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Integrated dynamical phase-variation diffractometry of single crystals with defects of three and more types

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Abstract. Generalization of the methods for the purposeful influence of the interrelated variations inherent to different experimental conditions on changes in the selectivity of the sensitivity of the azimuthal dependence of the total integrated intensity of dynamical diffraction to various types of defects in single crystals has been carried out. As a result, the improved phase-variation methods with additionally increased sensitivity and informativity of non-destructive structural diagnostics aimed at multi-parametrical single crystal systems have been developed.

Keywords: phase variation diagnostics, azimuthal dependence, defects.

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1. Introduction

This paper is a continuation of paper [1] and devoted to the analysis of fundamentally new selectivity features of the sensitivity of the azimuthal dependence (AD) of the total integrated intensity of dynamical diffraction (TIIDD) to different types of defects in single crystals. The physical nature of its occurrence, as well as the resulting possibilities of the purposeful influence of interrelated variations in different experimental conditions on changes in this sensitivity of selectivity are ascertained and analyzed.

Whereas the sensitivity of the integrated intensity of diffuse scattering to defects is researched, it should be noted that the intensity depends on the ways of instrumental integration of diffracted X-ray beams. Namely, the intensity can be a function of one or two angular variables, if this integration is performed on two or one angular deviation, *i.e.* on the Ewald sphere, when rocking curves from the imperfect crystals are measured using the double-crystal diffractometer with widely open detector window, or on a vertical divergence when reciprocal space maps are measured using the triple-crystal diffractometer, respectively. If integration is performed on all the three angular deviations, *i.e.* in a whole reciprocal lattice space, the integrated intensity will be a number (not function), and then the additional measurements are necessary for the successful characterization of defects. For example, one can point out the investigations of thickness dependences of the integrated diffraction intensity from thin crystals in the Laue diffraction geometry [2–4] or the measurements of the integrated diffraction intensity as a function of X-ray wavelength [5], the measurements of azimuth dependences of the integrated reflection power in the asymmetric Bragg diffraction geometry [6].

The aim of this paper is to increase the efficiency of practical applications of the dispersion mechanism discovered by the authors (see Refs in [1]) and the phase-variation principles developed by them on this basis. The use of phase-variation principles enhances the manifestation of the structural imperfections in the single crystals selective to the type of defects in the diffraction pattern of dynamically scattered radiation. On this base, a number of new possibilities have been already demonstrated in [1] by using the example of increasing the efficiency of the known diagnostic methods. The method is applicable for diagnostics of single crystals with a disturbed surface layer (DSL) and defects of different types by applying the measurements of azimuthal dependence inherent to TIIDD. The main feature of this approach is the complete suppression of the contribution from diffuse scattering related to 'large' randomly distributed dislocation loops (RDDL) to TIIDD by overlapping the angular region of total reflection in the Bragg diffraction geometry. As demonstrated in [1], due to this overlapping the number of defect parameters that determined at the same time from the experimental measurements is decreased. It was also proposed to replenish the measurements of azimuthal dependence of TIIDD on molybdenum X-ray source with measurements of azimuthal dependence of TIIDD on copper source. In this case, it was completely suppressed not only the contribution from diffuse scattering on RDDL, but also simultaneously from 'small' dislocation loops, as caused by different reasons. The effect of anomalous growth of diffuse scattering for copper radiation is suppressed due to the enhancement of absorption and the decreasing of the depth of formation of diffuse scattering. Therefore, the physical nature of the possibility of major increasing the selectivity of sensitivity to DSL of azimuthal dependence of TIIDD measured at the source of copper radiation is explained in [1]. It became the basis for the development of new improved approach of the phase-variation diagnostics with increased sensitivity and informativity, when determining the parameters of all types of defects. This work is aimed at generalization of proposed in [1] approach of the phase-variation diagnostics for the case of the presence of three or more different types of defects in a single crystal.

2. Experimental results and analysis of them

The presented experimental results were carried out using the Panalytical Philips X'Pert PRO diffractometer (V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine). All calculations presented in this paper were performed for Si single crystals with microdefects according to the formulas proposed in [8, 9], and the used designations coincide with those of [1].

