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Parametric X-rays from a polycrystalline target

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ABSTRACT

A theoretical description of parametric X-ray radiation (PXR) from a nanocrystal powder target is presented in terms of the orientation distribution function (ODF). Two models of ODF resulting in the analytical solution for the PXR intensity distribution are used and the characteristic features of this distribution are considered. A promising estimate of the number of the emitted photons is obtained for the case of a nanodiamond powder target using the parameters of ASTA Facility at Fermilab. The PXR spectra from polycrystal and single crystal targets are compared. The application scenarios of PXR from nanocrystals are discussed.

1. Introduction

Parametric X-rays (PXR) were theoretically predicted more than four decades ago [1,2]. First observed in 1985 [3–5], PXR is now thoroughly studied experimentally for the case of single crystal targets (for example, [6–10]). A simple model for the description of PXR features in this case was given in [11]. This radiation was shown to be quasi-monochromatic, tunable and observable at large angles to the velocity of a charged particle.

The research into X-rays emitted from polycrystals started about two decades ago from the theoretical description of the Polarization Bremsstrahlung [12]. Actually, the coherent Polarization Bremsstrahlung is equivalent to PXR and was observed later in the experiment [13]. Then PXR from similar polycrystals was observed at the REFER electron ring [14]. A molybdenum polycrystalline target proved to have its axis $(1,1,0)$ predominantly directed along the rolling direction [15]. Further studies [16,17] revealed that the intensity of the radiation was comparable with the characteristic K_α-line of Mo. This allowed considering PXR in a polycrystal as a promising radiation mechanism. The papers cited here claimed that the properties of the observed PXR spectrum were associated with the referred parameters of the polycrystal, but the theoretical analysis was made only for some particular configurations of the detector and the target [12].

This research is aimed at calculating the general form of the PXR intensity distribution in terms of the parameters of a nanocrystal target. This has become a timely research topic these days, since new nanocrystalline materials produced now are promising candidates as primary targets for PXR generation. It is well known [23] that the most general description of X-ray Diffraction (XRD) at nanocrystal powder uses the Orientation Distribution Function (ODF). So, the averaged PXR intensity distribution at nanocrystal powder is naturally calculated on the basis of ODF. Two major ODF models resulting in analytical solutions for the intensity distribution are considered in order to estimate the number of emitted X-ray photons. The PXR characteristics from polycrystal and single crystal targets are compared.

2. General approach

In the present consideration we used the nanodiamond film parameters reported in [18]: a 5×7 mm nanodiamond film of 500 nm thickness for the accelerator X-ray experiments with average crystallite size of primary nanodiamond particles varying around 100 nm, which is essentially less than the extinction length for the emitted radiation. Thus, the PXR kinematic theory is sufficient for calculating the PXR intensity that is proportional to the length of the electron trajectory in the film and is insensitive to the shape of the nanoparticle surface. However, it depends on the fraction of nanosized grains with parallel crystallographic planes. As it was mentioned above, in the case of polycrystals this value is defined by ODF $f(\varphi,\psi,\theta)$. Knowing ODF $f(\varphi,\psi,\theta)$, we can find the volume part of grains whose orientation corresponds to the Euler angles:

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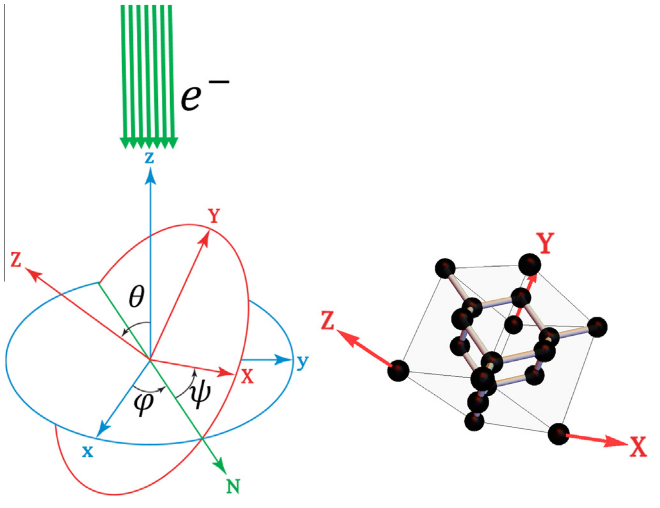


(a) (b)

Fig. 1. (a) Geometry of the case; (b) unit cell and crystallographic frame of reference.

$$\frac{dV}{V} = f(\varphi,\psi,\theta)\sin\theta d\varphi d\psi d\theta.$$

This function is constant for homogeneous polycrystals and has a nontrivial form if the orientation of grains has a certain direction (texture) [23]. In this research, we assume that the form of $f(\varphi,\psi,\theta)$ is known and depends on some characteristic parameters. This allows us to calculate the PXR intensity distribution averaged over ODF. The geometry of the case is shown in Fig. 1a. The (x,y,z) frame of reference corresponds to the sample system with xy-plane parallel to the film surface; the (X,Y,Z) frame of reference is the crystallographic system corresponding to the orientation of the unit cell in a nanocrystal, as in Fig. 1b.

