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EFFECT OF HEAT LOAD ON CRYO-COOLED MONOCHROMATORS AT THE EUROPEAN X-RAY FREE-ELECTRON LASER: SIMULATIONS AND FIRST EXPERIMENTAL OBSERVATIONS

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Abstract

Due to the high intensity of photon pulses generated at the European X-ray Free-Electron Laser facility, the heat load on silicon crystal monochromators becomes an issue. Here, first experimental data of heat load effects on the performance of a cryogenically cooled monochromator are presented. The measurements are compared with a model of X-ray diffraction taking beam absorption and heat deformation into account.

INTRODUCTION

A number of experimental techniques at hard XFELs require monochromators. Such devices reduce the spectral bandwidth, thus improving the temporal coherence of photon pulses. For instance, X-ray Photon Correlation Spectroscopy (XPCS) in wide-angle scattering benefits from increased speckle contrast enabled by a larger coherence time [1,2]. At European X-ray Free-Electron Laser (EuXFEL), several mJ of pulse energy can be reached in every femtosecond-long X-ray pulse. These pulses are arranged into trains containing from one to several hundreds of pulses. Within a train the pulses arrive at MHz repetition rate and ten trains are delivered per second. Currently, the facility operates at 1.1 MHz repetition rate. The planned 4.5 MHz repetition rate has recently been achieved [3]. Such intense radiation renders stable monochromator operation a challenge. Due to absorption and energy deposition in the crystals, the crystal lattice is deformed, which in turn affects the diffraction of X-rays. Here, we experimentally study the performance of cryogenically cooled Si(111) monochromator [4] for various numbers of pulses per train using first experimental data obtained at the Materials Imaging and Dynamics (MID) instrument of EuXFEL. Theoretical simulation results are also shown to estimate the heat load effect on XFEL pulse diffraction in crystals.

ROCKING CURVE MEASUREMENTS

Due to the stochastic nature of Self-Amplified Spontaneous Emission (SASE), the energy spectrum and temporal structure of XFEL pulses are irregular [5]. For example, a characteristic ~40 eV width of the energy spectrum results in ~0.2 fs coherence time.

At the MID instrument of EuXFEL a two-bounce artificial channel cut Si(111) monochromator in vertical scattering geometry has recently been commissioned and is available for user experiments in the range from about 6 to 18 keV. After two consecutive reflections, the spectral bandwidth is reduced from $\sim 5\cdot 10^{-3}$ to $\sim 10^{-4}$, which significantly increases the temporal coherence of pulses. The optical layout of the MID beamline (Fig. 1) includes offset mirrors, Si(111) and Si(220) monochromators and split-and-delay line (SDL) optics. For instance, the SDL (currently under production) will be used for the generation of pulses with the variable delay time. For the measurements presented in this paper, the Si(111) monochromator has been used.

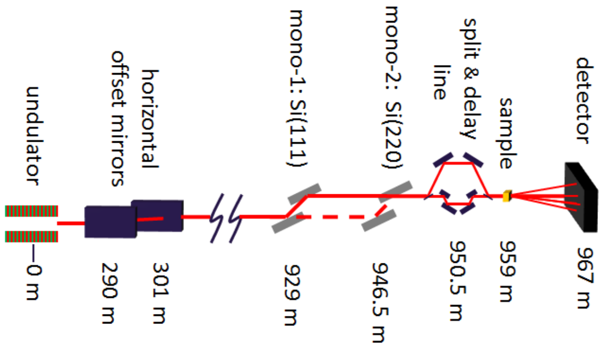

Figure 1: Sketch of MID beamline optical components. Relative positions of each component are shown under elements.

In order to analyse diffraction properties of the monochromator crystals, rocking curves have been measured for various numbers of pulses in the train, while the monochromator crystals have been cryo-cooled to 100 K. The energy of the hard X-rays in a pulse was ~0.25 mJ; the photon energy was 9 keV, the repetition rate 1 MHz, the beam size ~0.5 mm. The bunch charge was 250 pC, the electron energy 14 GeV. Rocking curve measurements were done with the pitch scan of the second crystal of the monochromator.