The azimuthal dependences of TIIDD for Bragg reflections (220) and radiation CuK_α are presented in Fig. 1. Here, the solid line shows the results of calculation at $t_{am} = 0.75$ μm, $k = 0.033$, $R_{\text{large loops}} = 20$ μm, $c_{\text{large loops}} = 2.5\cdot10^5$ cm^{-3}, $R_{\text{small loops}} = 0.02$ μm, $c_{\text{small loops}} = 2.086\cdot10^{13}$ cm^{-3}; the short dash line shows the results of calculation at $t_{am} = 0.75$ μm, $k = 0$, $R_{\text{large loops}} = 20$ μm, $c_{\text{large loops}} = 2.5\cdot10^5$ cm^{-3}, $R_{\text{small loops}} = 0.02$ μm, $c_{\text{small loops}} = 2.086\cdot10^{13}$cm^{-3}; markers are the data of experiments.

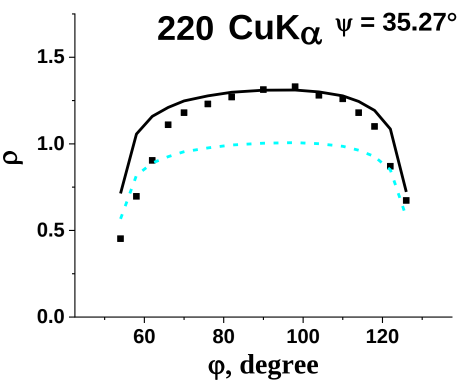

Fig. 1. The normalized azimuthal dependences of TIIDD (ρ) for Bragg reflections (220), radiation CuK_α.

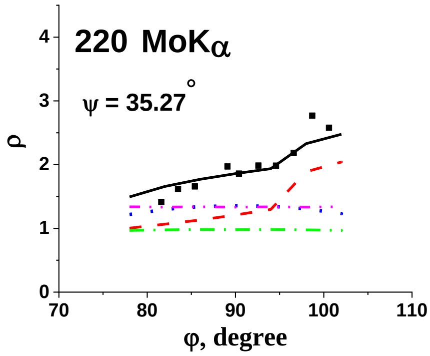

Fig. 2. Normalized azimuthal dependences of TIIDD (ρ) for Bragg reflections (220), radiation MoK_α.

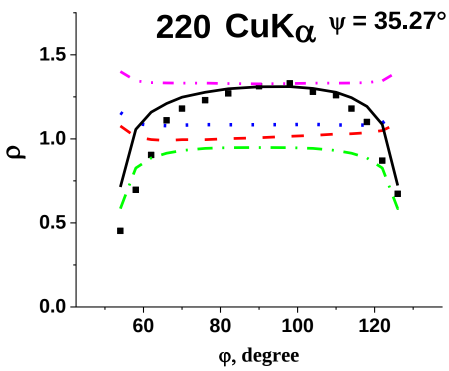

Fig. 3. The normalized azimuthal dependences of TIIDD (ρ) for different defect structures (Bragg reflections (220), radiation CuK_α).

It should be noted that, when using CuK_α radiation, the values of TIIDD calculated without account of the kinematically scattering DSL sublayer (short dash) are almost 30% less than the experimental values (markers). This behavior is observed for the largest values (right side) or the least ones (left side) of azimuthal angles. For these angles, the disagreement between the experiment values and solid line is maximum. The solid line is considerably higher than these experimental points, however, for all the rest points the solid line well coincides with experimental data. For these points, the short dash line practically coincides with IIDD for a perfect crystal. In addition, it should be taken into account the results obtained in [1], which are presented in Figs 2 and 3 for convenience of combined analysis (see [1], Figs 7 and 9, respectively). Here, the solid line shows the results of calculation at $t_{am} = 0.75$ μm, $k = 0.033$, $R_{\text{large loops}} = 20$ μm, $c_{\text{large loops}} = 2.5\cdot10^5$ cm^{-3}, $R_{\text{small loops}} = 0.02$ μm, $c_{\text{small loops}} = 2.086\cdot10^{13}$ cm^{-3}; while the dash line shows the results of calculation at $t_{am} = 0$, $k = 0$, $R_{\text{large loops}} = 20$ μm, $c_{\text{large loops}} = 2.5\cdot10^5$ cm^{-3}, $c_{\text{small loops}} = 0$; dot line shows the results of calculation at $t_{am} = 0$, $k = 0$, $R_{\text{small loops}} = 0.02$ μm, $c_{\text{small loops}} = 2.086\cdot10^{13}$ cm^{-3}, $c_{\text{large loops}} = 0$; the dash-dot line shows the results of calculation at $t_{am} = 0.75$ μm, $k = 0$, $c_{\text{large loops}} = 0$, $c_{\text{small loops}} = 0$; dash-double dot line shows the results of calculation at $t_{am} = 0$, $k = 0.033$, $c_{\text{large loops}} = 0$, $c_{\text{small loops}} = 0$; markers correspond to experimental data [1].

