

# The new principle for intensity calculation of X-rays dynamically diffracted in single crystals with defects

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**Abstract.** A new principle is introduced for X-ray intensity calculation dynamically scattered in single crystals with defects. The principle is based on Bragg diffraction dynamic theory for X-rays in ideal single crystals and small angle scattering theory. The principle is substantiated by juxtaposition of the corresponding formula with the particular solution of the integral-differential equation for a dynamically scattered X-ray wave in a weakly distorted single crystal.

## 1. Introduction

The further development of the dynamic theory for X-ray scattering in deformed crystals and crystals with defects is most important for the structural study of solid materials from the aspect of X-ray scattering phase problem solution. This leads to an unambiguous interpretation and decoding of X-ray diffraction and interference images on the purpose of precise determination of the structural distortions of the studied materials. This theory is quite developed and the integral-differential equation of the studied direct problem is obtained [1]. Nevertheless the integration of this equation is an uneasy task and the reverse problem formulation and solution for the determination of precise structures of materials with these equations is an unsolved problem. The direct problem solution, the calculation of complex amplitude of X-ray wave dynamically scattered in a distorted crystal for given analytic distortions is a difficult problem. Usually the problem is not solved analytically.

The numerical integration of the obtained equations strongly restricts the capabilities of developed strict dynamic theory of X-ray scattering in distorted crystals, in respect of new predictions, for experiment development in this spear. The uncertainty of the theoretical interpretation of experimental results, to some extent, is simplified when the crystal is distorted by definite external influences (a thermal gradient, ultrasound field). Therefore the further development of X-ray diffraction theory and experiment from the point of mutual supplementation, of course, is connected to the study of crystal distorted by definite external analytical influences [2, 3]. For the purpose of overcoming of above mentioned problems, in work [4] we suggest a new principle of calculation of X-ray intensities (or thermal neutrons) dynamically scattered in crystals with defects. This principle ensues from the juxtaposition of the dynamic theory of X-ray Bragg diffraction with the theory of their small angle scattering. The fairness of the new principle is substantiated by the juxtaposing of the corresponding formula with the particular solution of the integral-differential equation for a dynamically scattered X-wave in a weakly distorted crystal. .

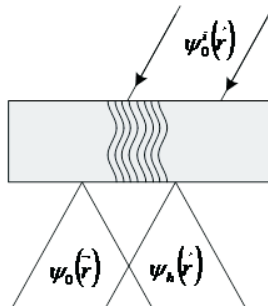


## 2. The Essence of the New Principle

Let's assume that a beam of X-ray falls at the Bragg angle on a single crystal with a defect (figure 1). We will consider the amplitude of the diffracted wave as a result of double-phase diffraction.

In the first phase a beam of X-ray dynamically scatters on an perfect single crystal (Bragg diffraction). In the second phase the waves diffracted in the first phase undergo a small angle scattering on a defect. In the first phase the dynamic Bragg diffraction of an X-ray beam takes place on an perfect single crystal, for what the amplitudes of the diffracted waves are known. In the second phase the waves diffracted in the first phase undergo Fraunhofer or Fresnel diffraction on a defect depending upon the defect size and the parameters of intensity registration geometry of the diffracted radiation. The essence of the new principle is that the amplitude of the X-wave diffracted in a crystal with a defect can be calculated by adding the scattered amplitudes of the two phases.

