ISSN 1062-8738, Bulletin of the Russian Academy of Sciences. Physics, 2011, Vol. 75, No. 2, pp. 226–228. © Allerton Press, Inc., 2011.
Original Russian Text © P.N. Zhukova, A.S. Kubankin, M.S. Ladnyh, N.N. Nasonov, 2011, published in Izvestiya Rossiiskoi Akademii Nauk. Seriya Fizicheskaya, 2011, Vol. 75, No. 2, pp. 244–246.

Defining the Distribution Function of Mosaic Crystal Grains on Orientation Angles Using Synchrotron Radiation

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Abstract—A new method of measuring the angular distribution function of grains in mosaic crystals is proposed and studied.

DOI: 10.3103/S106287381102033X

INTRODUCTION

Mosaicity is an important feature of the crystals used in X-ray devices, and the development of corresponding methods of diagnostics therefore remains a problem of interest [1]. As a rule, it is necessary to determine one characteristic parameter: the half-width of the distribution function for microassemblies of the crystal according to the orientation angles. To accomplish this, we perform angular measurements of the scattering quasi-monochromatic X-ray radiation in the investigated sample [2]. In this work, we show it is possible to obtain more detailed information on mosaicity using the energy-dispersion approach, which allows us to reconstruct the bidimentional distribution function for microassemblies according to their orientation angles.

EXPERIMENTAL

At the heart of the energy dispersion approach lies the process of measuring the spectra of the scattering broadband X-ray radiation in a sample (e.g., the synchrotron radiation) at the detector's fixed position. Let us consider the scattering of the quantum stream of the synchrotron radiation in a crystal consisting of ideal microassemblies, turned relative to one another at certain angles. We start with the Maxwell equations for the Fourier transform of a vector of the electric field:

$$\left(k^2 - \omega^2\right)\mathbf{E}_{\omega\,\mathbf{k}} - \mathbf{k}\left(\mathbf{k}\mathbf{E}_{\omega\,\mathbf{k}}\right) + \int d^3k'\,G(\mathbf{k}'-\mathbf{k})\mathbf{E}_{\omega\,\mathbf{k}'} = 0,$$
$$G = \frac{e^2}{2\pi^2 m}F(\mathbf{k}'-\mathbf{k})\sum_l \exp\left[i(\mathbf{k}'-\mathbf{k})\mathbf{r}_l\right], \tag{1}$$

where response function G, calculated at the high-frequency limit $\omega \gg I$ (I is the average potential of ionization of a target atom), includes the contribution from all atoms; $\mathbf{r}_l$ is the coordinate of the lth atomic nucleus; and F is the atomic form factor.

For further analysis, it is convenient to remove from G the average component

$$G = \bar{G} + \tilde{G}, \quad \bar{G} = \langle G\rangle = \omega_0^2\delta(\mathbf{k}'-\mathbf{k}),$$
$$\varepsilon(\omega) = 1 - \omega_0^2/\omega^2, \tag{2}$$

where ω_0 is the plasma frequency of the target, and ε is the usual dielectric capacitivity of a substance in the X-ray range. Substituting (2) into (1) and applying perturbation theory, we obtain the following solution for Eq. (1) in the form of the sum of an impinging non-monochromatic wave $\mathbf{E}^{(i)}_{\omega\,\mathbf{k}}$ and a scattered wave $\mathbf{E}^{(S)}_{\omega\,\mathbf{k}}$:

$$\mathbf{E}^{(i)}_{\omega\,\mathbf{k}} = \mathbf{e}_i E_\omega \delta(\mathbf{k} - \omega\sqrt{\varepsilon}\mathbf{n}_i),$$
$$\mathbf{E}^{(S)}_{\omega\,\mathbf{k}} = -\frac{1}{k^2 - \omega^2\sqrt{\varepsilon}}\left(\mathbf{e}_i - \frac{\mathbf{k}(\mathbf{k}\mathbf{e}_i)}{\omega^2\sqrt{\varepsilon}}\right)E_\omega\tilde{G}\left(\omega\sqrt{\varepsilon}\mathbf{n}_i - \mathbf{k}\right), \tag{3}$$

where $\mathbf{e}_i$ is the vector of polarization of the initial wave extending in direction $\mathbf{n}_i$, the spectrum of which is described by E_ω.