These facts are indicative of the negligible RDDL contribution to the TIIDD at most azimuthal angles and possibility of the refinement of both DSL parameters. The DSL parameters can be refined by achievement of optimal coincidence between the theoretical azimuthal dependences of TIIDD and experimental data at first for determination of the parameter of the kinematically scattering sublayer of DSL for azimuthal angles close to 90° and then for determination of the parameter inherent to the absorbing sublayer for the minimal or maximal azimuthal angles. Herewith the assumption of absence of the absorbing sublayer and RDDL are used (in the first case), and the assumption of absence of RDDL, but with account of the determined parameter for the kinematically scattering sublayer of DSL (in the second case). It should be also noted that these recommendations have already taken into account the differences between the dependences on the azimuthal angle for the sensitivity of the parameters of the DSL sublayers and the selectivity of these sensitivity values. As seen from Fig. 3, the sensitivity to the kinematically scattering sublayer of DSL practically does not depend on azimuthal angle. In addition, the sensitivity to the absorbing sublayer of DSL is practically absent at azimuthal angles close to 90° and increases with deflection of azimuthal angle from 90° (see also the discussion of Figs 4 and 5).

Fig. 4 illustrates the change of the sensibility of TIIDD to the thickness of absorbing DSL sublayer t_{am} for different reflections (radiation CuK_α). Fig. 4 shows that, at the given thickness of absorbing layer, the value of normalized TIIDD for the reflection (220) is four times less than that for reflections (224), (440) and 2.8 times less than the respective value for reflection (004) of radiation CuK_α. Thus, the azimuthal dependences of TIIDD are selectively sensitive to the thickness t_{am}.

Fig. 5 illustrates the change of the sensitivity of TIIDD to the thickness of kinematically scattering DSL sublayer (~$k\Lambda$, k = 0.033) when varying reflections of CuK_α-radiation (their extinction lengths in perfect crystals). Fig. 5 shows that at k = 0.033 the difference from unity of the normalized azimuthal dependences of TIIDD for reflection (220), radiation CuK_α, is already 15%. It is 2.8 times less than the differences from unity of the normalized azimuthal dependences of TIIDD for reflections (224) and (440), radiation CuK_α, and 1.75 times less than the difference from unity of the normalized azimuthal dependences of TIIDD for reflection (004), radiation CuK_α. Thus, the azimuthal dependences of TIIDD obtained for reflections (004), (220), (224) and (440), radiation CuK_α, are selectively sensitive to the parameter k.

Comparative analysis of the features of influence of parameters for two DSL sublayers on their contributions to TIIDD on the basis of results adduced in Figs 4 and 5 are carried out. The contributions of sublayers to TIIDD are large values and opposite signs, the changes of sensitivity of selectivity of the azimuthal dependences of TIIDD to parameters of two DSL sublayers, when varying the reflection, are also large.

