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Physical–mathematical model of Lorentz factor for the integrated intensity of single crystal diffraction

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ABSTRACT

The Lorentz factor is a sensitive issue of X-ray diffraction because it is taking into account some factors which influence the intensity of diffracted X-radiation, such as: (i) the geometry of the experiment and also (ii) the single crystal or poly-crystals size in the irradiation case of a set of crystallites (crystalline powder). The difficulty of the subject consists in the possibility of different interpretation of the influence of these factors and in modeling of them. Depending on the preferential orientation of the crystals, the relative error can be 3–10 times in comparison with the accepted classical model. The aim of this paper is to modeling Lorentz factor for the integrated intensity, in case of vertical divergence integrated intensity diffracted by a single crystal. The originality of paper consists in deducting expression of Lorentz factor, expression that correct the calculated value of intensity for real experimental conditions of X-ray diffraction, for a certain type of structural analysis.

1. Introduction

Future design of nanomaterials and nuclear materials requires structural materials that can withstand extreme environment conditions. There have been a number of experimental studies to characterize and understand the effects of radiation-induced in a number of irradiated metal systems as well as computational models the relations involved in the X radiation diffracted intensity [1–4].

In the X-ray diffraction experiments, the intensity of diffracted X-radiation is affected by 6 factors: (i) the polarization factor $P(2\theta)$; (ii) Lorentz factor, L; (iii) the structure factor $F(\vec{s})$; (iv) multiplicity; (v) temperature factor (Debye–Waller), $F_T(s)$; (vi) absorption factor [5–8].

The Lorentz–polarization factor is the most important of the experimental quantities that control X-ray intensity with respect to diffraction angle. This paper presents the results obtained from the analysis of the way in which full intensity reflected from a crystal plane is affected by the "geometry" experience, in case of vertical divergence integrated intensity diffracted by a single crystals; the results can be extended to the main types of methods used in structural analysis, similar with results presented in the literature data [5,8,9].

When defining factors enumeration characterizing coherent scattering of X-rays, it was assumed that the incident beam is plane parallel and monochromatic.

In all reality experiences, there are practical limitations to the feasibility of these conditions [5].

Geometric divergence (vertical and horizontal) of the beam incident, the deviation from ideal monochromatism and the diffraction geometry, leading to further enlargement of the widening of the observed diffraction peaks. The observed diffraction peaks, resulting from the expression of $G^2(\vec{s})$, where $G(\vec{s})$ is the interference function.

It is therefore necessary to find and introduce a "geometric factor" to correct the calculated value of X radiation diffracted intensity for "real" conditions experiences of a specific to a particular type of structural analysis.

In the following section, we will be discuss the "geometric factor" (Lorentz factor) in the case in which we define the integral intensity diffracted by a crystal plane.

The Lorentz–polarization factor is an important component of peak intensity, but it has little or no effect on peak shape except at low diffraction angles and the Lorentz–polarization factor is a factor whose values are controlled by the geometry of the

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instrument and the preferred orientation of crystallites within the crystal aggregate.

The Lorentz factor is a combination of two geometrical factors that we will deal with trigonometrically. The first factor is a formulation for the volume of the crystal that is exposed to primary irradiation. The second one relates the number of crystals favorably oriented for diffraction at any Bragg angle θ. The Lorentz factor is different for random powders and single crystals.

Difficulty Lorentz factor approach consists in the possibility of different interpretation influences of these factors, as well as in physical-mathematical modeling of these factors.

The mathematical modeling [10–16] are the scientific way of proposal and implementation of technology and instrumental analysis methods based on previously models tested in laboratory. So the mathematical formula can make use of hypotheses simplification proposals more or less justified as a result of the work of specialist [5,8,17–22].

Depending on the accuracy level and preferential orientation, we can be made relative errors of 3–10 times higher than the accepted classical model. For this reason, modeling of Lorentz factor is a subject which deserve a special attention, and in the context of this work, we will present an own mathematical modeling of Lorentz factor.

In accordance with the specialty literature [23–30] the diffracted intensity by a crystallite $I_c(\vec{s})$ irradiated with non-polarized monochromatic beam, in direction $\vec{u}$ has the expression:

$$I_c(\vec{s}) = I_e(0) \cdot \frac{1+\cos^2 2\theta}{2} F^2(\vec{s}) \cdot G^2(\vec{s}) \quad (1)$$

where $\vec{s} = \frac{\vec{u}-\vec{u}_0}{\lambda}$, $\vec{u}_0$ is the incident beam direction; $\vec{u}$ the diffracted beam direction; and λ = wavelength, and Ie(0) is the incident beam intensity, $P(2\theta) = \frac{1+\cos^2 2\theta}{2}$ the polarization factor, $F(\vec{s})$ is the factor structure, and $G(\vec{s})$ interference function.