In the expression following from (3) for the spectral angular distribution of scattering radiation,

$$\omega\frac{dN^{(S)}}{d\omega\, d\Omega} = 4\pi^2\left(1 - (\mathbf{n}_S\mathbf{e}_i)^2\right)\left|E_\omega\right|^2\left\langle\left|G\left(\omega\sqrt{\varepsilon}(\mathbf{n}_S - \mathbf{n}_i)\right)\right|^2\right\rangle \tag{4}$$

it is necessary to average over the coordinates of the atoms. We assume the microassemblies are large enough to produce Bragg diffraction. We also assume that the characteristic angle of the mutual disorientation of microassemblies exceeds the angular width of a reflex from one microassembly, while the radiation scattering on each microassembly is independent of other scattering. If we assume that

$$\mathbf{r}_l = \mathbf{R}_l + \bar{r}_{lm} + \mathbf{u}_{lm}, \tag{5}$$

where the first summand in the right-hand part denotes the coordinate of an elementary cell in the microassembly, the second summand corresponds to the coordinate of the mth atom in the lth cell, the last summand denotes the thermal shift of this atom. To average over the thermal vibrations in (5), Eq. (4) is transformed:

$$\omega \frac{dN^{(S)}}{d\omega\, d\Omega} = \frac{VZ^2 e^4 n_0}{m^2}\left(1-(\mathbf{n}_S\mathbf{e}_i)^2\right)|E_\omega|^2 \times\left[\frac{1-\exp\left(\omega^2\varepsilon(\mathbf{n}_S-\mathbf{n}_i)^2 u_T^2\right)}{\left(1+\omega^2\varepsilon(\mathbf{n}_S-\mathbf{n}_i)^2R^2\right)^2} + (2\pi)^3 n_0 \sum_{g\neq 0}\frac{|S(\mathbf{g})|^2\exp\left(-g^2u_T^2\right)}{\left(1+g^2R^2\right)^2}\delta\left(\omega\sqrt{\varepsilon}(\mathbf{n}_S-\mathbf{n}_i)-\mathbf{g}\right)\right], \tag{6}$$

where V is the volume of the target, Z is the number of electrons in an atom, n_0 is the density of the atoms, u_T is the root-mean-square amplitude of the thermal vibrations of the atoms, $S(g)$ is a structural factor of the cell, R is the radius of electronic shielding in the Thomas–Fermi nuclear model, and g is the vectors of the reciprocal lattice. The first summand in (6) describes the distribution of incoherent radiation scattered by the microassemblies, while the second corresponds to coherent scattering. It is easy to see that the incoherent component is quenched substantially, since in the field of the coherent contribution from atomic electrons to the scattering $\omega^2 R^2 < 1$, multiplier

$$1-\exp\left(\omega^2\varepsilon(\mathbf{n}_S-\mathbf{n}_i)^2u_T^2\right) < u_T^2/R^2 \ll 1,$$

and the coherent component is formed by the independent contributions of various crystallographic planes. It is therefore enough to analyze only one summand in (6) corresponding to the set vector of reciprocal lattice **g**. Let us show that measuring the number of quanta in a reflex allows us to determine the required function for the distribution of microassemblies according to vector orientation **g**.

We obtain the angular variables φ, χ, $\boldsymbol{\theta}$, and $\boldsymbol{\eta}$ in the figure, and determine the orientation in space of vectors $\mathbf{n}_i$, $\mathbf{n}_S$, and $\mathbf{g}$:

$$\mathbf{n}_i = \mathbf{e}_y, \quad \mathbf{n}_S = \mathbf{e}_2\left(1-\frac{1}{2}\theta^2\right)+\boldsymbol{\theta}, \quad \mathbf{e}_2\boldsymbol{\theta}=0, \\ \mathbf{g} = g\left[\mathbf{e}_1\left(1-\frac{1}{2}\eta^2\right)+\boldsymbol{\eta}\right], \quad \mathbf{e}_1\boldsymbol{\eta}=0. \tag{7}$$

To find the function of bidimentional angle $F(\boldsymbol{\eta})$ describing the desired distribution of microassemblies according to their orientation angles, we must express the vectors in (6) through the entered angular variables, multiply the right-hand part of (6) by $F(\boldsymbol{\eta})$, and integrate the resulting expression for the spectral angular distribution of a number of scattered quanta in the allocated reflex by angles $\boldsymbol{\theta}, \boldsymbol{\eta}$ and frequency ω.

We assume that the system probing the radiation crystal is close to the Bragg resonance (a condition achieved by the preliminary orientation of the crystal). Orientation angle φ is associated with angle χ (Figure) by the ratio

$$\varphi = \frac{\pi}{2}-\frac{\chi}{2}-\varphi', \quad \varphi' \ll 1. \tag{8}$$