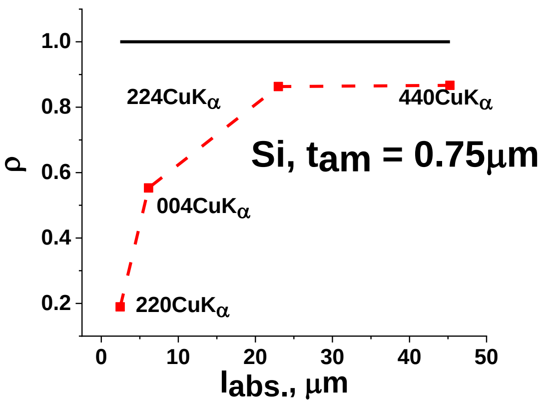

Fig. 4. Dependences of normalized TIIDD *vs* the length of beam path in the absorbing sublayer of DSL for different reflections calculated at t_{am} = 0.75 μm, k = 0 (dash line) and for perfect crystal (solid line).

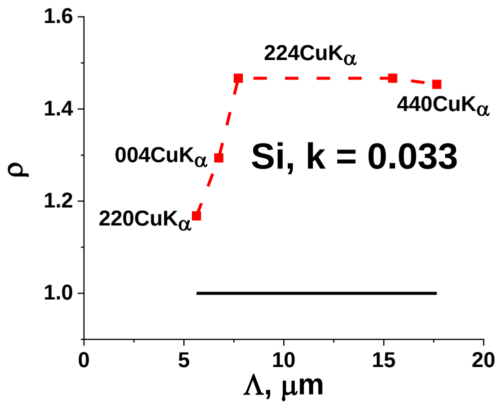

Fig. 5. Dependences of normalized TIIDD *vs* the extinction length calculated at t_{am} = 0, k = 0.033 (dash line) and for perfect crystal (solid line).

After refining the DSL parameters, the correction of microdefects parameters are carried out. The following values of defects parameters are obtained: 1) for DSL t_{am} = 0.75 μm, k = 0.033, 2) for large dislocation loops $R_{\text{large loops}}$ = 7 μm, $c_{\text{large loops}}$ = $3.31\cdot10^6$ cm^{-3}, 3) for small dislocation loops $R_{\text{small loops}}$ = 0.02 μm, $c_{\text{small loops}}$ = $8.9\cdot10^{12}$ cm^{-3}. The results are confirmed by literature data [7] obtained earlier using the destructive methods.

3. The additional functionality of the phase-variation diagnostics due to the anomalous absorption effect

The resources for additional increase of the diagnostics accuracy due to using the effect of anomalous absorption of diffuse scattering are illustrated by the results of the calculations presented in Figs 6 to 13.

The changes of sensitivity of the azimuthal dependences of TIIDD to different types of microdefects when changing the reflections are shown in Figs 6 to 8.

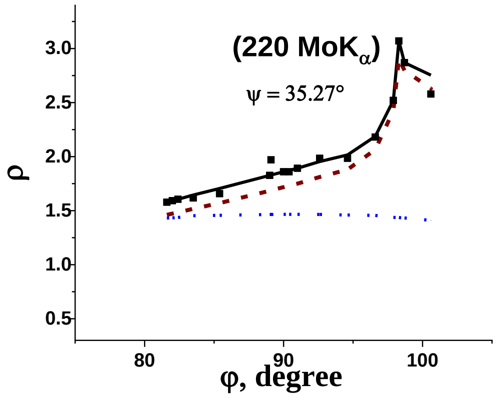

Fig. 6. Refined and normalized azimuthal dependences of TIIDD (ρ) for Bragg reflections (220), radiation MoK_α.

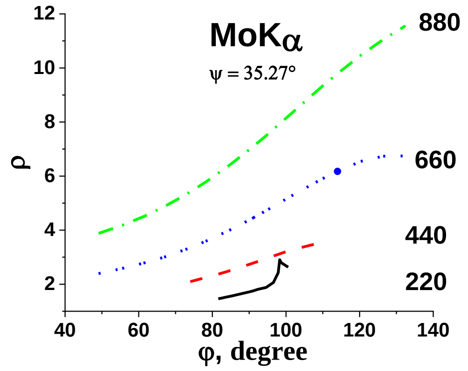

Fig. 7. Refined and normalized azimuthal dependences of TIIDD (ρ) for single crystal with ‘large’ microdefects (Bragg reflections (220), (440), (660), (880), radiation MoK_α).