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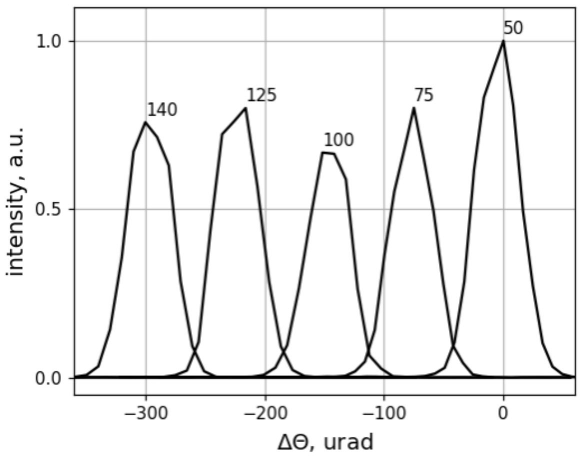

Figure 2: Rocking curves measured for various numbers of pulses per train, ΔΘ is the scan angle. Numbers of pulses are shown in the insets. The scan angles are shifted from the measured values for better visibility of the peaks.

The measured curves are shown in Fig. 2. After subtraction of a pedestal, the values are normalized to the numbers of pulses in trains. Due to the uncertainty in the calibration of crystal angle motor, the scan step is normalized to angles such that the width of the measured curve for 50 pulses in a train matches the width of double convolution of Darwin curve for the given reflection.

SIMULATIONS

An in-house developed code [6] has been used to estimate the radial distribution of temperature and deformations at a crystal surface. The used model considers temperature dependence of the specific heat and thermal expansion coefficient. Diffraction is modelled as described in [7], where the reflection amplitude at each point of the wavefront is defined by the local deformation caused by the heating. Rocking curves are considered as double convolution of a curve for one crystal. For the present simulations, heat flow is not considered. The incident beam is Gaussian with 0.5 mm full-width at half-maximum.

Crystal heating in the diffraction region leads to rocking curve widening and a shift towards smaller incidence angles. Figure 3 shows the theoretical rocking curve width widening for 0.25 mJ incident pulses and the measured widths calculated from experimental data in Fig. 2. Theoretical rocking curve width and shift caused by the heating are shown in Fig. 4. Since the initial temperature of the crystal is 100 K, the linear expansion coefficient of silicon changes from negative to positive values during heating. This leads to the peak in the shift curve and the plateau in the width curve. For larger intensities of the pulses, the heating effects are more pronounced. Sample theoretical rocking curves for various numbers of pulses in case of 1 mJ pulses are shown in Fig. 5. Rocking curve width and shift for this case are plotted in Fig. 6. The temperature at the beam center is shown in Fig. 7. For intensities and numbers of pulses considered here, the deviation from Bragg's law reaches several Darwin widths, as shown by horizontal lines in Fig. 7.

The simulations presented here enable to qualitatively predict the crystal heating under intense hard X-ray FEL pulses and its effect on the diffraction properties. However, for the full-scale modelling, heat flow, inhomogeneous distribution of the deformation and strain waves in three dimensions need to be taken into account and diffraction needs to be modelled using Takagi-Taupin equations. These results will be presented elsewhere.

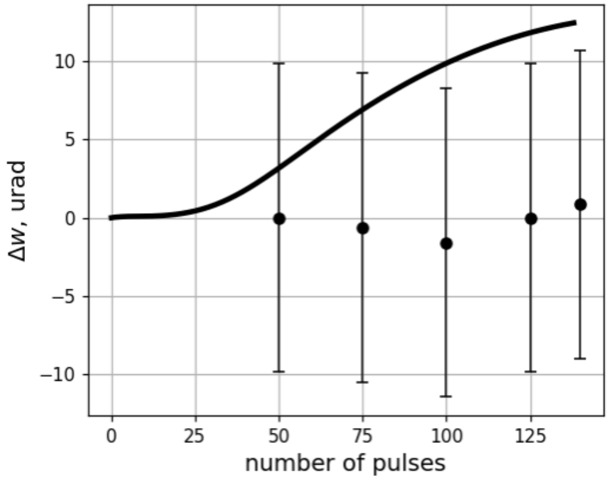

Figure 3: Difference of theoretical double-crystal rocking curve width from the width of double convolution of Darwin curve for a non-deformed crystal (solid line) and the widths calculated from measured data in Fig. 2 (dots). The error bars denote the scan step.

