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Grazing Incidence Off-Plane Lamellar Grating as a Beam Splitter for a 1-Å Free Electron Laser

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Abstract—A beam splitter based on the diffraction grating working in the grazing incidence conical diffraction is proposed for x-ray free-electron laser (XFEL) experiments with coherent beams in plasma and atomic physics. Such a beam splitter can provide undistorted wavefronts, high-power radiation scattering, and split beams with equal intensities, which propagate with delay along different paths to the target chamber of the XFEL end station. Using the PCGrate software based on rigorous electromagnetic theory and developed for the short-wavelength range, it is shown that the plane grating with lamellar groove profile of a certain depth, operating in grazing conical incidence mount (grooves are parallel to the incident beam), separates three beams in the –1, 0, and +1 orders with close diffraction efficiency. Numerical simulation predicts 23–27% absolute efficiency for 0.1-nm incident radiation in each separated order of a bulk or multilayer grating, taking into account the atomic level roughnesses and interdiffusion. When using a multilayer coating based on Ru/C or Ru/B_4C pairs, the optimum grazing angle providing approximately equal efficiencies is ~1.038° which is four times higher than for the Pt-coated grating. Such optimization of radiation geometry, groove profile shape, and multilayer coating parameters can be performed for various XFEL wavelengths. The proposed grating, in addition to diffraction, technological, and design advantages over the beam splitter based on a set of perfect crystals, can be fabricated and tested using currently available methods.

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INTRODUCTION

Radiation pulses from the x-ray free-electron laser (XFEL) are brighter by many orders of magnitude and shorter by several orders of magnitude than those obtained using any other source of coherent x-rays at the present time and for the near future. These unique characteristics make it possible to extend the frontiers of science in the field of detection of new matter states, real-time monitoring of chemical processes and biological reactions, determination of chemical and structural properties of material in the nanoscale, and visualization of noncrystalline biological materials with atomic resolution. Currently, two XFEL projects are being developed for hard x-ray generation: LCLS in the United States and XFEL in Germany [1, 2]. The typical parameters of the developed XFEL are as follows: the electron energy is 5–20 GeV, peak luminance is 10^{31}–10^{33} photon/s · mm^2 ·mrad^2 in 0.1% of the band, radiation wavelength $\lambda = 0.85$–15 Å, focused spot size is 10–100 μm, pulse duration is ~100 fs, and pulse frequency is 10 Hz. Although the peak power scattered by a single pulse reaches several gigawatts, the average radiation power in a 0.6-ms train consisting of 3000 electron bunches is an acceptable value of ~10 W/mm^2. A still lower power will dissipate in the optical system, taking into account a finite number of pulse bunches.

The brightness of XFEL pulses with a duration to 0.1 fs allows the unique opportunity to observe variation dynamics of a large groups of atoms in condensed matter systems in a wide range of time scales, using, e.g., x-ray photon correlation spectroscopy.

This makes it possible to obtain images of speckle distributions of scattering using various time delays; changes in speckle distributions as functions of the time delay are used to study the sample dynamics. Hence, a key element of such a device should be a device for generating repeated x-ray pulses with a precise time delay tunable in a wide range.

REQUIREMENTS ON THE BEAM SPLITTER AND OFF-PLANE GRATING DESIGN

For experiments with coherent beams in plasma and atomic physics, optical systems not distorting wavefronts should be used in XFEL end stations. This leads to the requirement that errors in the deviation from crystal and mirror planarity be smaller than 0.1 μrad in the hard x-ray region. Apparently, the most sensitive optical element is the beam splitter [1, 2]. It should provide splitting of the primary beam into several secondary ones with approximately equal intensities, which propagate with a delay to a target chamber along different paths. The splitting/delay line should provide a time difference for path traveling by separated pulses between 1 ps and 10 ns.

Hence, to prevent beam splitter destruction, it should be fabricated on the basis of a reflecting grazing-incidence coolable optical system. Beam splitters based on perfect crystals are conventionally used for such splitting. The splitting/delay line can include up to eight crystals [2]. In addition to rigid technological and design requirements on perfection of used crystals and their mounting, it was shown that ultrashort x-ray pulses 0.1–1 fs long significantly widen in time and are distorted in shape [3].

In this paper, we propose to use a plane high-frequency lamellar or trapezoidal grating operating in the conical diffraction grazing mount as a beam splitter (Fig. 1).