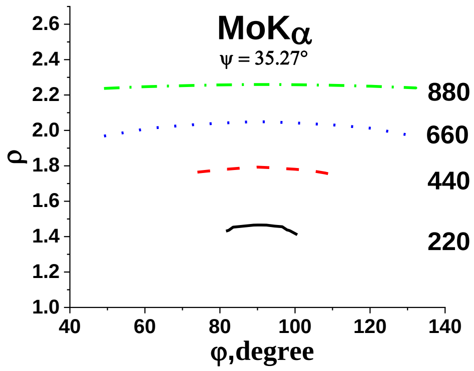

Fig. 8. Refined and normalized azimuthal dependences of TIIDD (ρ) for single crystal with ‘small’ microdefects (Bragg reflections (220), (440), (660), (880), radiation MoK_α).

Fig. 6 shows that contribution to TIIDD from ‘large’ microdefects contrary to ‘small’ microdefects has non-monotonic AD, which agrees with theoretical ideas about the anomalous transmission of the diffuse component of TIIDD. Here, solid line shows the results of calculation at t_{am} = 0.75 µm, k = 0.033, $R_{\text{large loops}}$ = 7 µm, $c_{\text{large loops}}$ = 3.31·10^6 cm^{-3}, $R_{\text{small loops}}$ = 0.02 µm, $c_{\text{small loops}}$ = 8.9·10^{12} cm^{-3}; the dash line shows the results of calculation at t_{am} = 0.75 µm, k = 0.033, $R_{\text{large loops}}$ = 7 µm, $c_{\text{large loops}}$ = 3.31·10^6 cm^{-3}, $c_{\text{small loops}}$ = 0; the dot line shows the results of calculation at t_{am} = 0.75 µm, k = 0.033, $R_{\text{small loops}}$ = 0.02 µm, $c_{\text{small loops}}$ = 8.9·10^{12} cm^{-3}.

The azimuthal dependences of TIIDD for single crystal with ‘large’ microdefects at different reflections of radiation MoK_α are adduced in Fig. 7. The calculations were carried out at t_{am} = 0.75 µm, k = 0.033, $R_{\text{large loops}}$ = 7 µm, $c_{\text{large loops}}$ = 3.31·10^6 cm^{-3}, $c_{\text{small loops}}$ = 0; the solid line shows the results of calculation for the reflection (220); the dash line shows the results of calculation for the reflection (440); the dot line shows the results of calculation for reflection (660); the dash-dot line shows the results of calculation for the reflection (880). As can be seen, the sensitivity of TIIDD to ‘large’ microdefects for the reflection (220) is ≈4 time less than for the reflection (880).

Fig. 8 presents the azimuthal dependences of TIIDD for single crystal with ‘small’ microdefects at different reflections of radiation MoK_α. The calculations are carried out at t_{am} = 0.75 µm, k = 0.033, $c_{\text{large loops}}$ = 0, $R_{\text{small loops}}$ = 0.02 µm, $c_{\text{small loops}}$ = 8.9·10^{12} cm^{-3}; the solid line shows the results of calculation for the reflection (220); the dash line shows the results of calculation for the reflection (440); the dot line shows the results of calculation for the reflection (660); the dash-dot line shows the results of calculation for the reflection (880). As can be seen, the sensitivity of TIIDD to ‘small’ microdefects at reflection (220) is ≈1.6 time less than for the reflection (880).

The changes in sensitivity of the azimuthal dependences of TIIDD to different types of microdefects, when changing the wavelength of characteristic radiation, are shown in Figs 9 to 11.

Fig. 9 shows that the sensitivity of TIIDD to ‘small’ microdefects for the reflection (220), radiation CuK_β is ≈1.2 time less than for the reflection (220), radiation AgK_β. The calculation are carried out at t_{am} = 0.75 µm, k = 0.033, $c_{\text{large loops}}$ = 0, $R_{\text{small loops}}$ = 0.02 µm, $c_{\text{small loops}}$ = 8.9·10^{12} cm^{-3}; the solid line shows the results of calculation for CuK_α; the dash line shows the results of calculation for MoK_α; the dot line shows the results of calculation for MoK_β; the dash-dot line shows the results of calculation for AgK_α; the dash-dot line shows the results of calculation for AgK_β.

