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THERMAL EFFECTS ON BRAGG DIFFRACTION OF XFEL OPTICS*

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Abstract

Crystal optical devices are widely used in X-ray free electron laser (XFEL) systems, monochromators, beam splitters, high-reflectance backscattering mirrors, lenses, phase plates, diffraction gratings, and spectrometers. The absorption of X-ray in these optical devices can cause increase of temperature and consequent thermal deformation, which can dynamically change in optic output. In self-seeding XFEL, the thermal deformation and strain in monochromator could cause significant seed quality degradation: central energy shift, band broadening and reduction in seed power. To quantitatively estimate the impact of thermomechanical effects on seed quality, we conduct thermomechanical simulations combined with diffraction to evaluate the seed quality with residual temperature field in a pump-probe manner. With our results, we show that a critical repetition rate could be determined, once the criteria for deviation of the seed quality are selected. This tool shows great potential for the design of XFEL optics for stable operation.

INTRODUCTION

The performance of the optics in synchrotron and XFEL applications has long been limited by the thermal load. To understand and relieve the thermal loading effects, many studies [1.2] have been performed. Different designs of the optics [3] have been proposed to improve their thermal performance. On the other hand, cooling and cryogenic operation [4, 5] are also reported to overcome the thermal difficulties. These technologies, unfortunately, have not been well adapted for some XFEL operating modes, such as the self-seeding mode.

In the self-seeding mode [6], one monochromator is implemented to separate the undulators into two segments. The self-amplified spontaneous emission (SASE) generated in the first segment of undulators passes through the monochromator to produce a coherent seed, which will then be amplified in the second segment of undulators. In this way, the coherence and brightness of the final XFEL can be significantly improved. However, the system performance can be severely undermined if the thermal load of the key component, the monochromator, exceeds the critical point. Bushuev [7, 8] demonstrated the thermal distortion of the rocking curves and indicated the possible degradation of the seed quality. Unfortunately, a quantitative description of the criterion, as well as a direct evaluation of the seed quality, is not yet clear.

In present study, we perform numerical simulation to quantitatively evaluate the seeding behaviour. This comprehensive thermal-mechanical-diffraction simulation is carried out in a pump-probe manner, but it can also be applied for quasi-steady multi-pulse situation. Our results provide insights to determine the critical parameters (such as repetition rate and single pulse dose) and implementation of the appropriate cooling techniques.

METHOD

The physical situation is illustrated by Fig. 1 below.

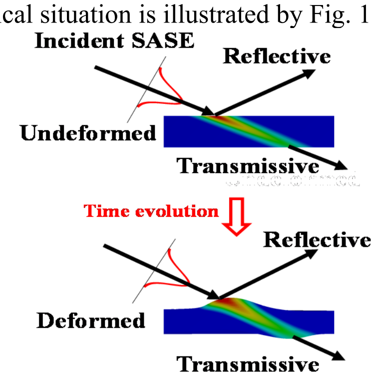

Figure 1: Schematic illustration of FEL induced thermal loads on crystal monochromators.

The incident SASE pulse from the first segment of the undulators interacts with the monochromator and splits into three parts: the reflected, transmitted and absorbed part. Among these parts, the reflected component contains the seed for reflective monochromator, while the transmitted part contains the seed for transmissive monochromator. The absorbed part, however, deposits energy into the monochromator, resulting in non-uniform temperature increase, which further develops into the strain field through thermal expansion. Next, when the second incident SASE pulse arrives, the interplanar distance between atoms in crystal monochromator deviates from the original status. This deviation causes the disturbance in wavelength of the seed, as governed by Bragg condition, thus undermines the seed quality.

Therefore, it is necessary to obtain the temperature and strain evolution in crystal monochromator. We employ 3D finite element analysis by ANSYS Mechanical APDL solver for thermal and mechanical simulation. On the other hand, to obtain the diffraction behavior (rocking curve) under thermal loads, Shvyd'ko's method [9] is employed. In this work, we only consider the first two FEL pulses in a pump-probe manner, but further investigation will be carried out to study the thermal loading effects at quasi-steady state.

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In detail, for the energy deposition by the first incident SASE beam, a Gaussian distribution is assumed for the beam transverse direction, while an exponential decay is assumed for beam longitudinal direction. This energy deposition is also assumed instantaneously in time since the heating process (typically finishes within tens of picoseconds) happens much faster than the thermal transport process. The laser induced temperature is then simulated and exported to static structural module at selected delay times. Based on the frozen temperature fields, static strain field can then be simulated and exported into an in-house MATLAB script to evaluate the thermally distorted rocking curves as well as the seed quality at the corresponding moment.

The above described process can be repeated with the energy deposition by the second, third and more SASE pulses considered. But to detour the expensive computational load, we take the results of the first two pulses to yield some direct estimation for the seed quality at different repetition rates (the reciprocal of the corresponding delay time in this case). Also, the strain waves induced by the FEL pules have not been included in this work yet but will be done in the future.

TEMPERATURE AND STRAIN FIELD

The deposited energy leads to an initial localized temperature increase, then gets dissipated into the material. The maximal temperature and temperature gradient drop quickly with time, and thus the strain.

Figure 2 displays an example of the temperature, deformation and strain field for SASE central photon energy of 8.5 keV, single shot dose energy of 100 µJ, beam transverse size of 47.1 µm (FWHM) and relative bandwidth of 1.2×10^{-3} (FWHM).

