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X-RAY DIFFRACTION ON THE EDGE-DISLOCATION NEIGHBORHOOD: FINITE-DIFFERENTIAL APPROACH

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Results of a precise calculation of X-ray diffraction on distorted edge-dislocation neighborhood in crystals are represented. Calculation of lattice sums of diffraction has been carried out with adherence to the classical scheme. So unlike to the previous approach, finite-differential distances of atomic pairs of diffraction were immediately taken into account here. The statistical form of their representation was used. Obtained results are compared with previous those based on identification of X-ray profiles with statistical strain distribution. It was found that accuracy of the previous result is sufficient for analyses of the dislocation structure with moderate inhomogeneity.
KEYWORDS: dislocations, strain, X-ray diffraction, theory of scattering, calculation

РЕНТГЕНІВСЬКА ДИФРАКЦІЯ НА ОКОЛИЦЯХ КРАЙОВИХ ДИСЛОКАЦІЙ: КІНЦЕВО-РІЗНИЦЕВИЙ ПІДХІД

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Представлено результати прецизійного розрахунку дифракції від спотвореної околиці крайової дислокації. Розрахунок решіткових сум дифракції проведено, максимально дотримуючись класичної схеми. Тож, на відміну від попередніх розрахунків, у цьому разі безпосередньо враховувалися кінцево-різницеві дистанції атомних пар дифракції. Використано статистичну форму їх подання. Зроблено зіставлення результатів з попередніми розрахунками, що засновані на ототожненні профілів рентгенівської дифракції зі статистичним розподілом спотворень. Встановлено, що точності попереднього результату достатньо для аналізу дислокаційної структури з помірною неоднорідністю.
КЛЮЧОВІ СЛОВА: дислокації, спотворення кристалічної решітки, рентгенівська дифракція, теорія розсіювання, розрахунок

РЕНТГЕНОВСКАЯ ДИФРАКЦИЯ НА ОКРЕСТНОСТЯХ КРАЕВЫХ ДИСЛОКАЦИЙ: КОНЕЧНО-РАЗНОСТНЫЙ ПОДХОД

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Представлены результаты прецизионного расчёта дифракции от искажённой окрестности краевой дислокации. Расчёт решёточных сумм дифракции проведен, максимально следуя классической схеме. Так, в отличие от предыдущих расчётов, в данной работе непосредственно учитывались конечно-разностные дистанции атомных пар дифракции. Использовалась статистическая форма их представления. Проведено сопоставление результатов с предыдущими расчётами, основанными на отождествлении профилей рентгеновской дифракции со статистическим распределением искажений. Установлено, что точности предыдущего результата достаточно для анализа дислокационной структуры с умеренной неоднородностью.
КЛЮЧЕВЫЕ СЛОВА: дислокации, искажения, рентгеновская дифракция, теория рассеяния, расчёт

Recent methods of X-ray (XRD) studies of dislocation structure in polycrystalline materials are reduced onto determination of density of dislocations by data of strain (microstrain) parameters of structure. The formula of Wilkens for determining the root-main-square (rms-) strain in dislocations neighborhood [1] was accepted as that basis. Up to now this approach is used in almost all the works of this area [2-5].

Generally, the numerical values of dislocation density obtained in this way are higher than those done by transmission electron microscopy (TEM). Leaving aside accuracy of TEM, we can note reasons for possible inaccuracies of XRD techniques in such tasks.

So, the expedient of square averaging of microstrain is accepted from classical tasks of extraction their effect from X-ray diffraction on distorted polycrystalline. In this case, both the microstrain distribution in itself (e_i) and the corresponded X-ray diffraction are finally described by the Gaussian function: $P(e) = A\exp(-ke^2)$ [6, 7]. However this is typical likely for random nature of intergranular strain (i.e. elastic strain in grain scale) than for distortions, which regularly change in the dislocations neighborhood. This is confirmed by studies of dislocation structure in deformed Zircalloy-2 [8], done by both the traditional XRD methods [1-3] and TEM [9]. By means of these studies, it is found that the XRD determination of the dislocation density in the alloy gives an overestimate value owing to an intergranular

part of strain. On the other hand, view of diffraction profiles for own dislocation strain occurs closed to the Cauchy function: $P(e) = A/(1+ke^2)$. This has been found on an irradiated single crystal of Zr in the same studies.