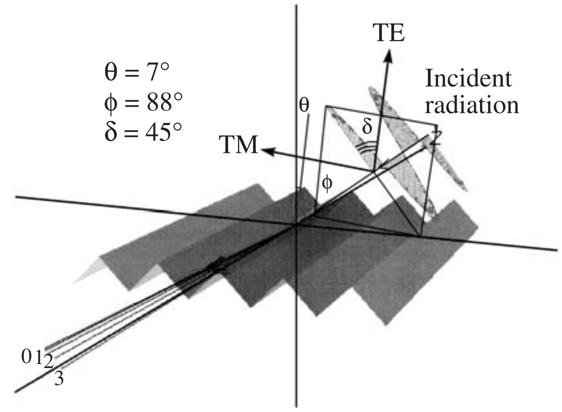

Fig. 1. Schematic representation of the off-plane grating and conical diffraction grazing incidence.

The choice of the conical configuration and a profile close to lamellar is caused by the necessity to achieve approximately equal high efficiencies in several diffraction orders simultaneously. The high grating frequency is required to increase dispersion of adjacent orders and to precisely fabricate grooves of small depth. To increase the grazing angle, it is proposed to use stable multilayer coatings with low atomic roughness and a small spread in thickness of identical layers. In the energy range of 10–22 keV, multilayer ruthenium-based coatings are the best choice. Calculations show that reflectances above 80% at a wavelength of ~1 Å can be achieved for Ru/C and Ru/B_4C mirrors with a roughness and/or interdiffusion root-mean-square deviation (RMSD) of several Angströms. Due to significant diffusion of carbon atoms in ruthenium, Ru/B_4C-based coatings seem to be preferable. In the case of insufficient stability of coatings and/or wavefront distortion by them, bulk gratings or gratings coated with metal can be used at the smaller grazing angles and small-size focused spots. The diffraction grating proposed for beam splitting must not necessarily be planar; however, extremely high requirements on the surface shape fabrication and grating replication precision lead to this choice. Apart from other advantages, the proposed solution is ready for implementation on the basis of modern techniques of fabrication and testing of high-frequency lamellar-profile gratings with atomic roughness [4]. Such a grating fabricated on a Si, SiO_2, or SiC substrate for removing the heat caused by intense radiation can be actively cooled in various ways using both water and liquid nitrogen [5].

EFFICIENCY OF THE BULK LAMELLAR GRATING IN CONICAL DIFFRACTION

The absolute diffraction efficiency of bulk and multilayer gratings was calculated using the PCGrate-SX 6.1 software [6] and the data on refractive indices of materials, taken from [7]. The PCGrate software based on the boundary integral equation approach with exact boundary conditions [8] was previously used for simulating bulk high-frequency gratings with variously shaped grooves, including real ones with various nanoroughnesses (i.e., measured using atomic-force microscopy (AFM)), operating under grazing and conical diffraction conditions in hard and soft x-ray ranges [9–12]. The results obtained in these studies showed a high accuracy and rate of the code used for simulation and a strong dependence of the efficiency on the groove shape profile and grating operation geometry, which was also shown previously [13]. In papers devoted to the design and study of off-plane gratings of the reflecting x-ray spectrometer of the Constellation-X mission (NASA), the calculated and measured (using synchrotron sources of polarized soft x-rays) efficiencies were compared and the necessity of using accurate numerical methods for its optimization was confirmed [12].

To solve the problems of this study, simulation using the PCGrate-SX code was directed to achieve equal maximum absolute efficiencies in three diffraction orders, i.e., –1, 0, and +1. Optimization calculations of gratings were performed for the off-plane (along grooves) angle of incidence φ (grazing φ_g) for lamellar-profile gratings with various depths, periods d = 100 and 200 nm, and λ = 0.1 nm. The angle θ in the dispersion plane (perpendicular to grooves) was chosen to be 0° to obtain equal efficiencies in the –1 and +1 orders at equal widths of lamellar profile ridges and grooves.

The calculation model assumed that gratings are coated with a sufficiently thick platinum layer; i.e., they are bulk and have high reflectances near the total external reflection angle for Pt.

The interface nanoroughness with RMSD σ = 0.1 and 0.2 nm was considered using the Nevot–Croce corrections [14]. The rigorous consideration of random roughnesses can be performed using the PCGrate-SX 6.2 software [15].

