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ВЗАИМОДЕЙСТВИЯ ИЗЛУЧЕНИЯ И ЧАСТИЦ С КОНДЕНСИРОВАННЫМ ВЕЩЕСТВОМ

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Models of Deformation Dependences of Total Integrated Intensity of Dynamical Diffraction in Single Crystals for Various Diffraction Conditions

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The paper shows the pattern of change in the deformation dependences (DD) of integrated intensity of dynamical diffraction (IIDD) with crystal thickness and with variation of other diffraction conditions by means of the Chukhovskii–Petrashen theory for the DD of IIDD in defect-free crystals. Relying on this and numerous other experiments with real defective crystals as well as the results of total integrated intensity of dynamical diffraction (TIIDD) in crystals with defects without bend, an analytical model of the DD of TIIDD in crystals with defects is developed, which is feasible for the diagnostics of structural defects in crystals. The heuristic model constructed for the DD of TIIDD in crystals with defects considers the DD of reflectivity and absorptive power of crystal, whose contribution is determined by model parameters (α, β, γ, ...) for both Bragg and diffuse components of TIIDD. As found, the sufficiently accurate DD description with fixed parameters and single description expressions is only achieved in certain narrow ranges of deformation radii. However, these parameters are selectively dependent on each set of parameters of diffraction conditions (wavelengths, crystal thicknesses, reflection indexes, diffraction geometries, etc.). As shown, the construction of the heuristic model of the DD of TIIDD in crystals with defects as a diagnostic method has only become possible because we were able to factorize the effect of microdefects and deformation parameter on coherent and diffuse components of TIIDD, separately; but it is important to save non-factorization of their effect on total IIDD.

В роботі за допомогою теорії Чуховського–Петрашеня для деформаційної залежности (ДЗ) інтеґральної інтенсивности динамічної дифракції (ІІДД) у кристалах без дефектів показано характер зміни ДЗ ІДД із товщиною кристалу та з варіяцією інших умов дифракції. На цій основі, а також при використанні ряду експериментів із реальними дефектними кристалами і результатів теорії повної інтеґральної інтенсивности динамічної дифракції (ПІДД) у кристалах з дефектами без вигину побудовано аналітичну модель ДЗ ПІДД у кристалах з дефектами, придатну для діягностики параметрів структурних дефектів у кристалах. Одержано евристичні вирази для ПІДД у кристалах з дефектами, що враховують ДЗ поглинальних і відбивних здатностей кристалів, внесок яких визначається параметрами моделі (α, β, γ, ...) як для Бреґґової, так і для дифузної складової ПІДД. Встановлено, що достатньо точний опис ДЗ досягається з фіксованими параметрами і єдиного виду виразами тільки у визначених вузьких діяпазонах радіюсів деформації. Проте ці параметри виявляються вибірково залежними від кожного набору характеристик умов дифракції (довжини хвилі, товщини кристалів, індексів відбивання, геометрії дифракції та ін.). Показано, що евристично побудувати модель ДЗ ПІДД у кристалах з дефектами як діягностичний метод виявилося можливим тільки завдяки тому, що вдалося факторизувати вплив мікродефектів і параметра деформації окремо на когерентну і на дифузну складові ПІДД, але вберегти нефакторизованість їх впливу на сумарну інтенсивність ІДД.

В работе с помощью теории Чуховского–Петрашеня для деформационной зависимости (ДЗ) интегральной интенсивности динамической дифракции (ИИДД) в кристаллах без дефектов показан характер изменения ДЗ ИИДД с толщиной кристаллов и с вариацией других условий дифракции. На этой основе, а также при использовании ряда экспериментов с реальными дефектными кристаллами и результатов теории полной интегральной интенсивности динамической дифракции (ПИИДД) в кристаллах с дефектами без изгиба построена аналитическая модель ДЗ ПИИДД в кристаллах с дефектами, пригодная для диагностики параметров структурных дефектов в кристаллах. Полученные эвристически выражения для ДЗ ПИИДД в кристаллах с дефектами учитывают ДЗ поглощательных и отражательных способностей кристаллов, вклад которых определяется параметрами модели (α, β, γ, ...) как для брэгговской, так и для диффузной составляющих ПИИДД. Установлено, что достаточно точное описание ДЗ достигается с фиксированными параметрами и единого вида выражениями только в определённых узких диапазонах радиусов деформации. Однако эти параметры оказываются избирательно зависящими от каждого набора характеристик условий дифракции (длины волны, толщины кристаллов, индексов отражения, геометрии дифракции и др.). Показано, что эвристически построить модель ДЗ ПИИДД в кристаллах с дефектами как диагностический метод оказалось возможным только благодаря тому, что удалось факторизовать влияние микродефектов и параметра деформации отдельно на когерентную и на диффузную составляющие ПИИДД, но уберечь нефакторизованность их влияния на суммарную интенсивность ИИДД.

Key words: total integrated intensity of dynamical diffraction, microdefects, deformation dependences.