Figs 10 and 11 show that the sensitivity of TIIDD to ‘large’ microdefects for the reflection (220), radiation MoK_α, is 12.5 time less than for the reflection (220), radiation AgK_β.

The sensitivity of the azimuthal dependences of TIIDD to ‘large’ microdefects of different sizes at reflection (220), radiation MoK_β, is illustrated by the results of the calculations presented in Figs 12 and 13.

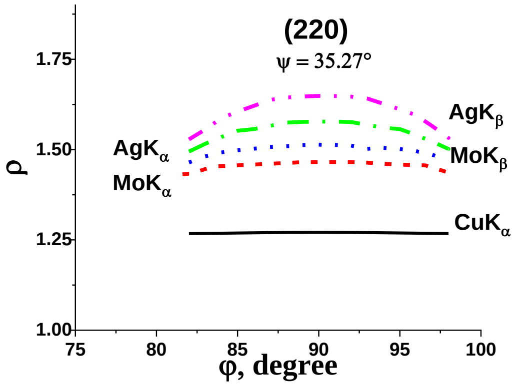

Fig. 9. Normalized azimuthal dependences of TIIDD (ρ) for the Bragg reflection (220), radiation AgK_α and AgK_β.

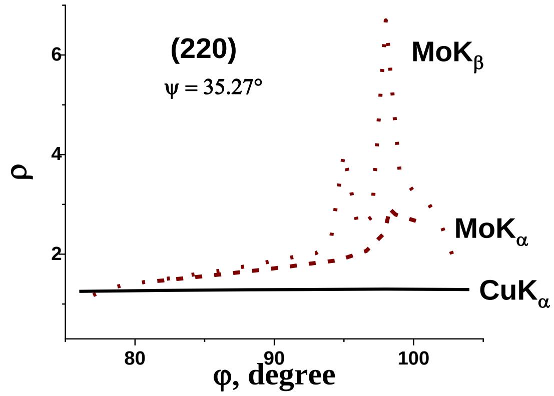

Fig. 10. Normalized azimuthal dependences of TIIDD (ρ) for the Bragg reflections (220), radiation CuK_α, MoK_α, MoK_β. These calculations were carried out at t_{am} = 0.75 μm, k = 0.033, $R_{\text{large loops}}$ = 7 μm, $c_{\text{large loops}}$ = 3.31·10^6 cm^{-3}, $c_{\text{small loops}}$ = 0; the solid line shows the results of calculation for CuK_α; the dash line shows the results of calculation for MoK_α; the dot line shows the results of calculation for MoK_β radiation.

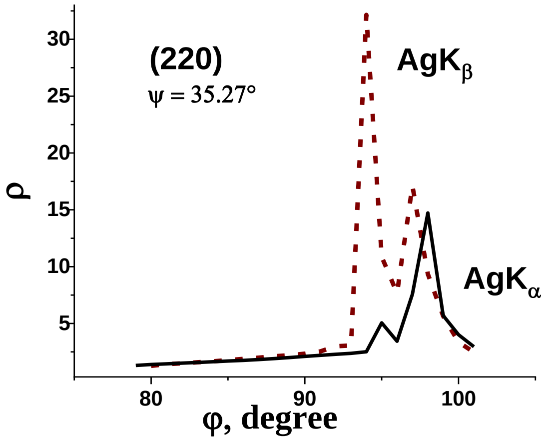

Fig. 11. Normalized azimuthal dependences of TIIDD (ρ) for the Bragg reflection (220), radiation AgK_α and AgK_β. These calculations were carried out at t_{am} = 0.75 μm, k = 0.033, $R_{\text{large loops}}$ = 7 μm, $c_{\text{large loops}}$ = 3.31·10^6 cm^{-3}, $c_{\text{small loops}}$ = 0; the solid line shows the results of calculation for AgK_α, the dash line shows the results of calculation for AgK_β.

