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NUMERICAL CALCULATION OF EXTINCTION COEFFICIENT FOR DISLOCATION LOOPS WITH A CERTAIN ORIENTATION

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Abstract. Approximation formulas for the calculation of extinction coefficients in a wide range of radii and concentrations of dislocation loops oriented in certain directions were obtained. It was shown that received expressions make it possible to quickly calculate with satisfactory accuracy the angular dependence of extinction coefficient and speed up the calculation of theoretical rocking curves.

Keywords: X-ray diffractometry, defects, extinction coefficient, dislocation loops.

1. INTRODUCTION

One of the methods of purposeful changing the properties of surface layers of materials used in electronic equipment is ion implantation. Ion implantation leads to the creation of point defects, which can associate into more complex defects, such as dislocation loops. These results in the formation of the crystal subsurface layer with a modified structure, characteristics of which depend on the distribution of stress fields, which parameters, in turn, are determined by shape, size, concentration of defects and in the case of dislocation loops, even their spatial orientation.

A common and express method to determine the numerical characteristics of radiation defects is the X-ray diffractometry. The reliability of the results is determined by the validity of the physical model of defects system used in estimating the angular distribution of intensity of X-rays diffracted by a real crystal with disturbed subsurface layer. In our studies, we used a statistical dynamical theory in the form of [1, 2], which makes it possible to take into account the types of defects and applicable to defects with any size. Nowadays for calculations of such structural sensitive to defects parameter as coefficient of absorption due to diffuse scattering μ_ds (extinction coefficient) correct in many instances assumption that dislocation loops can occur in all equivalent crystallographic planes with equal probability is used [3 - 5]. However, for example in the case of ion implantation, this assumption may be incorrect, and therefore a model in which dislocation loops are located only in certain crystallographic planes should be considered. Theoretical calculations in such cases are very

cumbersome and complex, so the aim of this article was to get the approximation formula for calculating the angular dependence of coefficient of absorption due to diffuse scattering.

2. Calculation of Coefficients in Approximation Formulas

In statistical dynamical theory of X-ray scattering coefficient of reflection from single crystals with uniformly distributed defects consists of coherent and diffuse components:

$$R(\Delta\theta) = R_{coh.}(\Delta\theta) + R_{diff.}(\Delta\theta)$$

Coherent component corresponds to the scattering by the "quasi-ideal" part of the single crystal, and diffuse component corresponds to the scattering by defects of various types. Existing in the crystal defects influence on the formation of both components. One of the parameters through which information about the characteristics of defects is included into the coherent and diffuse components of reflection coefficient of X-rays is the coefficient of absorption due to diffuse scattering $\mu_{ds}(\Delta\theta)$ [2]. It depends on such dislocation loops parameters as Burgers vector, radius and the concentration of dislocation loops.

For calculating the extinction coefficient taking into account the effects of anisotropy for each of them, just as in the work [2], the incident beam deviation from the exact Wolf-Bragg condition, the complex nature of momentum $\vec{q}$ transferred at diffuse scattering and different nature of the diffuse scattering in the Huang and Stokes-Wilson regions are taken into account. Values of coefficient $\mu_{ds}(\Delta\theta)$ for different reflections were calculated using mathematical package Maple 13, however, such calculations are very cumbersome, so the approximation was made and the approximation formula of the coefficient of absorption due to diffuse scattering was derived.

Materials with garnet structure are some of the common materials for which the ion implantation is used to modify their properties. Analysis of deformations that occur in the surface layers of the materials held by us in [6, 7], but taking into account the orientation of defects at X-ray analysis it was not implemented. In order to obtain the approximating functional dependence of the extinction coefficient on radius R and concentration c of dislocation loops and on the angular deviation of the incident beam from the exact Bragg position ($\Delta\theta$), analytical expressions obtained in [8] were used. Calculations were carried out for loops with Burgers vectors parallel to the [111] direction because the existence of such loops are the most likely in the investigated gadolinium gallium garnet (GGG) single crystals and ferrite-garnet films. As a result, arrays for a set of values of the angular deviation from the exact Bragg position ($\Delta\theta$) and radius R and concentration c of dislocation loops for (444), (888) and (880) reflections were received. Radius of dislocation loops ranged from 10 to 300 Å in increments of 2 Å, concentration ranged from $1\cdot10^{10}$ to $1\cdot10^{15}$ cm^{-3}.