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1. INTRODUCTION

The widely used X-ray defect diagnostics, based on the theory of kinematic scattering, though having a limited sensitivity, still makes it possible to determine the degree of crystal structure imperfection. However, it is non-informative for diagnostics of several defect types, which are simultaneously present in crystals. Here, for the total integrated intensity R_i as well as its Bragg R_{iB} and diffuse R_{iD} components, the following expressions are used:

$$R_i = R_{iB} + R_{iD}, \quad R_{iB} = R_{iP}e^{-2L}, \quad R_{iD} = R_{iP}(1 - e^{-2L}),$$
$$R_{iP} = \frac{C^2 Qt}{\gamma_0}, \quad Q = \frac{(\pi|\chi_{Hr}|)^2}{\lambda \sin 2\theta}, \tag{1}$$
$$R_i = R_{iB} + R_{iD} = R_{iP}, \quad \frac{R_{iD}}{R_{iB}} = \frac{(1 - e^{-2L})}{e^{-2L}} \approx 2L,$$

where L is an index of power of Krivoglaz–Debye–Waller factor, λ is a wavelength, t is a crystal thickness, θ_B is a Bragg angle, χ_{Hr} is an **H**-th Fourier component of the real part of crystal susceptibility, γ_0 is a cosine of incidence angle.

In this case, the Krivoglaz–Debye–Waller factor e^{-L} is the only structurally sensitive parameter, so the information on the total structural imperfection of the sample can only be found relying on it. Besides, as one can see from formulae (1), in the kinematic theory, the structure information is factorized with diffraction conditions, therefore any changes of experimental parameters on which the dependence is the same for Bragg and diffuse R_i components do not affect the ratio of coherent and diffuse components.

This makes the total integrated intensity of kinematic diffraction as non-informative in terms of structure, and defects diagnostics is only feasible if one manages to separate experimentally R_{iB} and R_{iD} components.

Several defect types can only be determined if crystals are investigated under dynamical diffraction conditions.

For example, in the expressions (2) and (3) for total integrated intensity of dynamical diffraction (TIIDD) in crystals with defects, the parameters describing diffraction conditions are mixed with parameters that are responsible for structure of sample;
for 'thin' crystal ($\mu_0 l < 1$, $l = t/\gamma_0$),

$$R_i = \exp(-\mu_0 l)[B_0 e^{-L} I_0(h_s)\exp(-\mu_{ds} l) + 2LR_{ip}\exp(-\mu^* l)], \tag{2}$$

where $B_0 = \pi C|\chi_{Hr}|/(2\sin 2\theta)$;

for 'thick' crystal ($\mu_0 l > 5,\ l = t/\gamma_0$),

$$R_{\rm i} = \frac{\sqrt{2\pi}Ce^{-L}\left|\chi_{\rm Hr}\right|}{4\sin 2\theta}\exp\frac{[-(\mu_0 - \mu_h Ce^{-L})l]}{\sqrt{\mu_h lCe^{-L}}}\left[i_0(h_s) + \frac{\alpha\mu_{\rm ds}}{\mu_h \sin 2\theta}Ce^{-L}\right], \quad (3)$$

$$i_0\left(x\right) = 1 + \frac{1}{8x} + \frac{9}{128x^2} + \ldots, \quad \alpha = \frac{3}{2}\frac{\exp(-\mu_{\rm ds}l) - \exp(-\mu_h Ce^{-L})}{1 - \mu_{\rm ds}Ce^{-L}/\mu_h}.$$

As a result, the coherent and diffuse components have much stronger and different sensitivity to diffraction conditions [1], unlike those in the kinematic theory (1).

The sensitivity of TIIDD to the thickness, wavelength, angle of beam orientation in respect to the crystal surface, which is unique and different for various types of defects, permits us to construct a new generation of diagnostic methods.

The proposed method is not based on the change in the diffraction conditions but, rather, on the study of defect structure, which is carried out by introduction of controlled crystal macrodeformation.

The theory developed by Chukhovskii and Petrashen [2], which describes the effect of elastic deformation on the integrated intensity of dynamical diffraction, is applicable only in the case of a defect-free sample; its extension to samples with damaged structure implies very complicated mathematical instruments, which questions the possibility to use this theory in practical defect diagnostics.

The purpose of this work is to study the basic possibility to describe deformation dependences (DD) of TIIDD in real crystals; it can also give results in characterizing crystal defects.

2. THEORETICAL DESCRIPTION

The solution [3] of the Takagi equations in partial derivatives makes it possible to determine the integrated intensity of dynamical diffraction for the elastically bent ideal crystal:

$$R_{\rm i}(M_0, M_\beta, M, D, B) = \pi^{-1}[1 - \exp(-\pi\left|B\right|/2)]e^{-M_0} \times$$
$$\times\int_{-1}^{+1}\frac{d\xi\,{\rm ch}(M_\beta\xi){\rm ch}[(M/D - 2)\ln(\sqrt{1-(D')^2} + D')]}{\sqrt{1-\zeta^2}\sqrt{1-(D')^2}}, \quad (4)$$

where $\zeta = x/t$, $\beta = \gamma_0/\gamma_{\rm H}$, $D = BT$, $D' = D\sqrt{1+\xi^2}$, $M = 2t\left|\chi_{\rm Hi}/\chi_{\rm Hr}\right|$,

$$M_0 = \frac{\chi_{0\rm i}(1+\beta)t}{\sqrt{\left|\beta\right|}C\left|\chi_{\rm Hr}\right|}, M_\beta = \frac{1-\beta}{1+\beta}M_0, B = \frac{\lambda^2\sin\psi\left[1 + \gamma_0\gamma_1(1+\nu)\right]}{2\pi\left|\chi_{\rm Hr}\right|^2 rd}, T = \frac{\pi t\left|\chi_{\rm Hr}\right|}{\lambda\sqrt{\gamma_0\gamma_1}},$$

ψ is the angle between the reflecting plane and the normal to the crystal surface, $\gamma_0 = \cos(\theta_B + \psi)$, $\gamma_1 = \cos(\theta_B - \psi)$, ν is Poisson's ratio, μ_0 is the linear photoelectric absorption coefficient, r is the radius of the curvature of crystal cylindrical bend, $d = a/(h^2 + k^2 + l^2)^{1/2}$, a is lattice constant, h, k, l are the Miller indexes, χ_{0i} is the imaginary part of the Fourier component of crystal polarizability.

