracting surface could change both the spacing of the lattice layers and change the angle of incidence, both of which can degrade the Bragg diffraction desired. These are only an issue if they are non-uniform across the diffracting surface, as a uniform change can be allowed for when aligning the monochromator crystal. As such we have calculated the radius of curvature of the diffracting surface at the centre of the surface for each design.

We also calculated the lattice spacing as a function of temperature, to see if a non-uniform temperature gave rise to a non-uniform lattice that would have affected the Bragg diffraction. However, this showed that between 150K and 80K the lattice spacing varied only by 5.5×10^{-15}m, a variance of approximately 0.001% compared to the room temperature spacing. This shows that the variance of the lattice spacing is less likely to impact the Bragg diffraction than the radius of curvature of the diffracting surface, as the change in incident angle would have far more effect on the Bragg diffraction than the direct thermal lattice deformation.



The eight crystal designs tested. Visible cooled faces are tinted blue, while cooled faces not visible are represented by a dropped shadow.

The crystal design used at Diamond's I20 Beamline. Bottom face and both sides held at 80K.

The crystal design used at Diamond's I20 Beamline. Bottom face only held at 80K.

The crystal design used at Diamond's I20 beamline with the "shoulder" section removed. Bottom face and both sides held at 80K.

The crystal design used at Diamond's I20 beamline with the "shoulder" section removed. Bottom face only held at 80K.

Square crystal design, conducting region increased by 5mm each side. Bottom face and both sides held at 80K.

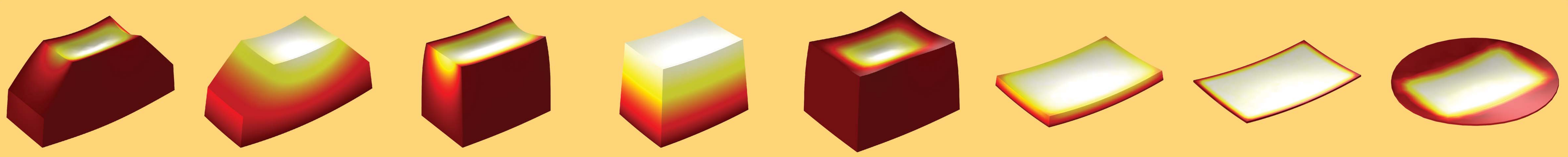
Square crystal design, flattened to 5mm thickness. Bottom face held at 80K.

Square crystal design, flattened to 0.5mm thickness. Bottom face held at 80K.

Standard silicon wafer, 0.5mm thickness. Bottom face held at 80K.

Three power loads were considered; 110 Watts, 550 Watts and 1100 Watts. This was to simulate the lowest, highest and future highest beam powers used at the I20 beamline at Diamond Light Source. These powers are applied as a beam profile using the Beer-Lambert Law, integrated across all of the energies produced by the I20 beamline. This models the intensity penetrating the surface and decreasing with position moving through the crystal.

We considered eight potential monochromator crystal designs at each power: the current monochromator design for Diamond's I20 beamline, a number of modifications to that crystal and then a silicon wafer. These designs were subjected to each incident power in both the minimum and maximum angles of the beam footprint, i.e. at a footprint of 36mm x 25mm representing an incident beam angle of 30° to the crystal and at a footprint of 5mm x 25mm representing an incident beam angle of 6° to the crystal. In each model the crystal was subjected to the beam for thirty seconds, after which it reached an equilibrium state.



The eight crystal designs after a thirty second exposure to a 1100W beam. Temperature represented by colour; red is coolest, white is hottest.

Cooling the side faces prevents them from deforming; this leads to a lower radius of curvature as the top face shrinks.

Not cooling the side faces allows the crystal to deform more uniformly, despite the diffracting surface reaching a higher temperature.

Trimming the crystal to just the active section actually increases deformation. This shows that the shoulders assist in heat dissipation.