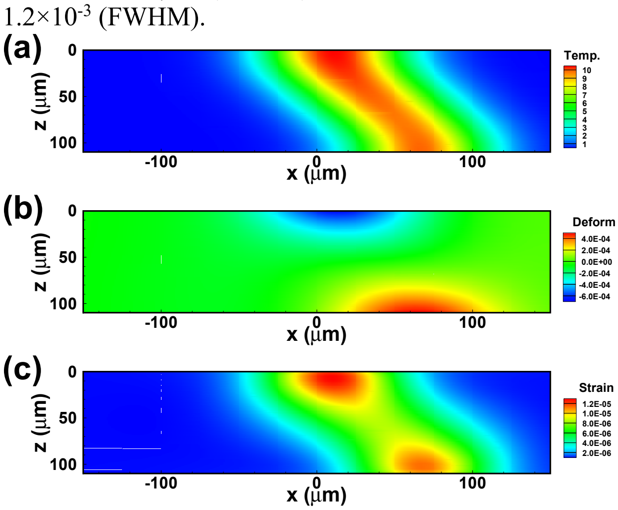

Figure 2: An example of thermal loads for transmissive monochromator with diamond (0 0 4) at 8.5 keV and delay time 0.2 µs: contours in central plane (symmetric plane) of (a) temperature increase in °C, (b) deformation in µm and (c) strain.

The temperature is initially tilted, since the incidence of the SASE is at certain Bragg angle. It then evolves towards in-plane directions (parallel to the crystal surface). Similar behaviour can be observed for the deformation and strain.

The thermal strain is dominant over the elastic strain. Compared to the Darwin width, which is about 10^{-5} for diamond (0 0 4), the strain is of a comparable order of magnitude. Therefore, it is expected that the rocking curve can be significantly distorted by the thermal loads.

ROCKING CURVES AND SEED QUALITY

After the deformation and strain are simulated by ANSYS, these results are then fed into an in-house MATLAB script to obtain the thermally distorted rocking curves using Shvyd'ko's method [9]. The thermally distorted rocking curves are further employed to evaluate the thermally affected seed quality. Figure 3 presents the results of the rocking curves and seed under the thermal load.

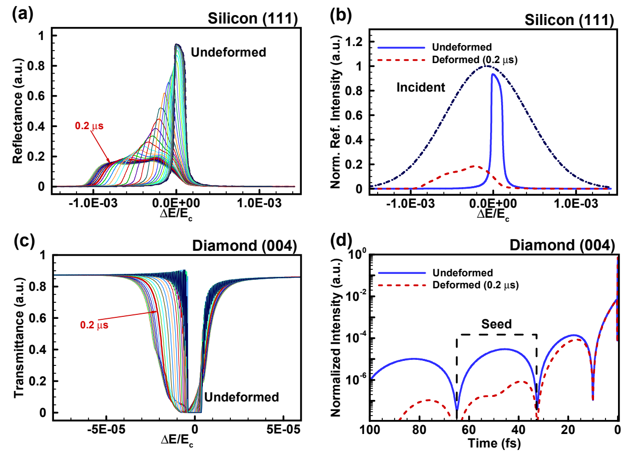

Figure 3: The rocking curve recovery history and the thermally distorted seed at delay time of 0.2 µs for reflective monochromator using silicon (1 1 1) in (a) and (b), and for transmissive monochromator using diamond (0 0 4) in (c) and (d).

Under thermal loads, the seed central photon energy, bandwidth and seed power are all significantly undermined, especially at short delay time, or effectively high repetition rate. We take the delay time of 0.2 µs as an example, which corresponds to a repetition rate of 5 MHz (close to the repetition rate of EuroXFEL machine). For reflective monochromator, as shown in Fig. 3(b), the relative seed central photon energy shift is -3.5×10^{-4}, and the seed spectrum experiences a severe broadening in FWHM (7.4×10^{-4} compared to 1.4×10^{-4} for the undeformed case or designed value). In addition, the peak power of the seed also drops to 19.8% of the designed value, though the total seed dose remains 77% of the designed total seed dose. For transmissive monochromator, the thermal load impact is different. The seed central photon energy (a relative shift of -1.5×10^{-5}) and bandwidth (1.6×10^{-5} compared to designed value of 1.8×10^{-5}) are not very significantly affected and consequently not shown here. However, the total seed dose drops to only 2% of the designed value, implying that there is almost no seed coming out of the monochromator.

As delay time increases, the rocking curves and seed quality gradually recover to its designed status. This is because the thermal load tends to homogenize due to the energy transport. However, in quasi-steady multi-pulse situa-

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tion, there could be an overall shift of the seed photon energy, as the whole piece of crystal is heated up and expands. We will continue studying the thermal loading effects in this situation.

Finally, a critical repetition rate can be simply determined once a criterion is selected. For example, for silicon (1 1 1) reflective monochromator, if the acceptable seed central photon energy shift is selected as 1.4×10^{-4}, the corresponding delay time could be determined from the simulation to be around 9 µs, or 111 kHz. But one should be reminded that the results may be different in a quasi-steady situation.

CONCLUSION

In conclusion, we perform finite element analysis to obtain the surface thermal slope and strain of both reflective monochromator using silicon (1 1 1) and transmissive monochromator using diamond (0 0 4), allowing a quantitative evaluation of the seed quality under thermal loads in a pump-probe manner. With specified criterion, critical delay time can be inversely determined and thus the critical repetition rate. Further investigation for thermal loading effects at quasi-steady state will be performed, and dynamic diffraction model will also be included to account for the non-uniform strain along the optical path.

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