Figure 1 shows DD of IIDD of the ideal crystal normalized to IIDD of unbent ideal crystal (solid lines): $R_{ib}(BT)/R_0$, these were calculated with the formula from the Chukhovskii and Petrashen paper for various thicknesses of the silicon sample and different wavelengths of the X-ray radiation used.

For different thicknesses of the silicon sample, when 220 Laue reflections of FeK_α-radiation are used, the calculated values of IIDD of

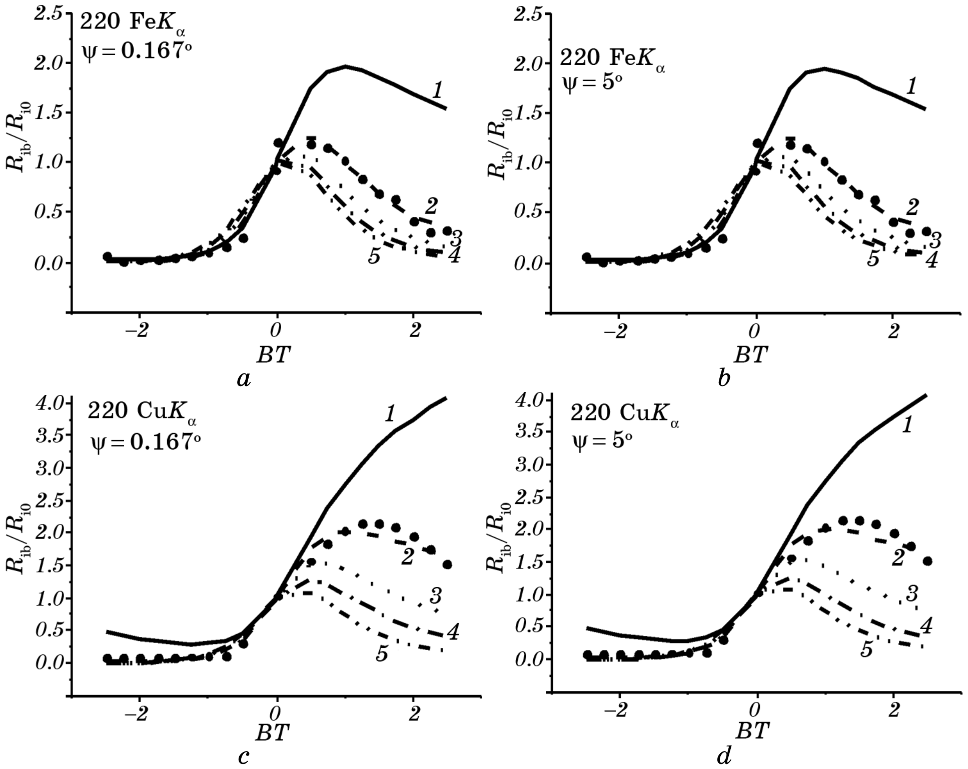
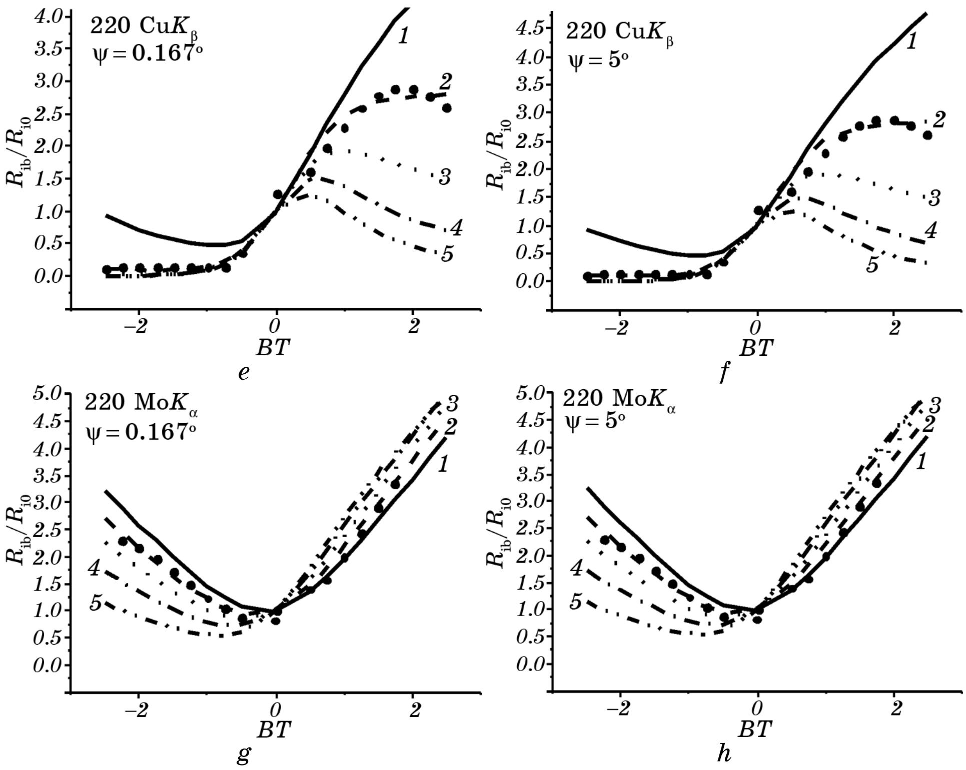