Let's assume that a monochromatic X-ray beam with amplitude  $\Psi_0^{(i)}(\mathbf{r})$  falls at the Bragg angle on a non absorbing single crystal with a static defect (figure 1). According to the new



**Figure 1.** The scheme of the incidence of a ribbon-like beam on the crystal

principle the amplitudes of waves  $\Psi_0(\mathbf{r})$  and  $\Psi_h(\mathbf{r})$  in the first approximation, can be represented in the form;

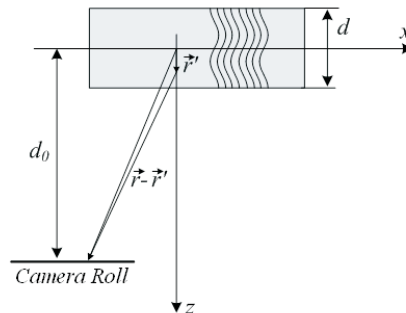
$$\Psi_{0,h}(\mathbf{r}) = \Psi_{0,h}^0(\mathbf{r}) \pm \frac{v}{4\pi} \int \Psi_{0,h}^0(\mathbf{r}') \frac{\exp(i\mathbf{k}|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} \mathbf{U}(\mathbf{r}') d\mathbf{r}' \quad (1)$$

where  $\Psi_{0,h}^0(\mathbf{r})$  – correspondingly, the amplitudes of the waves dynamically diffracted on a perfect crystal  $v$  – the parameter characterizing the strength of interaction of wave  $\Psi_{0,h}^0(\mathbf{r})$  - with the defect,  $\mathbf{U}(\mathbf{r}')$  the local replacement of the atoms from their equilibrium position in the perfect crystal,  $bfr$  the radius-vector of the observation point, the integration is made within the volume of the defect distribution.

The plus and minus signs difference follows from the energy conservation law as the observed strengthening of wave  $\Psi_h(\mathbf{r})$  scattered on a defect occurs at the expense of weakened wave  $\Psi_0(\mathbf{r})$

Expression (1) submits the solution of the volume problem. From the analysis of this solution it is possible, particularly, to predict the phenomenon of X-beam pumping from the passage direction to the reflection direction, the phenomenon of the beam focusing, diffraction on a defect in a crystal. In some cases, it is possible to set the reverse problem of determination of the local shift function  $\mathbf{U}(\mathbf{r}')$  of atoms from their equilibrium position in the perfect crystal, etc.

Particularly, let's consider the phenomenon of modulation of X-rays multiple times scattered on a perfect crystal of quartz where an acoustic standing wave exists. According to the experiment scheme [5] (figure 2) a ribbon-like monochromatic beam of X-ray falls on a single crystal of quartz at the exact Bragg angle when an acoustic standing wave exists along the



**Figure 2.** The scheme of the beam diffraction on the crystal in the presence of standing acoustic wave

crystal width. Under the conditions of the submitted experiment it is possible to admit that  $U = U_0 \cos(2\pi k_{ac}z)$ , where  $k_{ac}$  – the wave number of the acoustic wave.

Expression (1) is brought to the form;

$$\Psi_{0,h}(\mathbf{x}, \mathbf{y}) = \Psi_{0,h}^0(\mathbf{x}, \mathbf{y}) \mp \frac{\mathbf{v}U_0}{4\pi} \int_{-\frac{d}{2}}^{\frac{d}{2}} \Psi_{0,h}^0(\mathbf{0}, z) \frac{\exp(i\mathbf{k}|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} \cos(2\pi k_{ac}z) dz \quad (2)$$

where  $\Psi_{0,h}^0$  – the plane wave solution for the perfect crystal,  $d$  the width of the single crystal. Taking into account the numerical values of the parameters of geometry and radiation of the experiment, the integral in expression (2) is brought to a Fresnel integral, which real part, with the precision of the constant factor has the form:

$$\int_{-\frac{d}{2}}^{\frac{d}{2}} \cos\left[-kz \sin \theta_B \frac{\Delta x}{2d_0} + k \frac{z^2 \cos \theta_B}{4d_0}\right] \cos(2\pi k_{ac}z) dz, \quad (3)$$

where  $\theta_B$  – the precise Bragg angle,  $\Delta x$  – the distance of the viewed point on the photo plate from its center;  $k$  – the wave number of X-wave inside the crystal. The results of the numerical integration are submitted on figure 3.

From the numerical integration (9) follows that in the geometrical cross sections of both the passing and reflected beams occur certain amplitude oscillations, what precisely characterize the experimental results [5].

