Performance Prediction for a Hockey-Puck Silicon Crystal Monochromator at the Advanced Photon Source

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Abstract. One of the Key Performance Parameters of the upgrade of the Advanced Photon Source (APS) is the increase of the storage ring current from 100 to 150 mA. In order to anticipate the impact of this increased heat load on the X-ray optics of the beamlines, the APS has implemented a systematic review, by means of finite element analysis and computational fluid dynamics, of the thermal performance of the different types of monochromators installed at the highest-heat-load insertion device beamlines. We present here simulations of the performance of a directly liquid nitrogen-cooled silicon crystal, the hockey-puck design. Calculations of the temperature and slope error at multiple ring currents under multiple operational conditions, including the influence of power, cooling, and diffraction surface thickness are included.

1. Introduction
Cryogenically cooled silicon, high-heat-load monochromators have been successful at 3rd-generation radiation sources [1]. A directly cooled version, the hockey-puck design, has been in use for over ten years at three different beamlines at the Advanced Photon Source (APS) [2]. In general, these cryogenic X-ray optical components take advantage of the simultaneous reduction of thermal expansion coefficient and increase in thermal conductivity for Si [3] while avoiding boiling in the liquid nitrogen (LN₂) coolant. Finite element analysis (FEA) is used to calculate the thermal distortions and resulting surface slope errors of crystals [4-6] under varied operating conditions. As a rule of thumb, for double crystal monochromators, if the calculated slope error is comparable to half of the intrinsic Darwin width for that crystal, a sizable fraction of the flux is lost. In this report we present FEA simulations for the hockey-puck design. Calculations at different ring currents have been carried out for six operational conditions at a macromolecular crystallography beamline, APS Sector 19-ID.

2. The hockey-puck design
The main feature of the hockey-puck design is a flange-like silicon crystal elastically sealed to an Invar base [2], as shown in Figures 1 and 2. The crystal has a relief cut under the diffracting surface creating a thin web and decreasing the amount of power absorbed by the crystal [7]. On the cooling side, the crystal has fins that are sealed into the Invar base, allowing LN₂ to stream past. Sealing is provided by an In-foil-covered, elastic-metal “C-ring” seal clamped between the Si crystal and the
Invar base. This elastic ring compensates for the small thermal expansion mismatch between the parts during cooldown. No direct silicon bonding is required and no LN2 ports are intrinsic to the crystal.

**Figure 1.** The hockey-puck monochromator. a: crystal with undercut; b: cooling fins; c: cooling system; d: bench assembly (without shield). (As installed at SER-CAT)

**Figure 2.** Drawing of the hockey-puck monochromator. The flange-like crystal is mounted to an Invar base with a cut-out pocket.

### 3. Description of finite element analysis

#### 3.1. Power calculation

FEA calculations start with power generated by APS Undulator A, U33, propagating through a primary aperture of 4.2×2.1 mm² at 50.551 m to the crystal at 52.565 m without intervening windows or filters. Power absorption in the crystal by a layer of arbitrary thickness is calculated over the thermal footprint with SRUFF [8] using the source characteristics and corresponding Bragg angles for six selected energies. Differences in peak power density and total power as calculated by the SRUFF and XOP [9] codes are less than 1% [8]. The calculated power density is fit with a 4th-order Gaussian. Integration over the thermal footprint is the absorbed power by this layer of crystal.

#### 3.2. Heat transfer coefficient

Thermal input parameters for FEA analysis are calculated conventionally using i) the known crystal geometry, ii) experimentally set liquid nitrogen coolant conditions (volume, velocity, temperature, pressure), and iii) derived values of hydraulic diameter, Reynolds number, and Nusselt number, to yield a calculated heat transfer coefficient, $h=0.0043$ W/(mm² K). In this paper, a more conservative heat transfer coefficient of $h_{\text{eff}} = 0.003$ W/(mm² K) is used for the majority of the calculations.

#### 3.3. Model for finite element analysis

FEA analysis includes two steps: steady state thermal analysis followed by static structural analysis. For power absorption, a volumetric absorption model has been found to be better than either surface absorption or staggered layer models [5]. For absorption by a 1-mm-thick web, the absorption profile is split into ten 0.1-mm-thick layers, and the first layer is further split into ten 0.01-mm-thick layers, as shown in Figure 3. For the static structural analysis, zero vertical displacement is assigned at the location of the sealing ring and zero radial displacement at the geometric center of the sealing circle.

### 4. FEA predictions and discussion

A traditional FEA approach is used here, calculating surface temperatures, thermal strains, vertical displacements, and thermal slope errors along the meridian axis of the beam footprint.
4.1. Initial cooldown
A deformation calculation during cooldown from zero strain at room temperature to thermally strained at cryogenic temperature is –0.000231 from the FEA model and –0.000227 from analytical calculation; a reasonable agreement. The resulting slope change of the first crystal surface, due to the geometry of the system and cooldown deformation, is expected to be zero as confirmed by FEA.

