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X-ray acoustic resonance in real crystal

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ABSTRACT : The influence of crystal defects and ultrasound absorption on X-ray diffraction under the condition of X-ray acoustic resonance are theoretically investigated. It is shown that the rocking curve and integral intensity of diffraction are very sensitive to defect's type and concentration.

1 - INTRODUCTION

In the first papers [1, 2] devoted to the X-ray acoustic resonance the most fruitful results were obtained in case of dynamical X-ray scattering on thick ideal crystal ($\mu a > 6$, μ -linear absorption coefficient, a -thickness). It is well known that in that case a wave field corresponded to Bloch function (branch of dispersion surface, DS) with strong absorption can be neglected in comparison with Bloch function with weak absorption on the exit surface of the crystal. As result the rocking curve has not pendellosung oscillations (Borrmann effect).

In vibrating crystals anomalous transparency of X-ray (Borrmann effect) is disrupted for plane waves with such deviation from Bragg's law that the condition of X-ray acoustic resonance can be satisfied :

$$nK_S \approx \text{Re}(\delta K) \quad (1)$$

where $n = 1, 2, \dots$ - number of the phonon taking part in the diffraction, δK - distance between two sheets of the DS along the phonon wave vector K_S direction. Rocking curve has minimas for these deviations (see fig. 1). Convenient experimental scheme is shown on fig. 2.

Figure 1

Figure 2

2 - CRYSTAL DEFECTS

For simplicity we restrict ourselves in what follows to considering symmetric X-ray Laue diffraction with a Bragg angle θ and transversal ultrasonic standing wave. Taking account of multiple reflections of the ultrasonic wave from exit and entrance surfaces and absorption (with coefficient a) one can approximate displacement [3] in ultrasonic wave as :

$$u_s = w \cos(K_s z), \quad w = w_0 (A_1 \cos \omega t + i A_2 \sin \omega t) \quad (2)$$

where ω - ultrasound frequency, t - time, w - amplitude of the atom displacement in ultrasonic wave, K_s - is perpendicular to w , z - coordinate along normal to the entrance surface :

$$A_1 = (\exp \alpha a - \cos K_s a) / (2(\chi \alpha a - \cos K_s a)), \quad A_2 = \sin K_s / 2(\chi \alpha a - \cos K_s a)$$

We start by deriving a general expression for diffracted wave and then we estimate the influence of the defects. All distances are measured in what follows in units Λ/π , Λ - extinction length. We shall look for the solution of Takagi-Taupin's equations ($\chi_h = \chi_h^-$) in real crystal :

$$\partial E_0 / \partial s_0 - i \exp(ihu) E_h = 0, \quad \partial E_h / \partial s_h - i \exp(-ihu) E_0 = 0 \quad (3)$$

where we took into account atom's displacement due to ultrasonic vibration u_s and due to defects u_{def} .
 $u = u_s + u_{def}$.

It is convenient [4] for considered crystal with low defect concentration to treat the coherent and diffuse part of the diffracted wave separately :

$$E_g = E_g^c + E_g^{dif}, \quad g = 0, h \quad (4)$$

In what follows we shall be interested in coherent intensity [4], E_g^c , because diffuse part is relatively small. Omitting the diffuse part and substituting static Debye-Waller factor $E = \langle \exp(\pm ihu_{def}) \rangle$ instead of $\exp(\pm ihu_{def})$ allows us to use solution for ideal vibrating crystal with renormed extinction length $\Lambda' = \Lambda/E$. As result the form of the DS and the resonance condition are changed.

In summary, the influence of the defects on the diffraction arises from ultrasound absorption (amplitude w and absorption coefficient a) and from renormed extinction length. For example, minima positions on rocking curve of defect crystal are determined by condition (1) and consequently by extinction length and E but their depths are determined by amplitude w and consequently by ultrasound absorption.

