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Supporting information for article:

Performance of Quartz- and Sapphire-based double-crystal, high-resolution (~10 meV) RIXS monochromators under varying power loads

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S1. Finite Element Analysis

A 25×25×2 mm^3 bulk Quartz (309) crystal was modelled and analysed using ANSYS v17.2. The anisotropic properties of Quartz (thermal conductivity, thermal expansion, and Young's modulus) were taken into account[1]. The coordinates were defined so that the illuminated crystal face was the *x*-*y* plane, *z* points into the crystal and the *c*-axis lies in the *x*-*z* plane, 18.4° from surface normal (*z*), as shown in fig S1a. The beam intensity and power were modelled as a volumetric density function with Gaussian beam profiles for *x* and *y* and an exponential absorption decay in *z*. Incidence angle was taken to be normal (from 88.36°), any reflected or transmitted intensity were neglected. The power density *p* and total power *P* are calculated as:

$$p(x,y,z) = Ae^{-\left(\frac{x^2}{2\sigma_x{}^2}+\frac{y^2}{2\sigma_y{}^2}\right)}.e^{-\left(\frac{z}{l_z}\right)}, \qquad P = \int_{z>0} p\,dv = 2\pi A\sigma_x\sigma_y l_z$$

with the following parameters from actual beam profile measurements and attenuation length at 11.215 keV[2].

σ_x= 1.5mm FWHM/2.35 = 0.6383 mm

σ_y= 0.75mm FWHM/2.35 = 0.3191 mm

l_z=0.358 mm

where the value of *A* [Wm^{-3}] is adjusted to produce the beam power corresponding to the selected attenuation. The volumetric power input was implemented in ANSYS using the Mechanical APDL function generator. Natural convection in still air (h=10 Wm^{-2}K^{-1}) at 22°C was applied to the entire crystal surface, temperatures and strains were then recorded in their steady state. To model a strain free mounting, the "weak springs" constraint was used in ANSYS, where the unsupported object's rigid body motion resulting from small overall force imbalances is suppressed. The resulting "mounting strains" induced near the beam footprint were confirmed to be negligible compared to thermal strains even for the lowest power considered. A fine mesh was used for the center area (3×1.4×2 mm^3 *xyz*) with an element size of 0.15×0.175×0.0625 mm^3. Additional intermediate nodes were added when running the simulation to increase accuracy as needed but were not used in data post processing.

Data post-processing for the Finite-Element Model was done in Mathematica, where results for Normal Elastic Strain in the *z*-direction and Temperature distribution within the sample were evaluated. Simulated strained rocking curves are obtained from a weighted distribution of Bragg angle

displacements: the angular change $\Delta\theta$ [rad] of a volume element at position $\vec{\boldsymbol{r}}$ is directly proportional to the local normal strain $\boldsymbol{\epsilon}(\vec{\boldsymbol{r}})$ [m/m] via

$$\Delta\theta(\vec{r}) = \epsilon(\vec{r}) \tan\theta_{B0}$$

with θ_{B0} the unstrained Bragg angle and the local weight proportional to the power density times an exponential absorption factor to account for the reflected ray's exit path through the crystal. Note that for significant power loads the thermally strained crystal is not in the dynamical diffraction regime, therefore the depth dependence of the weights is approximated according to linear absorption, not to the dynamical extinction depth.

Assuming that thermal distortions only occur in the first crystal while the second crystal is essentially unaffected, measured widths of second-crystal rocking curves for practical power loads can be simulated by convolution of a broadened first-crystal reflectivity with an ideal second-crystal reflectivity. Representing the first-crystal reflectivity by its ideal width $\delta\theta$ plus a broadening $\Delta\theta_\sigma$ equal to the RMS value of the angular changes defined above, second-crystal rocking curve widths in Gaussian approximation are

$$\Delta\theta_2 \sim \sqrt{2\delta\theta^2 + \sqrt{8ln2}\,{\Delta\theta_\sigma}^2}$$