It follows from this, that to determine the dislocation density by XRD, a technique is required with a more coherent approach and detailed constructing of the diffraction pattern. The first step in this way was taken in [3]. However, in this work, a used approach was still applicable only for the random distortions. Thus, the calculated diffraction profile in this case was a little differed from the Gaussian.

A more coherent approach was done in [10]. So a subject for calculation was a model of crystal lattice distortions in neighborhood of an edge dislocation. With using both elasticity and boundary conditions, an exact and unambiguous mathematical solution was found. An only limitation further relates to postulated similarity between the shape of the diffraction profile on microstrain $I^e(h)$ in crystal lattice, and a function $P(e)$ of its statistical distribution, that is at the identity $e \equiv h$, where h is the relative coordinate in the reciprocal lattice (see later). Existence of such approximate similarity is implied in research tasks of this direction [11]. In particular, it is done for the random strain because the Gaussian function describes both its distribution and diffraction.

Because of this similarity, that calculation [10] was reduced to determination the function of strain distribution $P(e)$. A result was obtained for its universal analogue $f(e/\varepsilon_o) = \varepsilon_o P(e)$:

$$f(q) = \frac{2}{\pi}\int_0^{\pi/2} \frac{\left(\sqrt{q^2+\cos^2\varphi} - |q|\right)^2}{\cos^2\varphi\sqrt{q^2+\cos^2\varphi}}\,d\varphi = -\frac{\sqrt{2}}{\pi}\int_0^{\pi} \frac{\cos\phi\,d\phi}{\sqrt{1+2q^2+\cos\phi}}. \tag{1}$$

Parameter ε_o was a certain combination of module of the Burgers vector and the radius of own neighborhood of edge dislocation: $\varepsilon_o = b/\pi R$. For tasks limited by plane explication ($b \in (x,y)$), as it has been shown, the function $f(q)$ and their intrinsic parameter ε_o not depend on the direction of Burgers vector.

That result occurs acceptable for a satisfactory simulation of the shape of X-ray lines. Moreover, it did a principle agreement with the Voigt-function technique widely used for line approximation [12, 13].

A question stays open about definition of dislocations density, how accurate it may be on this pattern. In other words, how highly data of XRD and TEM will be divided. In investigations of hafnium substructure such data showed a satisfactory accordance [14], but gave a significant discrepancy for SHF-quenched alloy Zr-2,5%Nb [15, 16]. Methodical inaccuracy – a possible reason for these differences – may significantly be associated with both a sharp spatial inhomogeneity of strain in the neighborhood of dislocations and a great nonlinearity of its own statistical distribution. Thus, formal identification of the distribution functions with those of diffraction can give inaccuracy. This would be significant in relation to the dislocation strain.

The aim of this work is to resolve the problem concerned with such reason of inaccuracy, i.e. to determine the degree of accuracy in the similarity between the shape of the XRD-line profile on dislocations strain and its statistical distribution. To do this, a task of using a more precise approach for calculation of diffraction has outlined. It is meant an approach more coherent to the classical basis [17-20]. So, it is supposed to calculate the diffraction function including, instead of strain distribution, the distribution of real distances between the displaced atoms of the lattice. In fact it is implied to replace the differential approach onto finite-differential one, and to do this for case of edge dislocation.

FORMULATION OF PROBLEM

Well known classical basis of calculations is formal summation of reflection amplitudes $A(\boldsymbol{S})$ and X-ray intensities $I(\boldsymbol{S})$ (with a diffraction vector $\boldsymbol{S}$) in area of a grain, carried out on coordinates of all atoms $\boldsymbol{r}_j$ with accounting their real displacements [17-20]:

$$A\left(\vec{S}\right) = \sum_j^N \exp\left(\vec{S}\cdot\vec{r}_j\right); \tag{2}$$

$$I\left(\vec{S}\right) = \frac{1}{2}\left|\sum_j^N \exp\left(\vec{S}\cdot\vec{r}_j\right)\right|^2 = \frac{N}{2} + \sum_{j\neq j'}^N \cos\left[\vec{S}\cdot\left(\vec{r}_j - \vec{r}_{j'}\right)\right]; \tag{3}$$

wherein j and j' are, generally speaking, two independent numbering of atoms on all their multitude N in the grain. However, according to the known postulates [11, 21], the sum (3) is practically reduced to accounting only j-j'-pairs oriented along the diffraction vector. In this case, the account is convenient to carry on other pair of indices: let j be the position of the centers of the atomic pairs (in $\{N\}$), and $2n$ be their integer range (> 0).