Fig. 1. DD of IIDD of elastically bent ideal crystal normalized to IIDD of unbent ideal crystal: $R_{ib}(BT)/R_0$ curves are calculated with the formula from the Chukhovskii and Petrashen paper for various thicknesses of the silicon sample (*1*—195 μm, *2*—390 μm, *3*—565 μm, *4*—800 μm, *5*—1110 μm) and 220 Laue reflections of radiation with various wavelengths. Markers represent the DD $R_{ib}(BT)/R_0$, which were experimentally obtained by Kislovskii in Ref. [3].



Continuation of Fig. 1.

unbent ideal crystal are: R_{i0}(195 μm) = 1.11·10^{-5}, R_{i0}(390 μm) = 2.98·10^{-6}, R_{i0}(565 μm) = 2.4·10^{-7}, R_{i0}(800 μm) = 2.64·10^{-9}, R_{i0}(1110 μm) = 2.33·10^{-12}.

For different thicknesses of the silicon sample, when 220 Laue reflections of CuK_α-radiation are used, the calculated values of IIDD of unbent ideal crystal are: R_{i0}(195 μm) = 7.76·10^{-6}, R_{i0}(390 μm) = 7.55·10^{-6}, R_{i0}(565 μm) = 5.525·10^{-6}, R_{i0}(800 μm) = 2.05·10^{-6}, R_{i0}(1110 μm) = 2.48·10^{-7}.

For different thicknesses of the silicon sample, when 220 Laue reflections of CuK_β-radiation are used, the calculated values of IIDD of unbent ideal crystal are: R_{i0}(195 μm) = 6.755·10^{-6}, R_{i0}(390 μm) = 6.895·10^{-6}, R_{i0}(565 μm) = 6.38·10^{-6}, R_{i0}(800 μm) = 4.395·10^{-6}, R_{i0}(1110 μm) = 1.58·10^{-6}.

For different thicknesses of the silicon sample, when 220 Laue reflections of MoK_α-radiation are used, the calculated values of IIDD of unbent ideal crystal are: R_{i0}(195 μm) = 1.53·10^{-6}, R_{i0}(390 μm) = 2.42·10^{-6}, R_{i0}(565 μm) = 2.91·10^{-6}, R_{i0}(800 μm) = 3.32·10^{-6}, R_{i0}(1110 μm) = 3.65·10^{-6}.

In Figure 1, one can see the best fit with experimental DD of IIDD calculated for thickness of sample t = 390 μm. It is also understandable from Fig. 1 that any change in the asymmetry degree of reflection does not affect the shape of DD IIDD in the given interval of the range change. Their shapes change significantly with crystal thickness change.

Therefore, to develop the universal model of DD of IIDD it is necessary to introduce multipliers describing DD of both reflective and absorptive power of the crystal. For the coherent component, they must be such as to describe correctly all DD of IIDD calculated relying on the theory [2]; these DD of IIDD are shown in Fig. 1.

So, the analytical type of the proposed model is described as follow:

$$R_{\rm ib}/R_{\rm i0} = (1+\alpha BT+\beta B^2T^2)\left(1+\alpha'\frac{M_0}{r}+\beta'\frac{M_0^2}{r^2}\right)\exp\left(-\gamma'\frac{M_0^2}{r^2}\right). \quad (5)$$

3. DETERMINING COEFFICIENTS OF THE MODEL OF DEFORMATION DEPENDENCES OF IIDD

The results of determining the model of the deformation dependences of IIDD are presented by formulas (6)–(10), (6.1)–(10.1) and (6.2)–(10.2) for each case illustrated by Figs. 2–6 and Tables 1 and 2.

Solid lines in Fig. 2 are calculated according to theory [2]; the dashed line was calculated for model (6), the goodness of fitting (GOF) to the solid line is 0.0145, the dotted line is the calculation for model (6), GOF = 0.0321; the dash-and-dot line is the calculation for model (6.1), GOF = 0.112; dash-and-dot-dot line is the calculation for model (6.2), GOF = 0.109:

$$R_{\rm ib}/R_{\rm i0} = (1+1.16BT+0.74B^2T^2)(1-7.37\cdot10^5 M_0/r + \\ +1.1\cdot10^{12}M_0^2/r^2)\exp(-2.15\cdot10^{12}M_0^2/r^2), \quad (6)$$

$$R_{\rm ib}/R_{\rm i0} = (1+1.16BT+0.74B^2T^2)(1+7.05\cdot10^5 M_0/r + \\ +3.02\cdot10^{12}M_0^2/r^2)\exp(-2.325\cdot10^{13}M_0^2/r^2), \quad (6.1)$$

$$R_{\rm ib}/R_{\rm i0} = (1+1.16BT+0.74B^2T^2)(1-2.18\cdot10^5 M_0/r + \\ +1.26\cdot10^{12}M_0^2/r^2)\exp(-1.085\cdot10^{13}M_0^2/r^2). \quad (6.2)$$