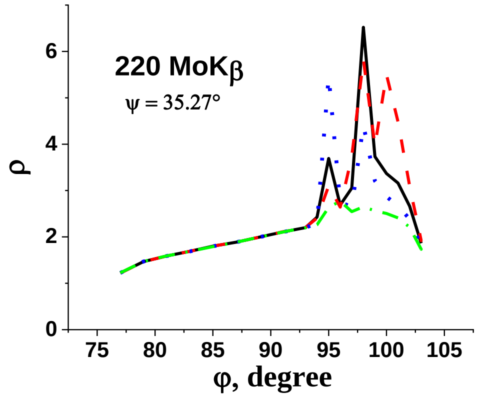

Fig. 12. Normalized azimuthal dependences of TIIDD (ρ) for 'large' loops ($R_{\text{large loops}}$ = 5…8 μm) (Bragg reflection (220), radiation MoK_β).

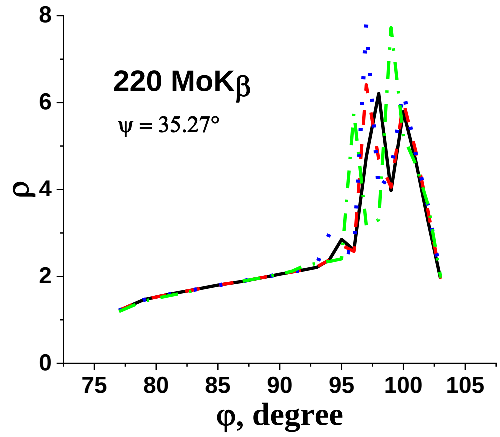

Fig. 13. Normalized azimuthal dependences of TIIDD (ρ) for 'large' loops ($R_{\text{large loops}}$ = 9…20 μm) (Bragg reflection (220), radiation MoK_β).

Fig. 12 shows that the peak in the azimuthal dependences of TIIDD at (220) reflection, radiation MoK_β ($\Lambda_{90°}$ = 5.75 μm) is practically absent at $R_{\text{large loops}}$ = 5 μm, appears at $R_{\text{large loops}}$ = 6 μm and increases at $R_{\text{large loops}}$ = 7 μm. Lines show the results of calculation at t_{am} = 0.75 μm, k = 0.033, $R_{\text{small loops}}$ = 0.02 μm, $c_{\text{small loops}}$ = 8.9·10^{12} cm^{-3}. The solid line shows the results of calculations at $R_{\text{large loops}}$ = 7 μm, $c_{\text{large loops}}$ = 3.31·10^6 cm^{-3}; the dash line shows the results of calculations at $R_{\text{large loops}}$ = 8 μm, $c_{\text{large loops}}$ = 2.5825·10^6 cm^{-3}; the dot line shows the results of calculation at $R_{\text{large loops}}$ = 6 μm, $c_{\text{large loops}}$ = 4.425·10^6 cm^{-3}; the dash-dot line shows the results of calculation at $R_{\text{large loops}}$ = 5 μm, $c_{\text{large loops}}$ = 6.25·10^5 cm^{-3}.

Fig. 13 shows that the peak in the azimuthal dependences of TIIDD at (220) reflection, radiation MoK_β ($\Lambda_{90°}$ = 5.75 μm) is present at any average radius of the 'large' microdefects exceeding the extinction length. Lines show the results of calculation at t_{am} = 0.75 μm, k = 0.033, $R_{\text{small loops}}$ = 0.02 μm, $c_{\text{small loops}}$ = 8.9·10^{12} cm^{-3}. The solid line shows the results of calculation at $R_{\text{large loops}}$ = 9 μm, $c_{\text{large loops}}$ = 2.0795·10^6 cm^{-3}, dash line shows the results of calculation at $R_{\text{large loops}}$ = 10 μm, $c_{\text{large loops}}$ = $1.7175\cdot10^6$ cm^{-3}, dot line shows the results of calculation at $R_{\text{large loops}}$ = 12 μm, $c_{\text{large loops}}$ = $1.2375\cdot10^6$ cm^{-3}, dash-dot line shows the results of calculation at $R_{\text{large loops}}$ = 20 μm, $c_{\text{large loops}}$ = $4.915\cdot10^5$ cm^{-3}.

As a result, the differences of the features of change in selectivity of sensitivity of the azimuthal dependences of TIIDD for sublayers of DSL to their parameters by varying the azimuth angles were determined. It enables to enhance the sensitivity and informativity of the developed phase-variation non-destructive structural diagnostics of multiparametrical systems.