Expression (1) presents the general expression for the amplitudes of neutrons and X-ray beams multiple times scattered on single crystals with defects of various forms. From this expression analysis, it is possible to predict and quantitatively evaluate different known and new dynamic phenomena while the diffraction of these beams.

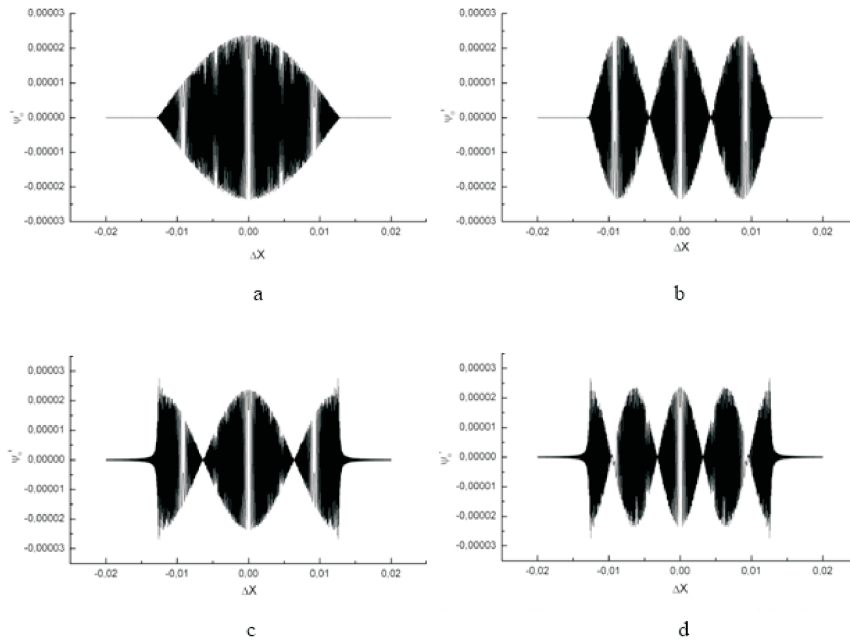
Let's reveal the physical essence of parameter  $v$ , characterizing the interaction power of the radiation with the defect. For this purpose, let's consider the problem of the dynamic scattering of a plane X-ray wave  $\Psi_0(\mathbf{r}) = \Psi_0^j(\mathbf{r}) \exp(-i\mathbf{k}_0^j \mathbf{r})$  in weakly deformed crystal with electric polarization  $\chi(\mathbf{r})$ . The fundamental equation of this scattering has the following form:

$$(\Delta^2 + k_0^2)\Psi = -\nabla \times \nabla \times (\chi\Psi) \quad (4)$$

where  $\Psi(\mathbf{r})$  – the vector of electric induction of the wave scattered in the crystal,  $k_0 = \frac{2\pi}{\lambda}$  – the wave number of the X-wave.

Differential equation (4) is equivalent to the following integral equation [1]:

$$\Psi(\mathbf{r}) = \Psi_0(\mathbf{r}) + \frac{1}{4\pi} \int d\mathbf{r}' \frac{\exp(-i\mathbf{k}|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} \nabla' \times \nabla' \times [\chi(\mathbf{r}')\Psi(\mathbf{r}')] \quad (5)$$



**Figure 3.** The results of numerical integration for the first (a), third (b), fifth (c) and seventh (d) harmonics

We search the solution of equation (5) by applying the method of sequential approximation. In the first approximation of the solution, in the integrand expression, we put, instead  $\Psi(\mathbf{r}')$ , the amplitude  $\Psi(\mathbf{r}')$  of the wave scattered in the perfect crystal. In weakly deformed crystal, the electric polarization  $\chi(\mathbf{r})$  can be presented in the form:

$$\chi(\mathbf{r}') \approx \chi_0(\mathbf{r}' - \mathbf{U}(\mathbf{r}')) \quad (6)$$

where  $\chi_0(\mathbf{r}')$  – the electric polarization of non-deformed crystal. According to Lagrange's formula, it is possible to write as:

$$\chi_0(\mathbf{r}' - \mathbf{U}(\mathbf{r}')) = \chi_0(\mathbf{r}') - \nabla \chi_0 \mathbf{U}(\mathbf{r}'). \quad (7)$$