Solid lines in Fig. 3 are calculated according to theory [2]; the dashed line is the calculation for model (7), GOF = 0.0145, the dotted line is the calculation for model (7), GOF = 0.0872; the dash-and-dot line is the calculation for model (7.1), GOF = 0.116; dash-and-dot-dot line is the calculation for model (7.2), GOF = 0.068:

$$R_{\rm ib}/R_{\rm i0} = (1+0.2BT+0.78B^2T^2)(1+1.54\cdot10^6 M_0/r + \\ +9.035\cdot10^{11}M_0^2/r^2)\exp(-1.385\cdot10^{12}M_0^2/r^2), \quad (7)$$

$$R_{\rm ib}/R_{\rm i0} = (1+0.2BT+0.78B^2T^2)(1+4.21\cdot10^6 M_0/r + \quad (7.1)$$

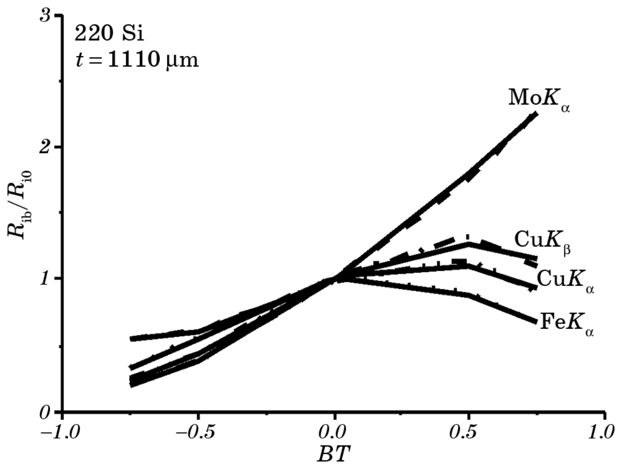


Fig. 2. DD of IIDD of elastically bent ideal crystal normalized to IIDD of unbent ideal crystal: $R_{ib}(BT)/R_0$.

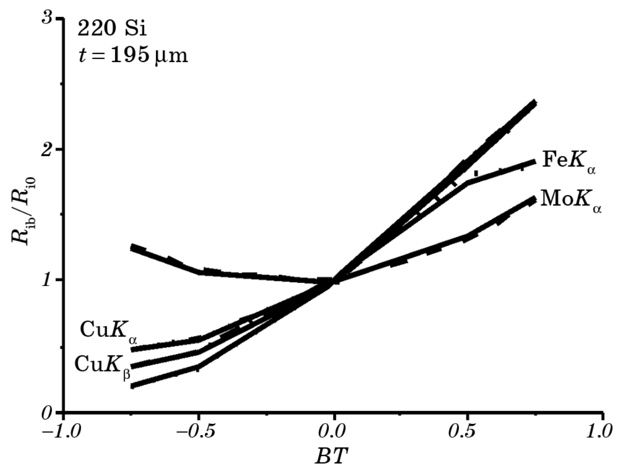


Fig. 3. DD of IIDD of elastically bent ideal crystal normalized to IIDD of unbent ideal crystal: $R_{ib}(BT)/R_0$.

$$+9.99\cdot 10^{12} M_0^2/r^2)\exp(-1.04\cdot 10^{13} M_0^2/r^2),$$

$$R_{ib}/R_{i0} = (1 + 0.2BT + 0.78B^2T^2)(1 + 3.306\cdot 10^6 M_0/r + +4.57\cdot 10^{12} M_0^2/r^2)\exp(-5.33\cdot 10^{12} M_0^2/r^2). \quad (7.2)$$

Solid lines in Fig. 4 are calculated according to theory [2]; the dashed line is the calculation for model (8), GOF = 0.0181, the dotted line is the calculation for model (8), GOF = 0.117; the dash-and-dot line is the calculation for model (8.1), GOF = 0.0362; dash-and-dot-dot line

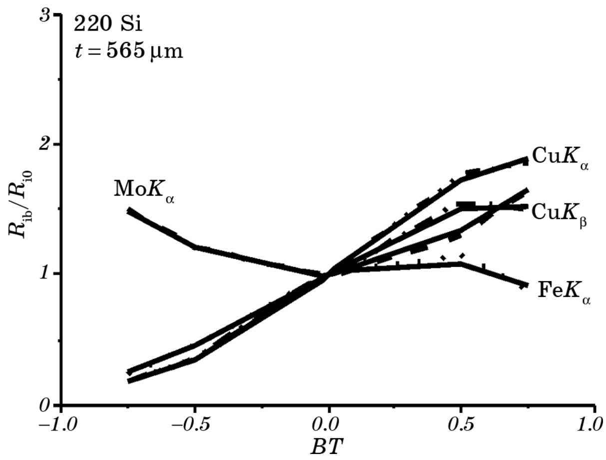


Fig. 4. DD of IIDD of elastically bent ideal crystal normalized to IIDD of unbent ideal crystal: $R_{ib}(BT)/R_0$.