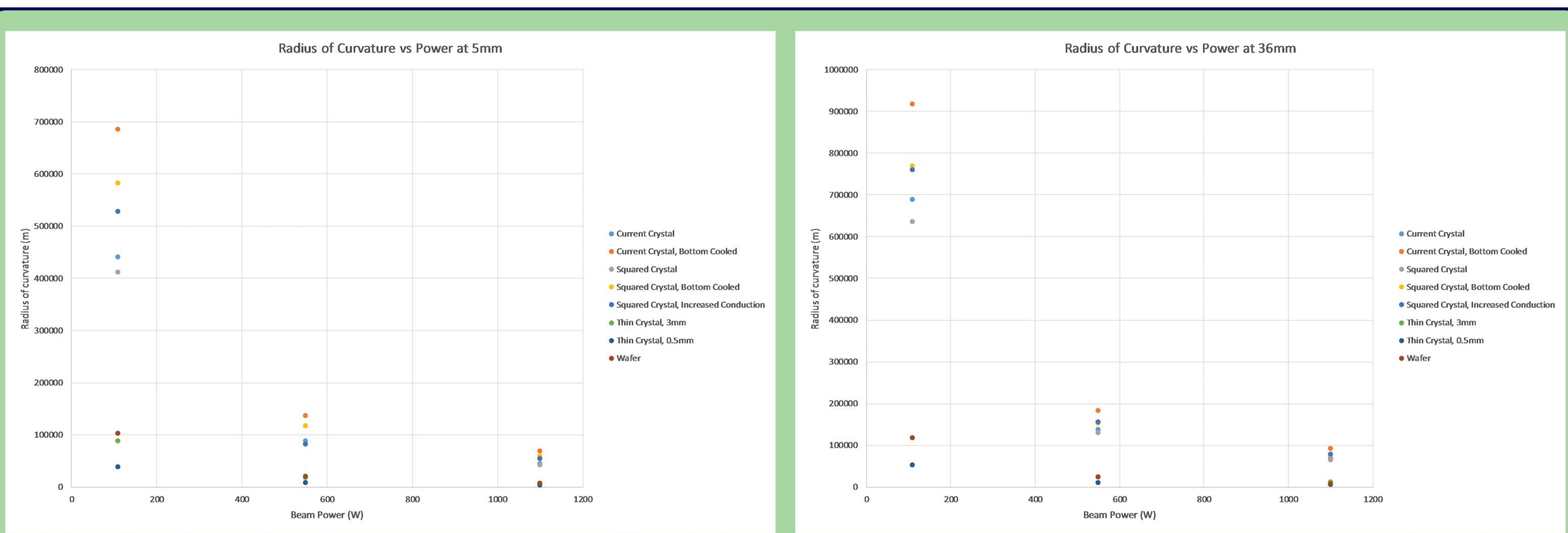
Cooling from the bottom alone results in a more uniform temperature. Not cooling the sides makes the surface more uniform.

Increasing the conducting region increases the total surface deformation. Less deformation is present in the diffracting region.

Thinner crystal design reduces the peak temperature, but the increased flexibility increases the bowing of the crystal.

Reducing the thickness further reduces the surface temperature by more and allows a more uniform temperature, but again causes the crystal to bow more.

The silicon wafer shows slightly less deformation than the rectangular crystal but still more than the larger designs.



Radius of curvature for both 36mm (left) and 5mm (right) beam footprints.

To help analyse the performance of the crystals the radius of curvature of each design at each power has been plotted on the two graphs to the left, showing the 36mm and 5mm footprints respectively.

A common feature found was that the thinner the crystal, the lower the maximum temperature. However, due to the innate flexibility of a thinner crystal they also show significant bowing with a lower radius of curvature.

The models with consistently the highest radius of curvature, and therefore the least bowing, are those cooled from the bottom alone. This setup allows the heat to dissipate more evenly, though more slowly, throughout the crystal, resulting in less variation in the deformation and a higher radius of curvature.

It is worth noting that all but the thinnest of the tested models fall well within Diamond's specified minimum radius of curvature of 40,000m. This suggests that far more important than the shape of the crystal is the thermal transport.

The crystal with the greatest radius of curvature throughout was the current I20 design cooled from the bottom only. This shows that bottom cooling does lead to less thermal deformation than cooling the sides, and that the shoulders on the design do improve the dissipation of heat through the crystal.

Future Work

The next step is to explore the mechanical side of these designs; how would they be held in good thermal contact with the heat exchangers and what steps can be taken to minimise mechanical stresses upon them. Many synchrotron facilities clamp their monochromator crystals between heat exchangers to hold them in the beam path; this design is not compatible with the concept of cooling the crystal from the base alone. However, bolting directly down to a heat exchanger or cooling the bolting plate itself could cause stresses to develop in the diffracting surface as the crystal contracts from the surface. Further work is needed to ascertain the feasibility of this approach.

By modelling more accurate mechanical and thermal boundary conditions we will be able to ascertain the feasibility of each of the above crystal designs, as well as see which parameters are most important. Using this information we will be able to design more suitable crystals.

Another future focus will be on the use of parametric sweeps, optimising the shape in order to reduce the thermal deformation.

Feedback

Any feedback, questions or just want to talk about the work? Please feel free to contact the lead author, Joshua Stimson, at: Joshua.Stimson@bcu.ac.uk