Search of function that would satisfactorily approximate calculated data was carried out using Origin application. The approximation was implemented in an environment of written in C++ Builder program that used a combination of a number of approximation methods.

Dependence of the extinction coefficient on ($\Delta\theta$) for all values of R and c looked like two branches of exponential function – increasing and decreasing – that mirror reflected one another. The functional dependence for the descending branch at the relative strain $\Delta d/d = 0$:

$$\mu_{ds}(\Delta\theta, R, c) = y_0(R, c) + A(R, c)\left(e^{-\frac{\Delta\theta}{t_1(R,c)}} + e^{-\frac{\Delta\theta}{t_2(R,c)}}\right) \quad (1)$$

Dependencies at other values of relative strain can be found by shifting this function along angular variable.

The coefficients $A(R, c)$, and $y_0(R, c)$ were approximated by functions of the form:

$$A(R, c) = a_1(c)R^{b_1(c)}, \qquad y_0(R, c) = a_2(c)R^{b_2(c)};$$

coefficients $t_1(R, c)$ and $t_2(R, c)$ – by pseudo-Voigt:

$$t_{1,2} = \eta_{1,2}(R,c)\, G_{1,2}(R,c) + \left(1 - \eta_{1,2}(R,c)\right) L_{1,2}(R,c),$$

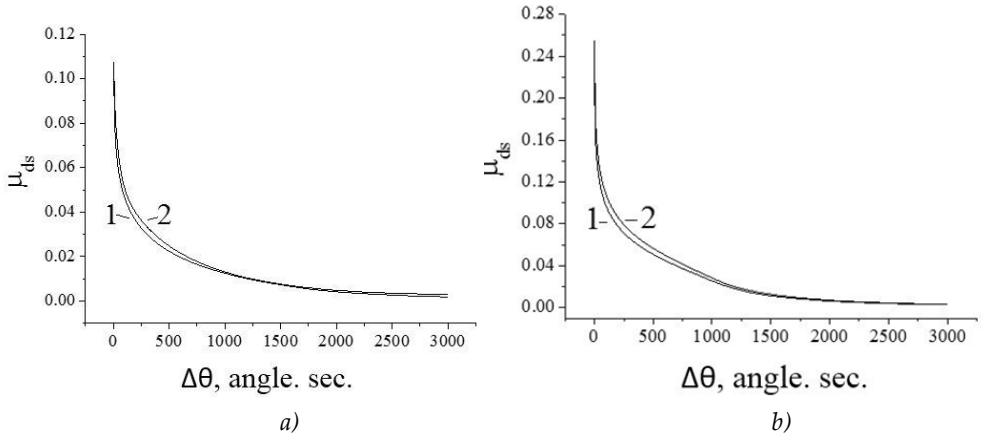
where:

$$L_{1,2}(R,c) = y_{01,2}(c) + \frac{2A_{1,2}(c)}{\pi} \frac{w_{1,2}(c)}{4(R - x_{c\,1,2}(c))^2 + w_{1,2}(c)^2},$$

$$G_{1,2}(R,c) = y_{01,2}(c) + \frac{A_{1,2}(c)}{w_{1,2}(c)} \sqrt{\frac{2\ln(4)}{\pi}}\, e^{-\frac{2(R - x_{c\,1,2}(c))^2 \ln 4}{w^2{}_{1,2}(c)}}.$$