is the calculation for model (8.2), GOF = 0.103:

$$R_{ib}/R_{i0} = (1 + 0.079BT + 1.025B^2T^2)(1 + 8.62 \cdot 10^6 M_0/r + +3.8 \cdot 10^{11} M_0^2/r^2)\exp(-2.038 \cdot 10^{12} M_0^2/r^2), \quad (8)$$

$$R_{ib}/R_{i0} = (1 + 0.079BT + 1.025B^2T^2)(1 + 5.78 \cdot 10^6 M_0/r + +1.08 \cdot 10^{13} M_0^2/r^2)\exp(-2.031 \cdot 10^{13} M_0^2/r^2), \quad (8.1)$$

$$R_{ib}/R_{i0} = (1 + 0.079BT + 1.025B^2T^2)(1 + 3.561 \cdot 10^6 M_0/r + +4.151 \cdot 10^{12} M_0^2/r^2)\exp(-1.092 \cdot 10^{13} M_0^2/r^2). \quad (8.2)$$

Solid lines in Fig. 5 are calculated according to theory [2]; the dashed line is the calculation for model (9), GOF = 0.007, the dotted line is the calculation for model (9), GOF = 0.062; the dash-and-dot line is the calculation for model (9.1), GOF = 0.02; dash-and-dot-dot line is the calculation for model (9.2), GOF = 0.09:

$$R_{ib}/R_{i0} = (1 + 0.489BT + 0.769B^2T^2)(1 + 7.61 \cdot 10^5 M_0/r + +1.435 \cdot 10^{11} M_0^2/r^2)\exp(-1.577 \cdot 10^{12} M_0^2/r^2), \quad (9)$$

$$R_{ib}/R_{i0} = (1 + 0.489BT + 0.769B^2T^2)(1 + 4.581 \cdot 10^6 M_0/r + +7.635 \cdot 10^{12} M_0^2/r^2)\exp(-1.418 \cdot 10^{13} M_0^2/r^2), \quad (9.1)$$

$$R_{ib}/R_{i0} = (1 + 0.489BT + 0.769B^2T^2)(1 + 3.02 \cdot 10^6 M_0/r + +2.85 \cdot 10^{12} M_0^2/r^2)\exp(-7.88 \cdot 10^{12} M_0^2/r^2). \quad (9.2)$$

Solid lines in Fig. 6 are calculated according to theory [2]; the

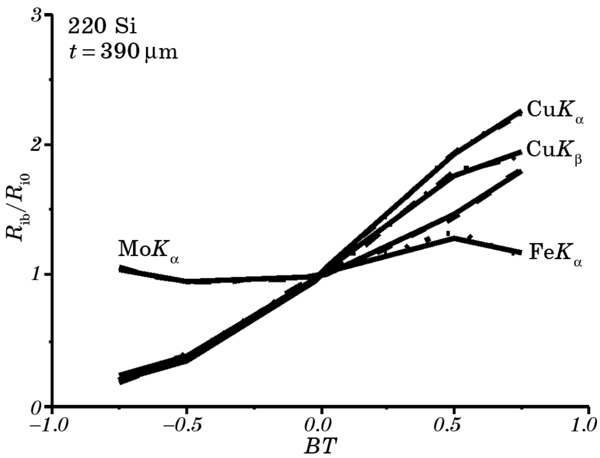


Рис. 5. DD of IIDD of elastically bent ideal crystal normalized to IIDD of unbent ideal crystal: $R_{ib}(BT)/R_0$.

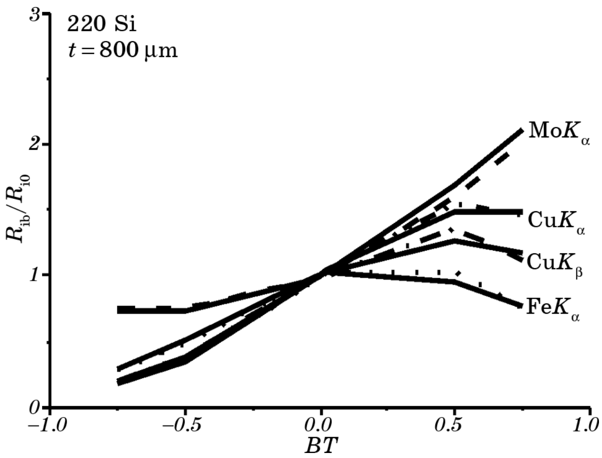


Fig. 6. DD of IIDD of elastically bent ideal crystal normalized to IIDD of unbent ideal crystal: $R_{ib}(BT)/R_0$.

dashed line was the calculation for model (10), GOF = 0.17, the dotted line is the calculation for model (10), GOF = 0.15; the dash-and-dot line is the calculation for model (10.1), GOF = 0.04; dash-and-dot-dot line - is the calculation for model (10.2), GOF = 0.16:

$$R_{ib}/R_{i0} = (1 + 0.848BT + 0.686B^2T^2)(1 + 1.7\cdot 10^2 M_0/r + \\ +1.82\cdot 10^{11} M_0^2/r^2)\exp(-1.76\cdot 10^{12} M_0^2/r^2), \tag{10}$$

$$R_{ib}/R_{i0} = (1 + 0.848BT + 0.686B^2T^2)(1 + 2.61\cdot 10^6 M_0/r + \tag{10.1}$$

TABLE 1. Deformation dependence coefficients for $BT \le 0.75$ interval for absorptive power.