4. Conclusions

The obtained results and the performed analysis demonstrate the possibility to develop new methods of phase-variation non-destructive structural diagnostics, in particular, by using the methods of the azimuthal dependences of TIIDD with appreciably advanced functional resources of the sensitivity and informativity of characterization aimed at multiparametrical monocrystalline objects. Among the most important new physical features of dynamical diffraction in single crystals with defects, it is proposed to practically use the following approaches:

1. For the developed technique of phase-variation diagnostics, two options are possible:

a) to determine the thickness of the absorbing sublayer of DSL from the most selective sensitivity to the thickness azimuthal dependences of TIIDD at (220) reflection, copper radiation and at the minimum and maximum azimuthal angles neglecting both RDDL and the kinematically scattering DSL sublayer. Thereafter, taking into account the thickness of the absorbing sublayer and neglecting RDDL, it has been determined the deformation parameter of the kinematically scattering sublayer of DSL from the most selective sensitivity to this parameter the azimuthal dependences of TIIDD at (220) reflection, copper radiation, but at azimuthal angles close to 90°.

b) However, in the case of defects considered in this work, it is rational to reverse the procedure for determining the parameters of DSL proposed in the previous item. Namely, this procedure should begin with determining the deformation parameter of the kinematically scattering sublayer by neglecting the absorbing sublayer and RDDL. As appropriate each of the proposed procedures for determining the parameters of sublayers of DSL can be continued using the parameters of the sublayer of DSL already determined in previous iteration.

It should be noted that the proposed approach is required of preliminary analysis and determining the main type of defects with the largest relative contribution to the measured TIIDD and necessary for this variations experimental conditions. After that, it is necessary to determine the type of defects with second relative contribution to TIIDD and so on until all the types of defects are enumerated.

2. After determination of the parameters of DSL by using the copper radiation source, it is necessary to determine the characteristics of RDDL from the azimuthal dependences of TIIDD measured on molybdenum radiation source, reflection (220). In this case, two ways are also possible:

a) at first, one needs to determine the characteristics of ‘small’ RDDL by measuring the minimum azimuthal angles and neglecting the ‘large’ RDDL. However, for refinement of the determined parameters, it can be also used the azimuthal dependences of TIIDD measured using copper radiation, which provides sensitivity to ‘small’ loops. After that, using the determined parameters of DSL and ‘small’ RDDL it is necessary to determine the characteristics of ‘large’ RDDL based on processing of the azimuthal dependences of TIIDD measured using the molybdenum radiation source, reflection (220) at maximum azimuthal angles and at maximum values of TIIDD.

b) the procedure is carried out similarly to the item (a) with taking into account the remarks made to the item (1). The parameters of ‘large’ dislocation loops are determined with neglecting the presence of ‘small’ loops. Then the parameters of ‘small’ dislocation loops are determined with account of the parameters for ‘large’ dislocation loops and so on until the required accuracy is achieved.

3. It can be also processed the azimuthal dependences of TIIDD measured with the molybdenum source for (440) and (660) reflections similar to the item (2). As a result, the profiles of distributions of RDDL over the depth of the sample can be determined.

Thus, the proposed phase-variation methods allow increasing (as compared to the traditional diagnostic methods) the sensitivity and informativity of non-destructive structural diagnostics of multiparameteric monocrystalline systems.

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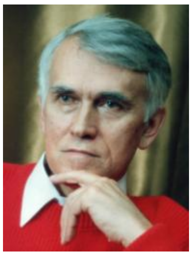

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Інтегральна динамічна фазоваріаційна дифрактометрія монокристалів з дефектами трьох і більше типів

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Анотація. Проведено узагальнення методів цілеспрямованого впливу взаємопов'язаних варіацій різних умов експерименту на зміну вибірковості чутливості азимутальної залежності повної інтегральної інтенсивності динамічної дифракції до різних типів дефектів у монокристалах. У результаті розроблено вдосконалені фазоваріаційні методи з додатково підвищеною чутливістю та інформативністю неруйнівної структурної діагностики багатопараметричних монокристалічних систем.

Ключові слова: фазоваріаційна діагностика, азимутальна залежність, дефект.