



## Diamond crystal optics for self-seeding of hard X-rays in X-ray free-electron lasers

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### ABSTRACT

We report design, fabrication, and results of X-ray topography characterization of thin synthetic type IIa diamond crystal plates and crystal-holder assemblies developed for the Hard X-ray Self-Seeding project at the Linac Coherent Light Source. The goal of the project was to achieve generation of fully coherent hard X-rays using the self-seeding concept and the single-crystal diamond wake monochromator [Geloni et al., *J. Mod. Opt.* 58, 1391 (2011)]. High crystal quality, crystal thickness of  $\approx 0.1$ – $0.2$  mm and strain-free crystal mount were the main requirements. Nearly defect-free diamond plates of (001) orientation, with thicknesses of 0.1 mm and 0.15 mm, and of a trapezoidal shape were fabricated and preliminarily evaluated. The plates were further characterized using X-ray topography. These tests helped to minimize strain in crystals induced by mounting in crystal holders and to determine defect-free crystal regions. Self-seeding experiments were conducted at the Linac Coherent Light Source using the diamond plates and crystal-holder assemblies selected by our studies. Fully coherent 8.33-keV X-rays with  $5 \times 10^{-5}$  relative bandwidth were produced [Amann et al., *Nat. Photonics* 6, 693 (2012)].

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### 1. Introduction

Self-seeding of X-ray free-electron lasers (XFELs) is an emerging technology to generate highly brilliant fully coherent X-rays that will have a broad range of scientific applications in the near future. Conventional operation of an XFEL is based on the phenomenon of self-amplified spontaneous emission (SASE), which results from the interaction of electron bunches traveling with relativistic velocity through a series of undulators with an electromagnetic field emitted by these electrons. The resulting SASE radiation is transversely coherent; however, the longitudinal coherence defined by the radiation bandwidth is rather poor, which is a consequence of the start-up from shot noise. To improve the longitudinal coherence, two-stage SASE FELs have been proposed where radiation produced in the first stage (by the first series of undulators) is monochromatized and used in the second stage to seed lasing in the second series of undulators (i.e., self-seeding) [1–3].

The monochromatic seed radiation for hard X-rays can be produced by means of X-ray diffraction on perfect crystals. A recently proposed simplest self-seeding monochromator for hard X-rays consists of a single diamond crystal where time dependence of forward diffraction is utilized to produce a monochromatic seed wake field [3,4]. Diamond is the preferable material for XFEL crystal optics due to its unique

material properties such as high thermal conductivity [5], high radiation hardness [6], low X-ray absorption and small coefficient of thermal expansion [7], as well as record high reflectivity for hard X-rays in Bragg diffraction [8]. These properties help to minimize variations in the crystal lattice exposed to intense XFEL radiation and, therefore, facilitate stable performance of the optical components.

Another parameter that substantially affects the performance is crystal quality. Nearly defect-free type IIa diamond crystals with sizes suitable for applications in XFEL and synchrotron X-ray crystal optics have recently become available [9–11]. Fabrication and detailed evaluation of such crystals for self-seeding of hard X-rays in XFELs deserves special attention since this is an example of X-ray optics that enables X-ray sources with unique characteristics.

The initial proposal [3] and a more detailed theoretical study [4] of the single-crystal diamond wake monochromator suggest that diamond thicknesses in the range 100–200  $\mu\text{m}$  are required to achieve optimal self-seeding conditions. Crystal strain, which can be easily induced by mounting of such thin specimens, can deteriorate crystal performance in Bragg diffraction. Therefore, a desired evaluation process of diamond crystal XFEL optics is twofold, which includes studies of crystal defects and crystal strain.

In this paper we report fabrication and detailed characterization of type IIa diamond crystal plates with (001) surface orientation and crystal-holder assemblies for self-seeding of hard X-rays in X-ray free-electron lasers. Several crystal plates of two different thicknesses (100  $\mu\text{m}$  and 150  $\mu\text{m}$ ) and two different types of crystal-holder

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assemblies were fabricated with the aim to select the best option for the Hard X-ray Self-Seeding Project (HXRSS) at the Linac Coherent Light Source (LCLS). White-beam synchrotron topography was performed to identify defect-free crystal regions. Strain-free mount was checked by mapping strain in the crystal plates placed into special graphite holders using double-crystal X-ray topography (Cu–K $\alpha$  X-ray source). In the final double-crystal topography experiments, angular variation of the reflectivity curve peak over representative crystal areas of  $1 \times 1 \text{ mm}^2$  was less than  $5 \text{ } \mu\text{rad}$ , which was smaller than the intrinsic angular width of the reflectivity curve  $\approx 13.5 \text{ } \mu\text{rad}$  of the working 004 reflection. Self-seeding experiments were recently conducted at LCLS using a crystal-holder assembly selected by our studies. Fully coherent 8.33-keV X-rays with  $5 \times 10^{-5}$  relative bandwidth were produced [12]. Thus, we demonstrate that careful fabrication, crystal selection, and minimization of mounting-induced strain can yield novel X-ray diamond crystal optics for self-seeding of XFEL.

## 2. Fabrication of crystal plates and crystal-holder assemblies

Type IIa diamond single crystals weighing up to 3 ct were grown at the Technological Institute for Superhard and Novel Carbon Materials (Troitsk, Russia) using the temperature-gradient method at high static pressure and high temperature (e.g., [10,13]). The temperature of crystallization was  $1460 \text{ } ^\circ\text{C}$  at a pressure of 5.5 GPa. After the crystallization process, diamond crystals were cut by a laser from the {001} growth sector furthest from the seed and mechanically polished to fabricate thin crystal plates. Nitrogen concentration measured by optical absorption was less than 0.1 ppm [10].