t, μm	$\alpha'_{\mathrm{Cu}K_\beta}\times 10^{-5}$	$\beta'_{\mathrm{Cu}K_\beta}\times 10^{-12}$	$\gamma'_{\mathrm{Cu}K_\beta}\times 10^{-12}$	$\alpha'_{\mathrm{Cu}K_\alpha}\times 10^{-5}$	$\beta'_{\mathrm{Cu}K_\alpha}\times 10^{-12}$	$\gamma'_{\mathrm{Cu}K_\alpha}\times 10^{-12}$	$\alpha'_{\mathrm{Fe}K_\alpha}\times 10^{-5}$	$\beta'_{\mathrm{Fe}K_\alpha}\times 10^{-11}$	$\gamma'_{\mathrm{Fe}K_\alpha}\times 10^{-12}$
1110	7.05	3.02	−23.25	−2.18	1.26	−10.85	−7.37	11.0	−2.15
800	26.1	11.8	−19.1	14.0	2.206	−11.94	0.0017	1.82	−1.76
565	57.8	10.8	−20.31	35.61	4.151	−10.92	8.62	3.8	−2.038
390	45.81	7.635	−14.18	30.2	2.85	−7.88	7.61	14.35	−1.577
195	42.1	9.99	−10.4	33.06	4.57	−5.33	15.4	9.035	−1.385

TABLE 2. Deformation dependence coefficients for $BT \le 0.75$ interval for reflective power.

t, μm	α	β
1110	1.16	0.74
800	0.848	0.686
565	0.079	1.025
390	0.489	0.769
195	0.2	0.78

$$+1.18\cdot 10^{12} M_0^2/r^2)\exp(-1.91\cdot 10^{13} M_0^2/r^2),$$

$$R_{\mathrm{ib}}/R_{\mathrm{i0}} = (1+0.848BT+0.686B^2T^2)(1+1.4\cdot 10^6 M_0/r + +2.206\cdot 10^{12} M_0^2/r^2)\exp(-1.94\cdot 10^{13} M_0^2/r^2). \quad (10.2)$$

Figures 2–6 show that model parameters are different for various wavelengths and crystal thicknesses, *i.e.* to build the model that could be used as a method of defect diagnostics, diffraction conditions and BT interval must be constant.

Deformation-dependence coefficients for interval of $BT \le 0.75$ are shown in Tables 1 and 2.

4. DETERMINING COEFFICIENTS OF THE DEFORMATION DEPENDENCES OF TIIDD MODEL FOR VARIOUS DEGREES OF STRUCTURE IMPERFECTION

According to the Chukhovskii–Petrashen theory, the DD of IIDD shown in Fig. 7 have been calculated for Si single-crystal plate of thickness $t = 530$ μm for the interval $-0.781 \le BT \le 0.744$ for 220 Laue-reflection MoK_α- and FeK_α-radiation with $\psi = 1.5°$.

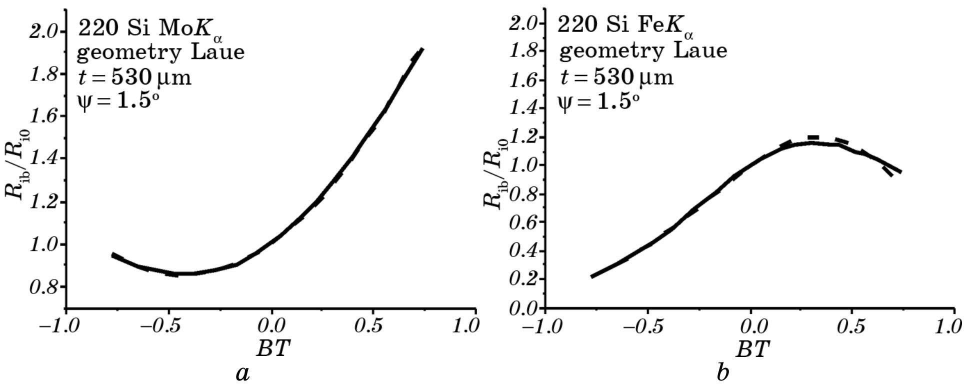


Fig. 7. DD of IIDD of elastically bent ideal crystal normalized to IIDD of unbent ideal crystal: $R_{ib}(BT)/R_0$.

The solid line in Fig. 7, *a* is calculated according to theory [2]; the dashed line is calculated for model (11), GOF = 0.000963; the solid line in Fig. 7, *b* is calculated according to theory [2]; the dashed line is calculated for model (11), GOF = 0.0147 and

$$R_{ib}/R_{i0} = (1 + 0.68BT + 0.8B^2T^2)(1 + 2.65\cdot 10^6 M_0/r + +4.71\cdot 10^{12} M_0^2/r^2)\exp(-9.31\cdot 10^{13} M_0^2/r^2). \quad (11)$$

Then, the factors of the model of DD of diffuse component of TIIDD have been determined for these diffraction conditions and the given interval of BT change by using a somewhat simplified model, with account being taken of its necessary accuracy (11), through fitting of the calculated DD of TIIDD (solid lines in Fig. 8) to the experimental ones (marker on Fig. 8).