Figure 2 shows the curves of the absolute efficiency of the zeroth and first diffraction orders in TE polarization as functions of the off-plane (azimuthal) grazing

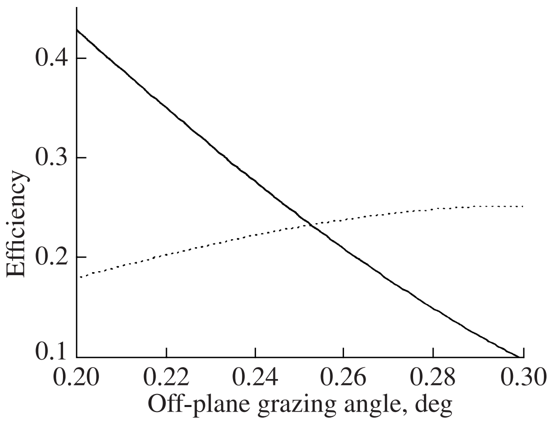

Fig. 2. Absolute efficiency of the zeroth (solid curve) and first (dashed curve) diffraction orders of the Pt grating (5000 lines/mm) with the lamellar profile of grooves of depth h_0 and roughness RMSD of 0.2 nm, calculated for incidence of TE polarized radiation with a wavelength of 0.1 nm at a polar angle of 0°, as a function of the azimuthal grazing angle.

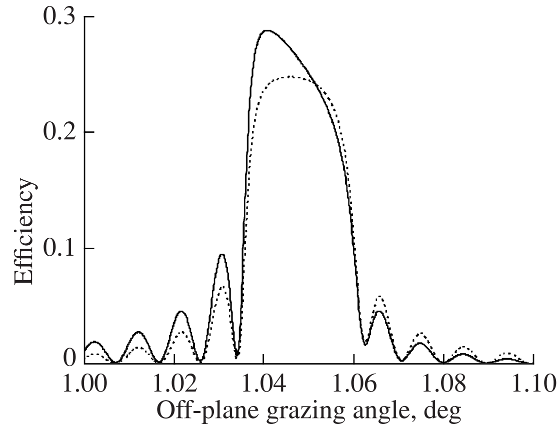

Fig. 3. Absolute efficiency of the zeroth (solid curve) and first (dashed curve) diffraction orders of the multilayer (100 Ru/C pairs, 5000 lines/mm) grating with lamellar profile of grooves of depth h_1 and roughness/interdiffusion RMSD of 0.2 nm, calculated for incidence of unpolarized radiation with a wavelength of 0.1 nm at a polar angle of 0°, as a function of the azimuthal grazing angle.

angle φ_g for the lamellar grating with d = 200 nm and optimized depth h_0. The zeroth-order curve intersects with the ±1-order curve (the efficiency curves of the –1 and +1 orders coincide) at a level of ~23.5% of the efficiency near φ_g = 0.253°. We can see that the curves diverge to the left and right of the intersection point; however, there is a certain angular range in which the efficiencies are still close and high.

Efficiencies of similar bulk gratings with d = 100 nm, σ = 1 and 0 Å, exposed under the same conditions were also calculated. The obtained absolute efficiencies differ from the data of Fig. 2 by less than one percent in the entire range of grazing angles, and are not presented in this paper. Similar optimization of the groove profile depth and incidence angle can be carried out for any other wavelength of the XFEL operating range.

EFFICIENCY OF THE MULTILAYER LAMELLAR GRATING IN CONICAL DIFFRACTION

Using the PCGrate-SX code, numerical optimization calculations of multilayer lamellar gratings operating in the grazing off-plane diffraction mount were also performed. Gratings with various depths were simulated at the angle φ_g for d = 100, 200 nm and unpolarized radiation wavelength λ = 0.1 nm. The angle θ in the dispersion plane, as in the case of the bulk grating, was chosen as 0°. The multilayer model assumed that gratings are fabricated in Si and are coated with 100 pairs of Ru/C films with parameters providing high reflectances near the first-order Bragg peak. The interface nanoroughness and diffusenesses with RMSD σ = 0.1 and 0.2 nm were considered using Nevot–Croce corrections under the assumption that interfaces are uncorrelated.

Figure 3 shows the curves of the absolute efficiency of diffraction orders as functions of the grazing angle φ_g for the lamellar grating with d = 200 nm, depth h_1, and optimized parameters of the Ru/C multilayer coating. The coating parameters are as follows: the multilayer structure period is 2.8 nm, the ratio of the Ru layer thickness to the period is 0.4286, and σ = 2 Å for all interfaces. As follows from the figure, the zeroth-order efficiency maximum exceeds the ±1-order efficiency maximum for this grating depth; in this case, there is an intersection point of efficiency curves (~24%) near φ_g = 1.051°. To the right of the intersection point, the efficiency curves are close in a rather wide range of grazing angles.

Figure 4 shows similar curves of the absolute efficiency for the lamellar grating with depth $h_2 > h_1$ and the same (as in Fig. 3) grating and radiation parameters. For a larger grating depth, the zeroth-order efficiency maximum is slightly lower than the ±1-order efficiency maximum; in this case, there is a convergence point of efficiency curves (~23%) near φ_g = 1.038°. To the left of this point, the efficiency curves almost coincide in a rather wide angular range.