From the angular shift data the weighted mean is calculated as

$$\overline{\Delta\theta} = \frac{\sum_{\vec{r}} \Delta\theta(\vec{r})\, p(\vec{r})\, e^{-z/l_z}}{\sum_{\vec{r}} p(\vec{r})\, e^{-z/l_z}} \cong \frac{2}{P}\sum_{\vec{r}} \Delta\theta(\vec{r})\, p(\vec{r})\, e^{-z/l_z}$$

and the (biased) standard deviation is then

$${\Delta\theta_\sigma}^2 = \frac{2}{P}\sum_{\vec{r}} \left[\Delta\theta(\vec{r}) - \overline{\Delta\theta}\right]^2 p(\vec{r})\, e^{-z/l_z}$$

The resulting second crystal widths are plotted as the green curve in Fig. 5.

S2. Analytical model

Crystal Temperature profiles are modelled by an idealized thermal spreader such as those used for high power electronic devices. The model consists of **[13]** a continuous, circular (radius *a*) power source *P* on the surface of a semi-infinite (*z*>0) medium of isotropic thermal conductivity *K*. There is no heat flow anywhere else, and the temperature rise is relative to that far from the source. The temperature rise profile (in cylindrical coordinates, *z*>0) and maximum temperature rise (at the origin) are

$$\Delta T(r,z) = \Delta T_{max} \cdot F(\vec{r},a), \qquad F(\vec{r},a) = \int_0^\infty e^{-\lambda z} J_0(\lambda r) J_1(\lambda a)\frac{d\lambda}{\lambda}, \quad \Delta T_{max} = \frac{P}{K\pi a}$$

These spatial profiles *F* are the same for all powers and materials, unfortunately, they cannot be expressed in a closed form. Nevertheless, an estimation can still be obtained, as normal strain is relatively small and found to be mostly proportional to the temperature rise.

With these approximations, the weighted RMS of the local angular shifts can be written as

$$wRMS[\Delta\theta(\vec{r})] \sim \tan\theta_{B0}\ \alpha\ \zeta\ \Delta T_{max}\ \ \sigma_F$$

Where $\zeta<1$ represents a reduction of the linear thermal expansion coefficient α since each element volume is mechanically constrained to different degrees by the surrounding elements at different temperatures, and σ_F is the weighted RMS value of the F-profiles. Numerical values for σ_F were obtained via Monte Carlo. Estimating the thermoelastic strain field of a semi-infinite heat spreader poses a much harder problem and is not necessary for an estimation, so values for ζ where obtained from FEA simulations as a weighted average of the effective linear thermal expansion relative to the unconstrained value.

These results are expected to be largely applicable to other cases since the constraints arise mostly from the semi-infinite geometry and the F-profiles, which, for beam sizes and attenuation lengths similar to those considered here, are not found to vary significantly.

Using the same Gaussian approximation as for the FEA results, a relative broadening figure is defined as the ratio of the full power second crystal rocking curve width to the reference width

$$\Delta\theta_{2,max}/\Delta\theta_{2,o} = \sqrt{1+S^2}$$

with

$$S = \frac{2\sqrt{ln2}\ \ wRMS[\Delta\theta(\vec{r})]}{\delta\theta}$$

Replacing

$$S = \frac{P}{a}\cdot\frac{\alpha}{K}\cdot\frac{\tan\theta_{B0}}{\delta\theta}\cdot\frac{2\sqrt{ln2}}{\pi}\ \sigma_F\ \zeta \sim \frac{P}{a}\cdot\frac{\alpha}{K}\cdot\frac{\tan\theta_{B0}}{\delta\theta}\cdot 0.03$$

The first factor depends on beam properties (power and size), the second on material properties (thermal conductivity and expansion coefficient), third on the selected reflection (Bragg angle and reflection width) and the last is a numerical factor containing constants and the numerical values mentioned above.