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THERMAL AND MECHANICAL STABILITY OF BRAGG REFLECTORS UNDER PULSED XFEL-RADIATION*

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Abstract

Free-electron laser (FEL) x-ray radiation can deliver pulses with a huge amount of energy in short time duration. X-ray optics like Bragg reflectors therefore must be chosen in a way that they can withstand radiation-material interaction without getting damaged so that they can maintain their technical functionality. Therefore thermal and mechanical reactions of Bragg reflectors to the radiation induced thermal strain and force (radiation pressure) have been considered in this study. The theory of thermoelasticity has been used to simulate the strain conditions at saturation of the amplifying process in an X-ray free-electron laser oscillator (XFELO). One aim of this study was to investigate, if the radiation pressure could be an effect that gives a considerable contribution to the strain propagation. The results of the simulations have shown that, if Bragg backscattering of the X-ray pulse by a diamond crystal with 99% reflectivity and 1% absorptivity is assumed, the value of the thermally induced strain is about two magnitudes higher than the radiation pressure induced strain. Also a measurement method which could be used to detect the simulated strain is shortly discussed at the end of this document.

INTRODUCTION

The European XFEL is under commissioning, the first lasing was achieved in May 2017. The facility provides radiation with high peak brilliance on the order of 10^{33} photons ($[s^{-1}mm^{-2}mrad^{-2}]$ / (0.1% BW)), with up to 27000 photon pulses s^{-1}, which are delivered in 600 µs long pulse trains with a repetition rate of 10 Hz [1]. These conditions give the possibility for the realization of an X-ray free-electron laser oscillator (XFELO) [2]. With the integration of an XFELO at the European XFEL longitudinally full coherent pulses and an increase of the peak brilliance by one order magnitude should be achievable. The bandwidth would reduce to a value of $\frac{\Delta E}{E} = 1.6 \cdot 10^{-6}$. The amount of energy in saturation of these photon pulses would be about 300 µJ to 1 mJ. The small bandwidth is in the order of the Darwin width and therefore nearly the whole amount of energy per photon pulse would be Bragg reflected. Shvyd'ko et al have shown that nowadays diamond crystals are available, which have reflectivity of more than 99% in case of Bragg reflection [3]. Hence, by considering such a Bragg reflector for saturated XFELO radiation the maximum amount of pulse energy which is absorbed inside the penetration depth (extinction length) can be at most 1%.

Under these radiation conditions the thermal and mechanical stability of Bragg-reflectors, which are necessary for the XFELO, have to be considered in detail. Therefore simulations of the strain induced by X-ray radiation in a diamond crystal have been performed in this study. Strain has a direct influence on the lattice parameter and therefore changes the Bragg reflection conditions, which can influence the stability of an XFELO.

When energy of electromagnetic radiation is interacting with a solid body in the timespan of femtoseconds, the system moves out of thermal equilibrium. Theoretical and experimental studies [4] [5] have shown that the dynamics of this thermal expansion, apart from heat transfer, can be explained as a mechanical disturbance. The absorbed energy creates thermal stress which is propagating as a longitudinal wave with the speed of sound into the irradiated material [6].

Besides the creation of a thermally induced strain wave, the radiation pressure could also create such a strain propagation. This could be important in cases where the amount of reflected energy is large and the absorbed portion is small. These conditions exist for Bragg reflected radiation that a saturated XFELO would deliver, because the thermal expansion is directly influenced by the amount of energy that is absorbed whereas radiation pressure occurs for absorption as well as for reflection. However, the force which is induced by radiation pressure is very small due to the small impulse of a photon and therefore the thermal effects are normally dominating this effect.

Mechanical deflection of micro beams caused by the radiation pressure have been investigated theoretically and experimentally by several authors [7–10]. However, in the present study the strain propagation and not the deflection is the parameter of interest. To the best knowledge of the authors this kind of strain propagation has not been considered by any other theoretical or experimental investigation so far.

PROBLEM FORMULATION

Stoupin *et al.* [11] have done experimental studies on the strain propagation caused by a ≈ 8 ps laser pulse in diamond. The strain has been assumed to propagate only along the z direction (Fig. 2 a), which is valid for $\sqrt{A} >> d$, where A is the radiated area of a crystal with the thickness d. In case of a low-flux laser pulse the heat dissipation can be neglected for the first tens nanoseconds after the radiation-material interaction and the formulas of thermoelasticity [12] yields:

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$$\sigma_{zz} = Y\frac{\partial u(z,t)}{\partial z} - \alpha Y \Delta T(z), \text{ and} \tag{1}$$

$$\frac{\partial \sigma_{zz}}{\partial z} + F(z,t) = \rho\frac{\partial^2 u(z,t)}{\partial t^2}, \tag{2}$$

where Y is the Young's modulus, α is the linear thermal expansion coefficient and ρ is the mass density. u is the displacement and its derivative is the strain $\epsilon_{zz} = \frac{\partial u(z,t)}{\partial z}$ and $F(z,t)$ the body force.