2. Theoretical aspects

To estimate the number of cells in a crystallite will consider a cubic crystallite of side 0.1 μm, which is the lattice parameter of approx. 5 Å. The crystal will contain 200 unit cells on each side, i.e. $8 \cdot 10^6$ unit cell. If considered crystal $I_c(\vec{s})$ is measurable only for $\vec{s}$, the vicinity of a vector $\vec{H}$ of reciprocal network care $F(\vec{H}) \neq 0$. In this case $\vec{s}$ can be written as:

$$\vec{s} = \vec{H} + \vec{\varepsilon} \quad (2)$$

where $\vec{H} = h_1\vec{b}_1 + h_2\vec{b}_2 + h_3\vec{b}_3$ and $\vec{\varepsilon} = \varepsilon_1\vec{b}_1 + \varepsilon_2\vec{b}_2 + \varepsilon_3\vec{b}_3(h_1\ h_2\ h_3)$ – Miller indices of crystallographic planes,

$$\vec{b}_1 = \frac{\vec{a}_2 x \vec{a}_3}{\Omega}, \quad \vec{b}_2 = \frac{\vec{a}_3 x \vec{a}_1}{\Omega}, \quad \vec{b}_3 = \frac{\vec{a}_1 x \vec{a}_2}{\Omega}$$

where $\vec{a}_i x \vec{a}_j$ is the multiplication product of the vectors, $\Omega = \vec{a}_1(\vec{a}_2 x \vec{a}_3)$ is the unit cell volume of the crystal or direct network.

$$G = \frac{\sin(\pi N_1 s_1 a_1)}{\sin(\pi s_1 a_1)} \cdot \frac{\sin(\pi N_2 s_2 a_2)}{\sin(\pi s_2 a_2)} \cdot \frac{\sin(\pi N_3 s_3 a_3)}{\sin(\pi s_3 a_3)}$$

The term G is also known in the literature as interference function [31].

N_1, N_2, and N_3 are the number of unit cells along a_1, a_2, and a_3 directions.

From the condition to cancel the interference function i.e. when it results from:

$\pi N_i s_i a_i \to \pm\pi$ results:

$$\frac{\sin^2(\pi N_i \vec{s}_i \vec{a}_i)}{\sin^2 \pi \vec{s}_i \vec{a}_i} = \frac{\sin^2 \pi N_i \varepsilon_i}{\sin^2 \pi \varepsilon_i} \quad (2.a)$$

with i = 1–3,

N_i are the number of unit cells along the a_i direction (i = 1, 2 or 3), so that the interval $\left[-\frac{1}{N_i}, \frac{1}{N_i}\right]$ or domain of $\bar{\epsilon}$ is about $1.25 \cdot 10^{-7}$ times smaller than the volume of the cube from respectively space, practically meaning that is a "node" point. It has been shown that $G^2(\vec{s})$ term plays a Dirac function better as the number of unit cells in the crystal is higher [32].

If the number of crystals from the crystallite increases to approx. 2000 cells per side, i.e. about 10^{10} cells, then the domain of $\vec{\epsilon}$ is reduced practically to a point. This led to the concept of Ewald sphere (Fig. 1) that diffracted beams can be obtained only when there is a vecor $\vec{s}$ of mutual network which is identical to that node must lie on the Ewald sphere with radius $1/\lambda$ (Fig. 1a and b).

Basically, if any node of the crystal does not intersect the Ewald sphere, then you cannot get any diffracted beam.

In order to prevent this, the crystal can rotate or oscillate about a position (axis) so that some components can end up in positions of diffraction, for example reach the Ewald sphere. All nodes that can generate diffracted beams are found in so-called sphere of inclusion that has radius $2/\lambda$.

3. The approached method

3.1. Experimental procedure

We used for experiments and modeling a modify diffractometer DRON3, equipped supplementary with computerized data acquisition and processing data of diffraction. In Fig. 2 is presented the image of the diffractometer goniometer DRON 3.

In general, the diffractometers comprises the following parts: the nuclear, mechanical, hydraulic, electric and electronics parts and the computerized data acquisition and processing of diffraction.

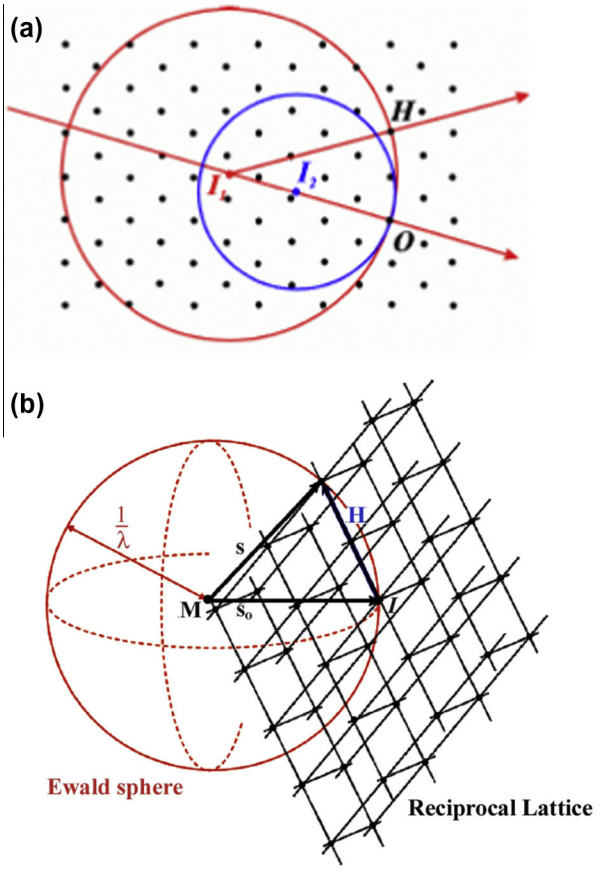

Fig. 1. Schematic representation of Ewald sphere with reciprocal lattice: (a) 2D representation; (b) 3D; [33].