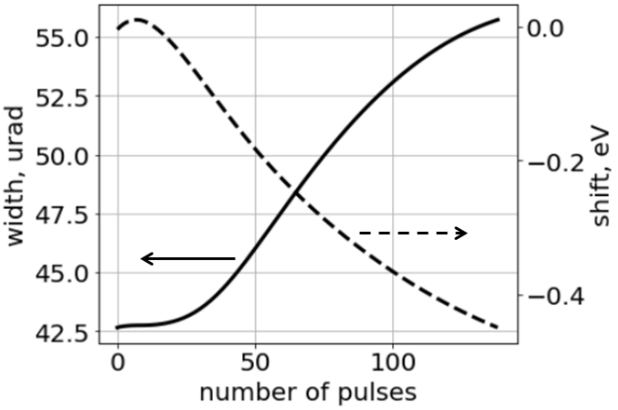

Figure 4: Shift of the center of the theoretical rocking curve for various numbers of pulses (dotted line, right vertical axis) and theoretical rocking curve width (solid line, left vertical axis). Values of the shift are normalized to energies using Bragg's law. Incident pulse energy is 0.25 mJ.

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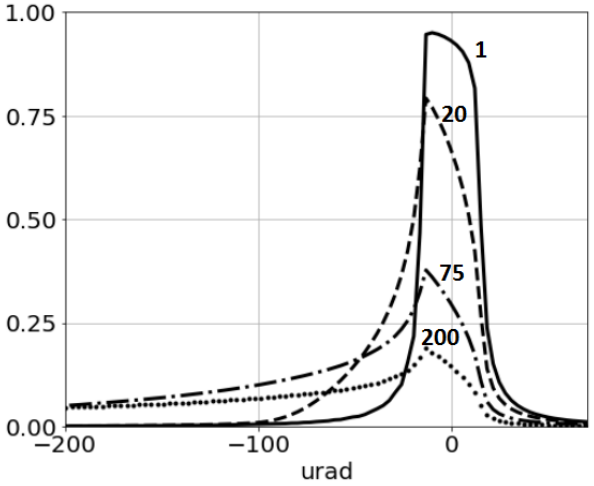

Figure 5: Theoretical rocking curves for various numbers of pulses and 1 mJ incident pulse energy.

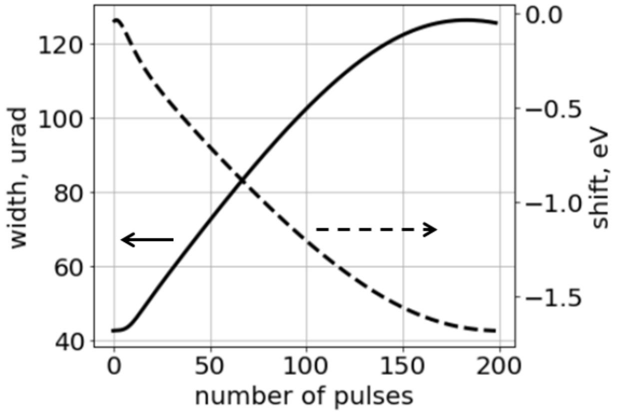

Figure 6: Rocking curve width and position for 1 mJ incident pulse energy.

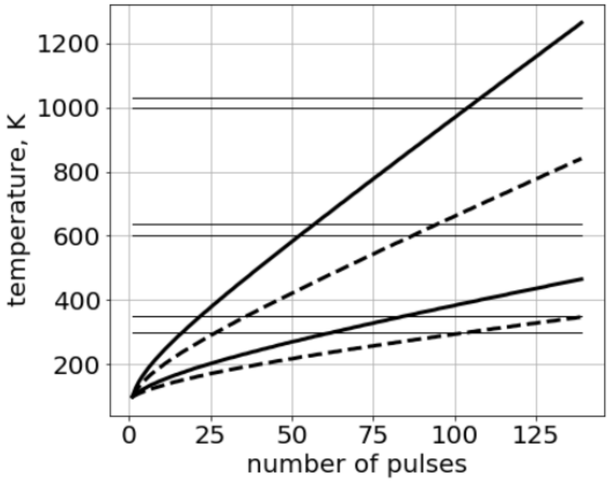

Figure 7: Temperatures at the center of the beam (solid lines) and at the distance corresponding to the σ of the beam profile (dashed lines) for 0.25 mJ pulses (bottom lines) and 1 mJ pulses (top lines). Horizontal lines denote the range of temperatures that cause the deformation within Darwin curve for various temperatures.

CONCLUSION

In conclusion, the monochromator has demonstrated stable operation under cryo-cooling and was tested at the repetition rate of 1 MHz and for up to 140 pulses per train; the energy of individual pulses was 0.25 mJ.

The simulated rocking curve widening during the train has not been observed at experiment. This might be due to losses in the beamline optics upstream of the monochromator, which might have led to an overestimation of the heating in the simulations. The account of the heat flow in the simulations will also lead to a smaller rocking curve widening.

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