Taking into account expressions (4–7), the solution of equation (5) can be presented in the form:

$$\Psi(\mathbf{r}) = \Psi^0(\mathbf{r}) - \frac{1}{4\pi} \int d\mathbf{r}' \frac{\exp(-i\mathbf{k}_0 |\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} \nabla' \times \nabla' \times (\nabla \chi_0 \mathbf{U}(\mathbf{r}') \Psi^0(\mathbf{r}')). \quad (8)$$

As  $\frac{\nabla \chi_0 \mathbf{U}(\mathbf{r}')}{\chi_0} \ll 1$  so for the double-wave approximation of scattering, from the corresponding to  $\chi$  equation (4), we'll obtain:

$$\nabla \times \nabla \times (\nabla \chi_0 \mathbf{U}(\mathbf{r}') \Psi^0(\mathbf{r}')) = \frac{\nabla \chi_0 \mathbf{U}(\mathbf{r}')}{\chi_0} 2\mathbf{k}_0^2 \Psi^0(\mathbf{r}'). \quad (9)$$

By inserting expression (9) into (8), we'll obtain the final solution of the formulated problem.

$$\Psi(\mathbf{r}) = \Psi^0(\mathbf{r}) - \frac{1}{4\pi} \int d\mathbf{r}' \frac{\exp(-i\mathbf{k}_0 |\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} \frac{\nabla \chi_0 \mathbf{U}(\mathbf{r}')}{\chi_0} 2\mathbf{k}_0^2 \Psi^0(\mathbf{r}') \quad (10)$$

From the juxtaposition of solution (10) and expression (1), the physical essence of parameter  $v$  is reveal, which characterize the interaction strength between a wave and a defect:

$$v = \frac{2k_0^2}{\chi_0} |\nabla\chi_0| \cos\theta \quad (11)$$

where  $\theta$  - the angle between the bftors  $\nabla\chi_0$  and  $\mathbf{U}(\mathbf{r}')$ .

Taking into account the obtained expression for parameter (11), according to the new principle, the amplitude of the wave diffracted on a defect in a single crystal can be calculated with the formula:

$$\Psi_{0,h}(\mathbf{r}) = \Psi_{0,h}^0(\mathbf{r}) \pm \frac{2k_0^2}{\chi_0} |\nabla\chi_0| \cos\theta \int \Psi_{0,h}^0(\mathbf{r}') \frac{\exp(i\mathbf{k}_0|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} \mathbf{U}(\mathbf{r}') d\mathbf{r}' \quad (12)$$

Particularly, in the far region of the diffraction of a plane monochromatic wave on a defect (Fraunhofer diffraction), the second member presents the Furrier-image of the distribution of the local displacement of the atoms  $\mathbf{U}(\mathbf{r}')$ . Consequently, if the amplitude  $\Psi_{0,h}(\mathbf{r})$  of the diffracted on a defect wave is known, then it possible to solve the reverse problem of the determination of the field  $\mathbf{U}(\mathbf{r}')$  by calculating of the reverse Furrier-image of the amplitude  $\Psi_{0,h}(\mathbf{r})$ .

### 3. Conclusion

In the end it is possible, particularly, to study the phenomenon of the pumping of X-rays into the reflection direction and to predict new phenomena, it is possible to study the focusing of X-ray beams diffracted on defects in crystals. In some cases it possible to formulate the reverse problem of the determination of the function of local replacement of atoms  $\mathbf{U}(\mathbf{r}')$  from their equilibrium location in the perfect crystal, etc.

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