We may start the consideration from the relation

$$N_{hkl} = \frac{\alpha|\cos 2\Theta_B|}{4\sin^2\Theta_B}\frac{J}{e}|\chi_{\vec{g}}(\omega_B)|^2\frac{\omega_B L}{c}((1+\cos^2 2\Theta_B)\ln(\xi_D+\sqrt{\xi_D^2+1})-\cos^2 2\Theta_B) \tag{1}$$

given in [19] that yields the number of photons that reach the detector per second from one PXR peak in the case of a single crystal target. Here $\xi_D = \gamma\theta_D$ and θ_D is the angular size of the detector (in radians); the centers of the peak and the detector are supposed to coincide; $\gamma = E/mc^2$ is the Lorentz factor of the electron with the energy E; $\vec{g}$ is the reciprocal lattice vector, $\alpha = 1/137$, J is the electron beam current, e is the electron charge, L is the length of the electron path in the crystal; ω_B, $\chi_{\vec{g}}(\omega_B)$ are the frequency and the X-ray polarizability, respectively. These values are defined by the angle Θ_B (see Fig. 2a), where $\vec{v}$ is the electron velocity and $\vec{k}$ is the wave vector corresponding to the PXR peak. It is important that in the case of a polycrystal target, we can observe several PXR peaks simultaneously (Fig. 2b).

To consider PXR from a polycrystal target, let us make several assumptions:

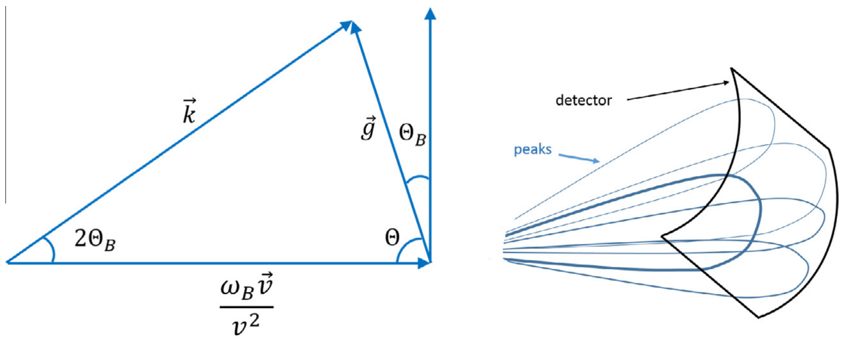
1. ODF is a rather smooth function of the angles in comparison with the width of the PXR peak from a single crystal;
2. the detector is rather large, and so the measured intensity depends mainly on the number of the detected peaks rather than on the structure of a single peak from a nanodiamond particle that is considered as a single crystal;
3. N_{hkl} is proportional to the number of PXR peaks generated in various nanoparticles in the direction of the detector, see Fig. 2b;
4. the relation (1) holds for the peak in the center of the detector, whereas it does not apply to the peaks on the periphery due to different geometry. This effect is taken into account by using the effective value ξ_{Deff} instead of real ξ_D. It is supposed to allow for tails of peaks from outside the detector as well;
5. ξ_{Deff} slightly depends on the parameters of the case and is close to the value of $\gamma\theta_D$ with logarithmic accuracy.

This allows us to relate the number of quanta dN to $d\varphi d\psi d\theta$ corresponding to nanocrystals, PXR peaks of which are in the direction of the detector:

$$dN = \alpha L\frac{J}{e}\frac{|\cos 2\Theta_B|}{|\vec{g}|^3}|\kappa_{\vec{g}}|^2((1+\cos^2 2\Theta_B)\ln(\xi_{Deff}+\sqrt{\xi_{Deff}^2+1})-\cos^2 2\Theta_B)\times f(\varphi,\psi,\theta)\sin\theta d\varphi d\psi d\theta. \tag{2}$$

We consider one separate peak defined by the vector $\vec{g}$. Here L is the total length of electron path in the polycrystal including a lot of intercepts in nanocrystal grains and Θ_B is the function of the Euler angles φ,ψ,θ which define the positions of the sample and the detector. The value of $\kappa_{\vec{g}} = \chi_{\vec{g}}(\omega)\omega^2/c^2$ is independent of ω if the radiation absorption and the anomalous dispersion corrections are not considered. However, $|\kappa_{\vec{g}}|$ is the function of $|\vec{g}|$ because of the atomic scattering and the Debye–Waller factor [20]. Thus we can rewrite the above-mentioned relation as

$$dN = T(|\vec{g}|,\Theta_B)f(\varphi,\psi,\theta)\sin\theta d\varphi d\psi d\theta. \tag{3}$$



(a) (b)

Fig. 2. (a) Geometry of PXR; (b) characteristic view of PXR from a polycrystal.