4.2. Power effect
The slope error vs. power curve can generally be divided into three regions: linear, transition, and nonlinear [5, 6]. In the linear region, slope error increases with power. As power continues to increase, the slope error decreases in the transition region because the silicon expansion coefficient changes from negative to positive. Here, the thermal contraction (negative expansion) dominates the thermal deformation. In the third (nonlinear) region, the slope error increases rapidly with power as the contraction no longer dominates the thermal deformation. Since the slope error vs. power curve varies with the footprint size [5, 6], a modified linear power density (MLPD) was proposed to replace the total absorbed power [6]. The calculated peak-valley thermal slope error (Table 1) versus MLPD for the hockey-puck design is shown in Figure 4. It also generally falls into three categories: linear (< 35 W/mm), transition (~35 - 53 W/mm), and nonlinear (>53 W/mm).

Increasing the cooling efficiency, $h_{eff}$, changes these transitions (Figure 5). If the maximum value of slope error from the linear region is treated as one of failure criteria for the crystal, the hockey-puck crystal will work well at 150 mA. The thermal slope error is less than half of the Darwin width for a majority of the cases tested. It is known that the slope error is independent of the cooling coefficient in the linear region but not in the nonlinear region [5, 6]. For example, the slope errors at 13.474 keV in Table 1 show a strong nonlinear relationship when the storage ring current increases from 100 mA to 200 mA.

5. Summary
The hockey-puck crystal works well at 150 mA in terms of temperature and thermal slope error. The results in Table 1 predict that the temperature at the cooling fins will remain less than 85 K, the boiling point of LN$_2$ at 27 psi, for all energy selections at storage ring currents up to 200 mA. The thin-web undercut aids in maintaining this low interface temperature by lowering absorption and by elongating the thermal conduction path. Increasing web thickness causes a corresponding increase in temperature at the convection interface and an expected decrease of peak temperature and slope error at the diffraction surface. If the maximum value of slope error from the linear region is treated as an acceptable value for the crystal, the hockey-puck crystal works well for all energy selections at 150 mA and for 12.66 keV up to 200 mA.
### Table 1. Effect of power on the hockey-puck crystal with a 1-mm-thick web.

| Energy (keV) | Current (mA) | Peak power density* (W/mm²) | Power (W) | MLPD (W/mm) | Peak temperature (K) | Lowest temperature (K) | Slope error (arcsec) | Darwin width (arcsec) |
|-------------|--------------|-----------------------------|-----------|-------------|----------------------|------------------------|-----------------------|---------------------|
| 6.5 (1st harm.) | 100          | 1.52                        | 216       | 35.84       | 114.11               | 80.364                 | 2.55                  | 8.52 (Si-111)       |
|              | 150          | 2.28                        | 324       | 53.76       | 144.14               | 81.68                  | 1.65                  |                     |
|              | 200          | 3.04                        | 432       | 71.68       | 195.54               | 82.985                 | 8.23                  |                     |
| 12.66 (1st harm.) | 100         | 0.24                        | 48        | 4.99        | 82.21                | 78.299                 | 0.19                  | 4.22 (Si-111)       |
|              | 150          | 0.36                        | 72        | 7.48        | 84.992               | 78.595                 | 0.32                  |                     |
|              | 200          | 0.48                        | 96        | 9.97        | 87.656               | 78.893                 | 0.42                  |                     |
| 13.47 (3rd harm.) | 100         | 0.99                        | 304       | 30.15       | 113.69               | 81.456                 | 1.74                  | 3.96 (Si-111)       |
|              | 150          | 1.49                        | 456       | 45.23       | 141.58               | 83.278                 | 1.29                  |                     |
|              | 200          | 1.98                        | 613       | 60.75       | 192.21               | 85.119                 | 5.25                  |                     |
| 19.50 (3rd harm.) | 100         | 0.87                        | 253       | 18.99       | 99.967               | 80.813                 | 0.83                  | 2.72 (Si-111)       |
|              | 150          | 1.31                        | 380       | 28.49       | 115.05               | 82.348                 | 1.14                  |                     |
|              | 200          | 1.75                        | 507       | 37.99       | 134.12               | 83.865                 | 1.02                  |                     |
| 30.0 (3rd harm.) | 100         | 0.72                        | 132       | 16.24       | 93.542               | 79.334                 | 0.75                  | 0.37 (Si-333)       |
|              | 150          | 1.07                        | 198       | 24.36       | 104.2                | 80.145                 | 1.14                  |                     |
|              | 200          | 1.43                        | 264       | 32.48       | 116.13               | 80.952                 | 1.39                  |                     |
| 30.0 (5th harm.) | 100         | 1.30                        | 250       | 30.80       | 111.55               | 80.78                  | 1.29                  | 0.37 (Si-333)       |
|              | 150          | 1.94                        | 376       | 46.21       | 138.2                | 82.299                 | 0.89                  |                     |
|              | 200          | 2.59                        | 501       | 61.61       | 182.13               | 83.801                 | 3.86                  |                     |

*: The peak power density is for absorption by the first layer of 10 μm.

Figure 5. Cooling value effect, $h_{\text{eff}}$, on (a) temperature, (b) thermal strain and (c) slope error (Condition: energy 13.474keV, 3rd undulator harmonics, Si-111, current 100mA).

Acknowledgments
The authors thank Mati Meron for utilizing his code SRUFF and Catherine Eyberger for edit. The Advanced Photon Source and the Structural Biology Center at Sector 19 are Office of Science User Facilities operated for the U.S. Department of Energy, Office of Science and Office of Biological and Environmental Research by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

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