The Dirichlet boundary conditions are that the stress σ_{zz} vanishes at the crystal boundaries and the initial conditions at t=0 are that the spatial and temporal derivative of the displacement is zero.

Absorption and reflection of saturated XFELO X-ray radiation at a diamond Bragg reflector

In this study a Bragg reflection under the following conditions is considered: a diamond crystal C 444 in backscattering $\Theta = 90°$ configuration, FEL radiation with $E = 12.04keV$ ($\lambda = 1.03$ Å), a beam radius of $r \approx 40\,\mu$m, a pulse duration of $t_p \approx 70$ fs, an amount of energy per pulse of E_p= 1 mJ, a bandwidth of ≈ 20 meV equal to the Darwin width (≈ 20 meV for C 444), a reflectivity of 99%, an absorptivity of 1% , an extinction length $l_{ext} \approx 20\,\mu$m and a crystal thickness of 150 µm.

Following the work of Thomson *et al.* [5] the temperature rise can be described by

$$\Delta T(z) = \Delta T_{0,R} e^{-z/l_{ext}}, \text{ where} \tag{3}$$

$$\Delta T_{0,R} = \frac{0.01 E_p}{A \rho c_v l_{ext}}. \tag{4}$$

In this Formula c_v is the specific heat capacity which is 509 J/(kg K) for diamond.

The body force $F(z,t)$ which is induced by radiation pressure [10] is

$$F(z,t) = F_{0,R} e^{-z/l_{ext}} \cdot tri(t), \text{ where} \tag{5}$$

$$F_{0,R} = \frac{0.99 \cdot 2E_p}{t_p c_o A l_{ext}}, \tag{6}$$

and c_0 is the speed of light. Unlike the thermal gradient $\Delta T(z)$ the body force $F(z,t)$ must be time dependent, because it only exists when the photons interact with the material. To consider this, a triangular function $tri(t)$, whose full width half maximum (FWHM) is the photon pulse duration, has be multiplied to the equation.

Another point that has to be considered in case of radiation pressure induced body force is, that the energy transferred to the lattice will cause a constant velocity of the entire considered system due to Newtons laws. To consider this the boundary conditions for the stress have been modified in this study to be:

$$\sigma_{zz}|_{z=0} = D \cdot u \text{ and } \sigma_{zz}|_{z=d} = -D \cdot u, \tag{7}$$

where, u is the displacement and D is a spring constant the value of which depends on the clamping of the crystal. Using the assumptions of the Euler–Bernoulli beam theory the spring constant for a cantilever beam yields:

$$D = \frac{3 Y I_y}{L^3}. \tag{8}$$

In this study a rectangular crystal with $I_y = b \cdot d^3/12$ is considered, where $d = 150\,\mu$m is the thickness and b is the width with a value of 0.5 mm. The length L is 5 mm, so D becomes 4.1 kN/m.

RESULTS OF THE SIMULATED STRAIN PROPAGATION

Simulations of the stress propagation are calculated by solving Eq. 2 with the finite element (FEM) software COMSOL Multiphysics®. A FEM calculation of the strain in the case where the body force $F(z,t)$ in Eq. 2 is zero, is compared to an analytical solution which is presented in the study of Stoupin *et al.* [11]. Calculations using the same system parameters are show in Fig. 1. Both calculations give the same results for the strain values and the temporal function. However, the FEM solution shows some minor oscillations on the main signal which could be reduced by using a smaller mesh size, but this would significantly prolong the calculation time.

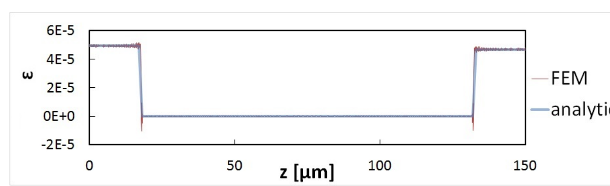

Figure 1: Comparison of numerical and analytical calculation of strain for a fixed time value

The heat expansion and the body force induced by the radiation pressure will create a longitudinal strain wave that is assumed to propagate with the speed of sound in z direction (illustration Fig. 2 a). The diagram that is used to illustrate the strain propagation can be explained by Fig. 2 b. The strain will propagate with the speed of sound between the boundaries of the crystal. In this study only a time duration of a strain wave that travels through the crystal once (back and forth) is considered.

The results of the discussed situations of the section "Problem Formulation" are show in Fig. 3. The maximum value to the strain caused by dynamical thermal expansion is about two magnitudes higher than the one due to radiation pressure in the considered case. However, the propagation of radiation pressure could be a considerable effect if the situation would be created were the absorption is even smaller than

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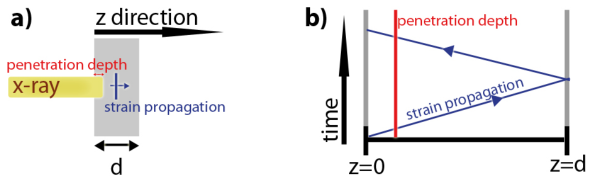

Figure 2: a) Illustration of the radiation-material interaction with a penetration depth smaller than the crystal thickness b) description of the plots used in the present study

1%. For example this could be the case if Bragg reflection of a diamond crystal far form backscattering would be chosen where the reflectivity is up to 99.9% [3]. Also the clamping of the crystal could perhaps increase the value of the strain. To find situation were the radiation pressure is the dominating effect and therefore a direct measurement would be feasible, further simulations are necessary.