	$A(R,c) = a_1(c) R^{b_1(c)}$					$y_0(R,c) = a_2(c) R^{b_2(c)}$				
	$a_1(c) = a_{11}c^2 + b_{11}c + d_{11}$			$b_1(c) = a_{12}c + b_{12}$		$a_2(c) = a_{21}c^2 + b_{21}c + d_{21}$			$b_2(c) = a_{22}c + b_{22}$	
	a_{11}	b_{11}	d_{11}	a_{12}	b_{12}	a_{21}	b_{21}	d_{21}	a_{22}	b_{22}
(444)	$-1\cdot10^{-4}$	$1\cdot10^{10}$	$2\cdot10^{21}$	$-1\cdot10^{-15}$	3,89	$-7\cdot10^{-13}$	201,94	$2\cdot10^{14}$	$-4\cdot10^{-16}$	2,84
(888)	$-9\cdot10^{-6}$	$3\cdot10^{8}$	$3\cdot10^{18}$	$-3\cdot10^{-15}$	3,51	0	$1\cdot10^{-4}$	$-1\cdot10^{8}$	$-5\cdot10^{-19}$	1,73
(880)	$-8\cdot10^{-5}$	$5\cdot10^{9}$	$1\cdot10^{21}$	$-2\cdot10^{-15}$	3,79	$-8\cdot10^{-12}$	960,75	$3\cdot10^{14}$	$-8\cdot10^{-16}$	2,97
	$t_1(R,c) = \eta_1(R,c) G_1(R,c) + \left(1 - \eta_1(R,c)\right) L_1(R,c)$									
	$A_1(c) = a_{31}c + b_{31}$		$w_1(c) = a_{32}c + b_{32}$		$\eta_1(c) = a_{33}c + b_{33}$	$y_{01}(c) = a_{34}c + b_{34}$			$x_{c1}(c) = a_{35}c + b_{35}$	
	a_{31}	b_{31}	a_{32}	b_{32}	a_{33}	b_{33}	a_{34}	b_{34}	a_{35}	b_{35}
(444)	$-5\cdot10^{-24}$	$1\cdot10^{-8}$	$-5\cdot10^{-22}$	$2\cdot10^{-6}$	$9\cdot10^{-26}$	$1\cdot10^{-6}$	$7\cdot10^{-19}$	$9\cdot10^{-4}$	$2\cdot10^{-22}$	$2\cdot10^{-7}$
(888)	$-5\cdot10^{-22}$	$7\cdot10^{-8}$	$-3\cdot10^{-21}$	$2\cdot10^{-6}$	$-9\cdot10^{-16}$	0,28	$3\cdot10^{-18}$	$3\cdot10^{-4}$	$5\cdot10^{-21}$	$-2\cdot10^{-6}$
(880)	$-4\cdot10^{24}$	$1\cdot10^{-8}$	$-3\cdot10^{22}$	$1\cdot10^{-6}$	$2\cdot10^{-24}$	$1\cdot10^{-6}$	$5\cdot10^{-19}$	$8\cdot10^{-4}$	$1\cdot10^{-22}$	$-1\cdot10^{-8}$
	$t_2(R,c) = \eta_2(R,c) G_2(R,c) + \left(1 - \eta_2(R,c)\right) L_2(R,c)$									
	$A_2(c) = a_{41}c + b_{41}$		$w_2(c) = a_{42}c + b_{42}$		$\eta_2(c) = a_{43}c + b_{43}$	$y_{02}(c) = a_{44}c + b_{44}$			$x_{c2}(c) = a_{45}c + b_{45}$	
	a_{41}	b_{41}	a_{42}	b_{42}	a_{43}	b_{43}	a_{44}	b_{44}	a_{45}	b_{45}
(444)	$-1\cdot10^{-25}$	$5\cdot10^{-10}$	$-2\cdot10^{-22}$	$2\cdot10^{-6}$	$4\cdot10^{-24}$	$1\cdot10^{-6}$	$2\cdot10^{-20}$	$9\cdot10^{-5}$	$5\cdot10^{-23}$	$3\cdot10^{-7}$
(888)	$-4\cdot10^{-23}$	$9\cdot10^{-9}$	$-9\cdot10^{-22}$	$1\cdot10^{-6}$	$-4\cdot10^{-16}$	0,78	$4\cdot10^{-20}$	$3\cdot10^{-5}$	$2\cdot10^{-21}$	$-2\cdot10^{-6}$
(880)	$-6\cdot10^{-26}$	$6\cdot10^{-10}$	$4\cdot10^{-24}$	$1\cdot10^{-6}$	$1\cdot10^{-23}$	$1\cdot10^{-6}$	$4\cdot10^{-21}$	$2\cdot10^{-4}$	$5\cdot10^{-23}$	$-8\cdot10^{8}$