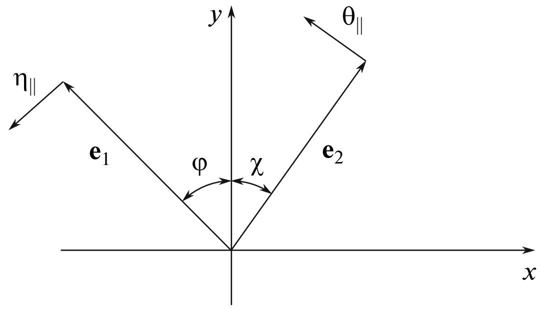
The integration result has the form

$$N_g(\varphi') = \pi V \frac{\omega_0^4}{g^3}\frac{|S(\mathbf{g})|^2\exp(-g^2u_T^2)}{\left(1+g^2R^2\right)^2}\frac{\sin^2(\chi/2)\sin^2(\chi)}{\cos(\chi/2)}\int_{-\infty}^{\infty} d\eta_{\parallel}F_{\parallel}(\eta_{\parallel}) \times\int_{\omega_-}^{\omega_+}\frac{d\omega}{\omega}|E_\omega|^2\,\delta\left(\varphi'-\eta_{\parallel}+\tan(\chi/2)\left[\frac{\omega}{\omega_g}-1\right]\right), \tag{9}$$

where $\omega_g = g/2\sin(\chi/2)$ is the Bragg frequency in whose vicinity the spectrum of the scattering radiation's reflex is concentrated, $\omega_\pm = \omega_g\left(1\pm\frac{\Delta\theta}{4\,\mathrm{tg}(\chi/2)}\right)$, $\Delta\theta$ is the angular width of the radiation detector, and function $F_{\parallel}(\eta_{\parallel})$ is determined by equation

$$F_{\parallel}(\eta_{\parallel}) = \int_{-\frac{\Delta\theta}{4\,\mathrm{tg}(\chi/2)}}^{\frac{\Delta\theta}{4\,\mathrm{tg}(\chi/2)}} d\eta_{\perp}F(\boldsymbol{\eta}) \approx \frac{\Delta\theta}{2\mathrm{tg}(\chi/2)}F(\eta_{\parallel},0). \tag{10}$$

The approximate equality in (10) denoting the smoothness of the change in mosaicity distribution for an interval of angles on the order of the collimation



Geometry of the process of synchrotron radiation dispersion on a microassembly.

angle is used repeatedly in the analysis below. (It is always possible to satisfy to the specified condition with the selection of the collimator.)

Equation (9) is the convolution of required function F with the δ function, and can thus be solved using the Fourier transform

$$N_{g\xi} = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\varphi' \exp(i\xi\varphi') N_g(\varphi') = \pi V \frac{\omega_0^4}{g^3} \frac{|S(\mathbf{g})|^2 \exp\left(-g^2 u_T^2\right)}{\left(1+g^2R^2\right)^2} \frac{\sin^2(\chi/2)\sin^2(\chi)}{\cos(\chi/2)} \times F_{\|\xi} \int_{\omega_-}^{\omega_+} \frac{d\omega}{\omega} |E_\omega|^2 \exp\left(-i\xi \tan(\chi/2)\left[\frac{\omega}{\omega_g} - 1\right]\right). \tag{11}$$

The last integral in (11) is easily addressed in the case of a sufficiently smooth change of the primary radiation spectrum in the interval $\Delta\omega = \omega_+ - \omega_-$, whose condition of infinitesimality is again reduced to the requirement $\Delta\theta \ll 2\,\mathrm{tg}(\chi/2)$. Inverting the Fourier transform, we obtain following formula:

$$F(\eta_\|, 0) = \frac{1}{A}\int_{-\infty}^{\infty} d\xi \exp(-i\xi\eta_\|) \frac{\xi}{\sin\left(\frac{1}{4}\Delta\theta\xi\right)} N_{g\xi} = -\frac{2}{A}\frac{d}{d\eta_\|}\left[N_g\left(\eta_\| + \frac{\Delta\theta}{4}\right) + N_g\left(\eta_\| + \frac{3\Delta\theta}{4}\right) + N_g\left(\eta_\| + \frac{5\Delta\theta}{4}\right) + \ldots\right], \tag{12}$$

where coefficient A is obviously determined from (11).

We are easily convinced that when the smoothness of the change in measured orientation function $N_g(\eta_\|)$ in an angular range on the order of $\Delta\theta/4$, series (12) is reduced to the integrated sum

$$F(\eta_\|, 0) = -\frac{4}{A\Delta\theta}\frac{d}{d\eta_\|}\int_{\eta_\|+\Delta\theta/4}^{\infty} dx N_g(x) = \frac{4}{A\Delta\theta} N_g\left(\eta_\| + \frac{\Delta\theta}{4}\right) \equiv \frac{4}{A\Delta\theta} N_g\left(\varphi' + \frac{\Delta\theta}{4}\right). \tag{13}$$

Formula (13) shows that measuring the orientation dependence of a number of quanta in a particular reflex of the collimated scattering radiation allows us to determine directly the of distribution function for the microassemblies of a mosaic crystal according to the orientation angle in one plane. By rotating the crystal around the incident radiation axis and repeating the measurements, it is easy to determine the distribution function in the orthogonal plane.

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