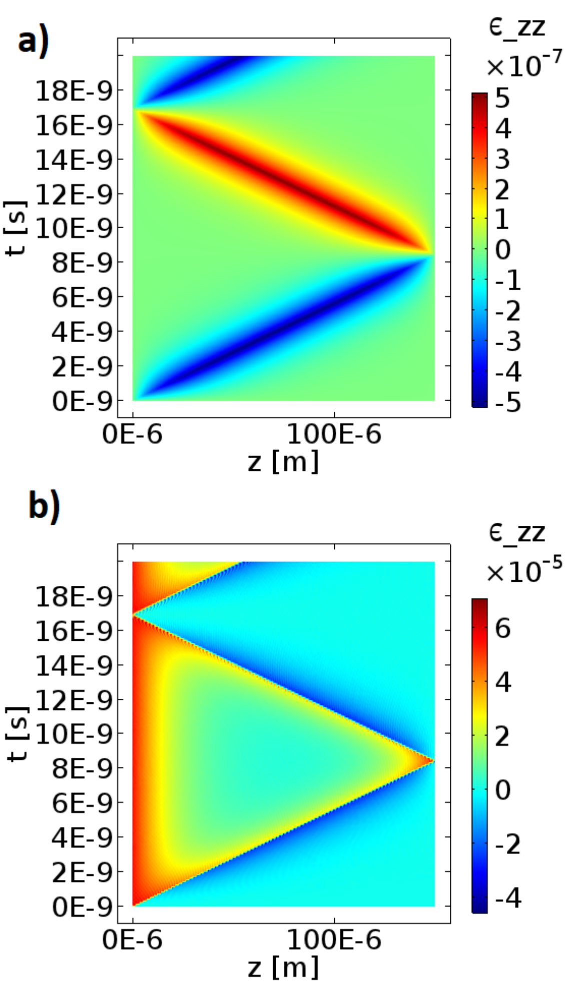

Figure 3: FEM calculations of the cases discussed in section “Problem Formulation” **a)** strain propagations due to body force induced by radiation pressure **b)** strain propagation due to dynamical thermal expansion.

A general problem that has to be mentioned in the presented simulation is that the considered beam radius is so small that a 1D simulation would not be exact anymore. However, the results give a first estimation on the order of magnitude of the strain induced by an XFELO pulse.

Investigation of the strain during the first nanoseconds as presented in this paper provides information about the important physics at the creation of strain and its initial propagation in diamond. The relaxation of this strain taking place on larger time scales was not part of the present study. However, it is of paramount relevance for the operation of an XFELO since it determines the amount of strain remaining after a round trip in the oscillator. This aspect is experimentally investigated by Maag *et al.* [13].

Experimental setup for strain detection

Stoupin *et al.* [11] have measured the transient strain by observing the temporal change of Bragg reflection. The strain has a direct effect on the local lattice parameters and therefore changes a diffraction pattern the shape of which can be simulated with the dynamical diffraction theory and can then be compared with the measured signal. A great advantage of this method is that the strain, which is the value of interest, has a direct influence on the measured signal. However, this method needs coherent x ray radiation which can only be created with monochromatised synchrotron or FEL radiation. A different method to measure the strain is proposed by Thomson et al. [5] and is based on the change of reflectivity ΔR of an optical probe laser after absorption of a pump laser. This is caused by the change of the optical constants as a result of the propagating strain ($\Delta n(z,t) = \frac{\partial n}{\partial \epsilon_{zz}} \epsilon_{zz}$ and $\Delta\kappa(z,t) = \frac{\partial \kappa}{\partial \epsilon_{zz}} \epsilon_{zz}$) induced by the pump pulse. Here $\Delta n(z,t)$ and $\Delta\kappa(z,t)$ are the changes of the real and imaginary parts of the complex index of refraction, respectively, from their values n and κ in the absence of strain. The problem with this method is that values of $\frac{\partial n}{\partial \epsilon_{zz}}$ and $\frac{\partial \kappa}{\partial \epsilon_{zz}}$ have to be known. One possibility would be a calibration measurement of the reflectivity for a fixed wavelength for a material of interest. If such a measurement would be done, the presented experimental setup build up by Maag et al. [13] could be used to measure the strain propagation simulated in this study.

CONCLUSION

The results of the strain simulations in this study have shown, that for the considered XFELO setup the strain which is induced by dynamical thermal expansion is about two magnitudes higher than the strain induced by radiation pressure. However, for X-ray radiation with an bandwidth similar to the Darwin width and even smaller values of absorptivity, the radiation induced strain may become a considerable and experientially measurable effect in strain propagation.

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