Tab. 1 The coefficients of the approximating functions for (444) (888) and (880) reflections from GGG single crystals.



a) *b)*

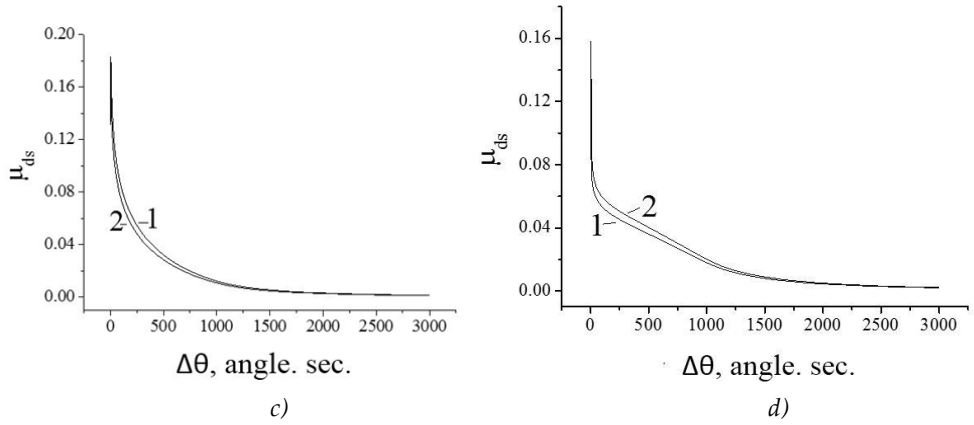


Fig. 1. Angular dependencies of $\mu_{ds}(\Delta\theta)$ for GGG single crystals in assumption of the presence of dislocation loops of radius R = 100 Å (1 – calculated by statistical dynamical theory considering anisotropy, 2 – calculated by approximation formula), a – reflection (444), b – reflection (888), c – reflection (880) (strongly absorbed wave fields), d – reflections (880) (weakly absorbed wave fields).

Dependence of the most coefficients of Pseudo-Voigt and exponential function on concentration is linear and others – parabolic. Analytical dependences of coefficients of approximation function on the radius and concentration of prismatic dislocation loops with Burgers vector parallel to the [111] direction, and the values of the numerical coefficients for reflections (444), (888) and (880) from the GGG single crystals are shown in the Table 1.

Approximation formula (1) gives a satisfactory approximation of the function $\mu_{ds}(\Delta\theta)$ at the concentrations ≤ $1 \cdot 10^{12}$ cm^{-3} (Fig. 1), but slightly worse – at large values of concentration. Obviously, this is related to the total error resulting from the multiple approximations.

3. CONCLUSION

Functional relationships were derived and coefficients by means of which it is possible to calculate the extinction coefficient μds, which takes into account the effects of anisotropy in the orientation of the dislocation loops in the crystal were calculated. Obtained approximation formula within the statistical dynamical theory enables to calculate with a satisfactory accuracy the theoretical rockin curves, which takes into account the effects of anisotropy in the orientation of dislocation loops.

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Яремій І.П., Томин У.О., Яремій С.І., Луканюк М.М., Годовська Г.М., Катрич Ю.І. Чисельний розрахунок коефіцієнта екстинкції для дислокаційних петель з певною орієнтацією. *Журнал Прикарпатського університету імені Василя Стефаника*, **3** (1) (2016), 75–79.

Отримано апроксимаційні формули для розрахунку коефіцієнтів екстинкції у широкому діапазоні радіусів і концентрацій дислокаційних петель, при їх орієнтації в певних напрямках. Показано, що дані залежності із задовільною точністю дають можливість швидко розрахувати кутову залежність коефіцієнта екстинкції та пришвидшити розрахунок теоретичних кривих дифракційного відбивання.

Ключові слова: Х-променева дифрактометрія, дефекти, коефіцієнт екстинкції, дислокаційні петлі.