The solid line DD of TIIDD in Fig. 8, *a* is calculated according to model (12); the dashed line DD of coherent component of TIIDD is calculated for model (12), the dotted line DD of diffuse component of TIIDD is calculated for model (12), GOF = 0.208:

$$R_{ib} = 3.39\cdot 10^{-7}(1 + 0.61BT + 0.64B^2T^2)(1 + 2.81\cdot 10^6 M_0/r)\times \times\exp(-8.22\cdot 10^{13} M_0^2/r^2) + 0.009\cdot 10^{-7}(1 + 0.49BT)\times \times(1 + 2.6\cdot 10^6 M_0/r)\exp(-6.2\cdot 10^{13} M_0^2/r^2). \quad (12)$$

The solid line DD of TIIDD in Fig. 8, *b* was calculated according to model (13); the dashed line DD of coherent component of TIIDD was calculated for model (13), the dotted line DD of diffuse component of TIIDD was calculated for model (13), GOF = 0.158:

$$R_{ib} = 2.6\cdot 10^{-8}(1 + 0.61BT + 0.64B^2T^2)(1 + 2.81\cdot 10^6 M_0/r)\times$$

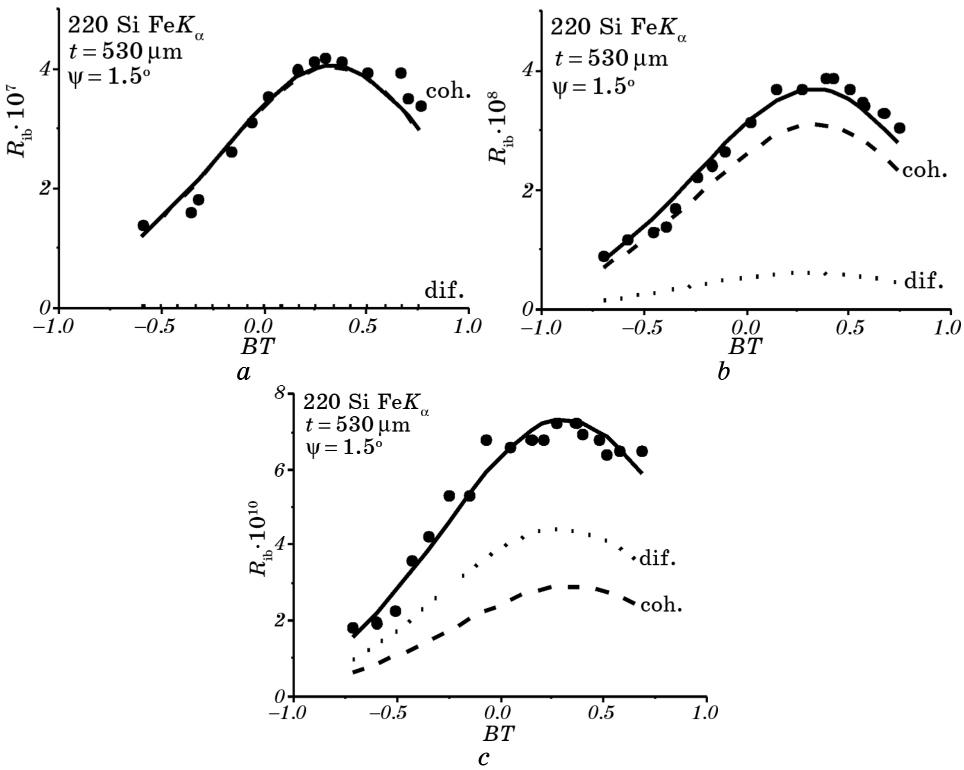


Fig. 8. Deformation dependences (DD) of TIIDD of elastically bent crystal with defects: $R_{ib}(BT)$.

$$\times\exp(-8.22 \cdot 10^{13} M_0^2/r^2) + 0.53 \cdot 10^{-8}(1 + 0.49BT)\times \\ \times(1 + 2.6 \cdot 10^6 M_0/r)\exp(-6.2 \cdot 10^{13} M_0^2/r^2). \quad (13)$$

The solid line DD of TIIDD in Fig. 8, *c* is calculated according to model (14); the dashed line DD of coherent component of TIIDD is calculated for model (14), the dotted line DD of diffuse component of TIIDD is calculated for model (14), GOF = 0.149:

$$R_{ib} = 2.44 \cdot 10^{-10}(1 + 0.61BT + 0.64B^2T^2)(1 + 2.81 \cdot 10^6 M_0/r)\times \\ \times\exp(-8.22 \cdot 10^{13} M_0^2/r^2) + 3.91 \cdot 10^{-10}(1 + 0.49BT)\times \\ \times(1 + 2.6 \cdot 10^6 M_0/r)\exp(-M_0^2/r^2 \cdot 6.2 \cdot 10^{13}). \quad (14)$$

5. CONCLUSION

A heuristic theoretical model of DD of TIIDD in single crystals with defects has been developed.

To determine the factors of the model, we use the Chukhovskii–Petrashen theory for IIDD for bent defect-free crystals and the results of the TIIDD theory in crystals with defects without bending as well as real samples with varying degrees of imperfections and with measured deformation TIIDD dependences.

The paper shows that by fixing the conditions of diffraction, samples that differ by defect structure only are described by the same model and the same factors for DD.

Thereby, it has been proved that the effects of both deformation and defects on the coherent and diffuse components are factorized separately in the model.

At the same time, a marked difference of this effect on R_{iB} and R_{iD} components permits one to use DD of their total value (TIIDD) for determining the structure of samples with various types of defects.

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