Preliminary selection of crystal plates with low density of crystal defects was made using Lang X-ray topography. Four plates with thicknesses of  $\approx 100 \text{ } \mu\text{m}$  and two plates with thicknesses of  $\approx 150 \text{ } \mu\text{m}$  were selected and trimmed by a laser into a trapezoidal shape with height 4 mm and bases of 4 mm and 5 mm. One of the 100- $\mu\text{m}$ -thick plates was repolished, which resulted in thickness reduction to  $75 \text{ } \mu\text{m}$ .

The trapezoidal shape was chosen in order to constrain motion of the crystal inserted into a slit (also trapezoidal shape) of a special holder while minimizing induced strain due to crystal mounting. The holders were fabricated out of polycrystalline graphite with slits

machined individually for each plate. The holders were of two types, which provide slightly different boundary conditions for crystal support (Fig. 1). Additional details on the design of the crystal holders and diamond wake monochromator can be found in [14].

## 3. X-ray topography

In the first step of X-ray characterization, double-crystal topography using a Cu K  $\alpha$  rotating anode X-ray source was performed to map the rocking curve of diamond crystals placed into the holders. A Si(135) beam conditioner first crystal with an asymmetry angle  $\eta_{\text{Si}} \approx 56.4^\circ$  was used to collimate an X-ray beam incident on the diamond crystal (Fig. 2). The diamond crystal was set for the 004 reflection, which was the working reflection in the HXRSS project. The Bragg angle of the diamond crystal was  $\theta_{\text{C}} \approx 59.8^\circ$ , which was close to the Bragg angle of the collimator crystal  $\theta_{\text{Si}} \approx 57.1^\circ$ . A CCD camera (with a resolution  $60 \times 60 \text{ } \mu\text{m}^2$ ) was used to obtain a series of X-ray diffraction images at different angular positions of the diamond crystal through the rocking curve of the 004 reflection. This setup was previously used for evaluation of the crystal strain in type Ib diamond crystals with  $\approx 10^{-6}$  strain sensitivity [15].

A software program has been written to combine the diffraction images at different angles and sort data for every pixel, thus making it possible to map the rocking curve over the crystal (i.e., rocking curve imaging [16]). The full width at half maximum (FWHM) of the ideal rocking curve of the diamond crystal in the utilized double-crystal configuration can be estimated as follows (see e.g., [17]):

$$\Delta\theta \approx \sqrt{\left(\frac{\Delta\lambda}{\lambda} (\tan\theta_{\text{C}} - \tan\theta_{\text{Si}})\right)^2 + \left(\epsilon_{\text{C}}^{(s)} \tan\theta_{\text{C}}\right)^2}, \quad (1)$$

where  $\frac{\Delta\lambda}{\lambda} \approx 3 \times 10^{-4}$  is the relative spectral width of the incident radiation (Cu K  $\alpha$  source) and  $\epsilon_{\text{C}}^{(s)} \approx 8.7 \times 10^{-6}$  is the relative intrinsic bandwidth of the 004 reflection. Although the resulting value  $\Delta\theta \approx 50 \text{ } \mu\text{rad}$  is larger than the intrinsic angular width of the reflection  $\Delta\theta_{\text{i}} \approx 13.5 \text{ } \mu\text{rad}$ , the sensitivity of the method to strain in the crystal is defined by resolution in the angular position of the curve and signal statistics. In our

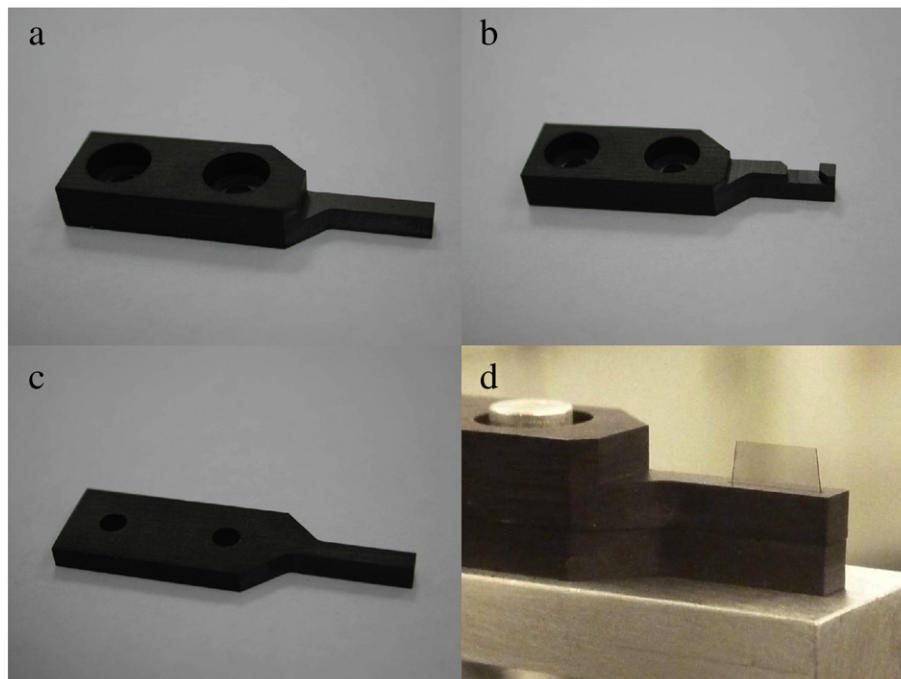


Fig. 1. Graphite crystal holders and diamond mounting. (a) Holder type 1 (top part). (b) holder type 2 (top part). (c) Holder base (common for type 1 and type 2). (d) Trapezoidal diamond plate inserted into holder type 1.

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