Figure 5 shows the absolute efficiency curves for the lamellar grating with depth $h_3 > h_2$ and the same (as in Figs. 3 and 4) grating and radiation parameters. For a larger grating depth, the zeroth-order efficiency maximum is smaller than the ±1-order efficiency maximum; in this case, the convergence region of the efficiency curves is only near low efficiencies to the left.

The author also calculated efficiencies of similar gratings with d = 100 nm, σ = 1 and = 0 Å, exposed under identical conditions. The obtained absolute efficiencies differ from the data of Figs. 3–5 by a few percent in the entire angular range, and are not presented in this paper. Similar optimization of the grating groove

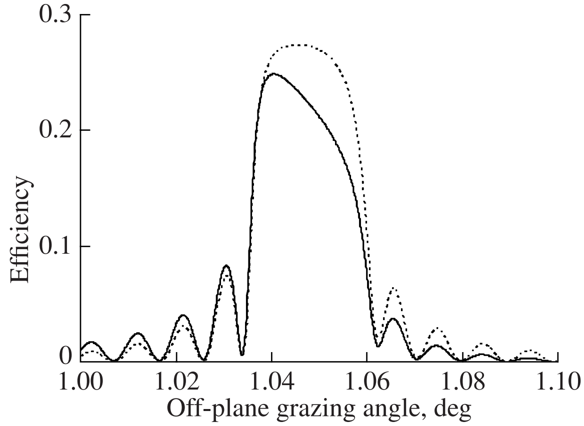

Fig. 4. The same as in Fig. 3, but for the grating with depth $h_2 > h_1$.

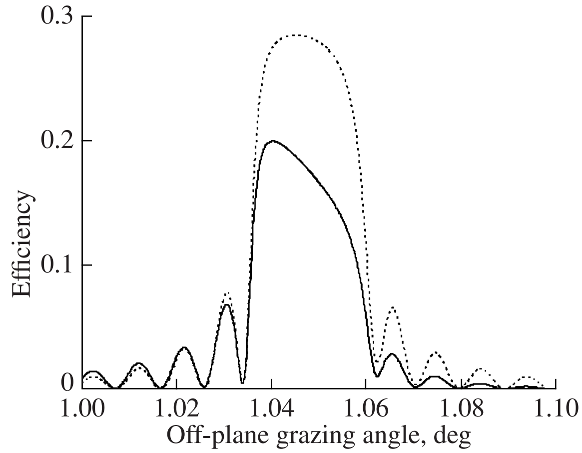

Fig. 5. The same as in Fig. 4, but for the grating with depth $h_3 > h_2$.

profile, grazing angle, and multilayer coating parameters can be carried out for other wavelengths of the XFEL operating range.

All calculations presented in this paper were performed using 200 collocation points at the interface and turned-on options of convergence acceleration [15]. The error found from the energy balance is no worse than 1×10^{-5} and 1×10^{-3} for bulk and multilayer gratings, respectively. The calculation time of a single point for a dual processor workstation with an Intel Pentium 4, 2-GHz CPU, 400-MHz Bus Clock, 2-MB Cache, 2-GB RAM, and operating with Windows XP Pro is ~1 s, taking into account paralleling and caching of identical matrix elements.

CONCLUSIONS

The high-frequency reflecting diffraction grating with a symmetric lamellar profile of small depth, operating in conical diffraction at small grazing angles, can split the zeroth and first orders with approximately equal efficiencies and without wavefront quality loss at an operating wavelength of ~1 Å. The use of the metallized (Pt) grating makes it possible to achieve absolute efficiencies of ~24% for split orders at a grazing angle of ~0.25° and near it. It is clear that such a bulk grating does not cause significant wavefront distortions; however, small grazing angles should be used.

The use of multilayer coatings based on Ru/C or Ru/B_4C pairs makes it possible to increase approximately fourfold the grazing angle of incidence and to achieve a maximum efficiency of ~24% for three orders. The close order efficiencies are observed in a rather wide range of grazing angles. Diffraction at a nonideal multilayer grating structure can cause wavefront distortions; it seems that such a grating requires efficient cooling.

For all XFEL operating wavelengths, grating setup, groove profile, and multilayer coating parameters, including the grazing angle, profile depth, multilayer coating period, the ratio of pair layer thicknesses, roughness, and interdiffusion, should be optimized. The use of real interface profiles, e.g., those measured using AFM, will allow simulation improvement.

Thus, the use of the high-frequency lamellar-profile grating operating in the conical diffraction grazing mount as a beam splitter for experimental XFEL end stations can have a significant effect due to modern technology of diffraction grating fabrication, deposition of high-quality multilayer x-ray coatings, and accurate calculation and measurement of the diffraction efficiency.

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