3 - PERTURBATION THEORY

We shall look for the solution in the form of an expansion :

$$E_g(x, z) = \int_{-\infty}^{\infty} (ipx/\sin \theta) E_g(p, z) dp, \quad g=0, h \quad (5)$$

where parameter p is correlated with deviation from Bragg's angle $\delta\theta$, $p = \delta\theta \sin 2\theta (\Lambda/\lambda)$ and $E_g(p, z)$ is sum of the two Bloch's waves with excitation amplitude $\phi_m(z)$, $m = 1, 2$.

$$E_m(r) = \phi_m(z) \{E_{0m}(p) + E_{hm}(p) \exp(-ihr)\} \exp(i \pm Qz) \quad (6)$$

where $Q = \delta Q/2 = \sqrt{p^2 + (1+i\eta)^2}$, E_{0m} , E_{hm} are solutions of the Takagi-Taupin's equations for unvibrating crystal.

One can derive the closed set of equations related on functions ϕ_2, ϕ_1 :

$$\begin{aligned} v_1 \partial \phi_1 / \partial z &= iK_s(hw) \sin K_s z (\exp(-i\delta Qz) \phi_2 - \phi_1, \\ v_2 \partial \phi_2 / \partial z &= iK_s(hw) \sin K_s z (\exp(i\delta Qz) \phi_1 - \phi_2 \end{aligned} \quad (7)$$

where $v_{1,2} = 2Q/(\pm Q - p)$, h - diffraction vector.

According I.R. Entin [1] for case $K \approx \delta Q$, one should omit a fast oscillating part in [6] and the set of the equations reduces to the simple form :

$$\begin{aligned} 2v_1 \partial \phi_1 / \partial z &= K_s (hw) \exp[i(-K_s + \delta Q)z] \phi_2, \\ 2v_2 \partial \phi_2 / \partial z &= -K_s (hw) \exp[-i(-K_s + \delta Q)z] \phi_1 \end{aligned} \quad (8)$$

Using perturbation theory and neglecting the amplitude of strong absorbed wave ϕ_2 in comparison with ϕ_1 I.R. Entin obtained :

$$\phi_2 \approx i c \phi_1 \exp[i(-K_s + \delta Q)z] / v_2 (-K_s + \delta Q), \quad \phi_1 \approx \phi_1(0) \exp\{-c^2 / v_1 v_2 (-K_s + \delta Q)\} \quad (9)$$

The developed perturbation theory was valid only in case of a rather small ultrasonic amplitude, $(hw)^2 / \text{Im}(\delta Q) \ll 1$, where $\text{Im}(\delta Q)$ dynamical absorption coefficient $\{\text{Im}(\delta Q) \approx 0.15\}$.

4 - EXACT SOLUTION

Exact solution [5] consists of four terms corresponding to four sheets of the DS :

$$\phi_{m,j=1,2} = \sum f_{mj} \exp[\lambda_{mj}z], \quad m = 1, 2 \quad (10)$$

where

$$\lambda_{mj} = i/2 [(-1)^m G + (-1)^j \sqrt{G^2 + K_s^2} J_1(hw)(1 + i\eta)^2 / 4Q^2] \quad (11)$$

Additional splitting between new sheets of DS are proportional Bessel's function of the first order $J_1(hw)$. We note here that formula (11) describes diffraction on crystal with high displacement amplitude ($hw \geq 1$) and reduces to the well known result [1] in the limiting case when $hw \ll 1$. As result we can define w with high accuracy.

Theoretically and experimentally it is known that the integral intensity of the diffraction (IID) on vibrating crystal goes monotonically beyond kinematic limit when hw increases. On the basis of the exact theory anomalous dependance (minimum) of the IID on ultrasonic amplitude was explained. It was found that minimum depth depends on static DW factor and increases with annealing [6].

Summarising, we can say that X-ray resonance can be considered as a very accurate ($\approx 10^{-6}$) method for investigation of the defect structure through extinction length determination and through ultrasonic absorption.

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