Just as in the previous calculations, we may use a system of dimensionless variables: $\Delta\boldsymbol{r}_{j,j'} \to 2n + (u_{j,n} - u_{j,-n})/d_o$ and $\boldsymbol{S} \to 2\pi(H + h)$, wherein $u_{j,\pm n}$ are displacements of atoms of the pair from the ideal positions, d_o is the spacing, H is the order of reflection, and h is the relative coordinate in the neighborhood of reflecting position in the reciprocal lattice. As a result, the formula (3) is transformed onto the following expression:

$$I(h)=\frac{N}{2}+\sum_{2n>0}\sum_{j}^{N}\cos\left\{2\pi\left[2n+\left(u_{j,n}-u_{j,-n}\right)/d_0\right](H+h)\right\}. \quad (4)$$

Mentioned limitation followed from linear approximation, whereby the previous calculations have been simplified. This is a linear representation of the distances between a pair of atoms in the formula (4): $u_{j,n} - u_{j,-n} = 2nd_0e_j$; $\Delta\boldsymbol{r}_{j,j'} \rightarrow 2n(1+e_j)$. Because e_j and h are small quantities, the argument of cosine (4) was reduced to expression $4\pi n(e_jH + h)$. If additionally to include, as it was done, the statistical distribution $P(e)$ of values e_j, formula (4) will be simplified:

$$I^e(h)=\frac{N}{2}+\sum_{2n>0}\int_{-\infty}^{\infty}P(e)\cos 4\pi n(eH+h)de. \quad (5)$$

Fourier inversion of it leads to the following expression:

$$\int_{-\infty}^{\infty}I^e(h)\cos 4\pi nh\cdot dh=\int_{-\infty}^{\infty}P(e)\cos 4\pi neH\cdot de. \quad (6)$$

As follows from the similarity of representation of the left and right side of (6), when $h \equiv eH$, identity occurs between the intensity function and the strain distribution. As mentioned, it was taken as a basis for the previous calculation [10].

The essence of the comments is that: to describe the diffraction on strain, use of the distribution $P(e)$ is virtually restricted by limits of small values of $2n$. It is acceptable for the functions with no high non-linearity, but real distribution $P(e)$ must be not that, especially at small e.

Thus, it is provided to reiterate the calculation with accounting real interatomic distances without any limitations, as much as it is possible. It is supposed for this to calculate numerous distributions of the interatomic distances (function $P_n(\varepsilon)$) with fixed values $2n$ for each one, performing calculations on own neighborhood of edge dislocation and presenting these functions through the value of strain (ε_n) averaged inside a pair of atoms: $\Delta\boldsymbol{r}_{j,j'} \rightarrow 2n(1+\varepsilon_n)$. It is adequate to some substitution into the formula (5):

$$I^e(h)=\sum_{2n}\int_{-\infty}^{\infty}P_n(\varepsilon_n)\cos\left[4\pi n(\varepsilon_nH+h)\right]d\varepsilon_n. \quad (7)$$

CALCULATION RESULTS

Formulas for calculation. Just as in the previous task, the calculations are based on mathematical description of field of elastic displacements $\boldsymbol{u}$ in the neighborhood of an edge dislocation, which Burgers vector is oriented along the coordinate y. The expression was obtained in polar and Cartesian coordinates - (r, φ) and (x,y) [10, 21]:

$$u_y=\frac{b}{2\pi}\left(\varphi-\frac{r^2}{2R^2}\sin 2\varphi\right)=\frac{b}{2\pi}\left(\arctan\frac{y}{x}-\frac{xy}{R^2}\right); \quad (8)$$

$$u_x=\frac{b}{2\pi}\left(-\ln r+\frac{r^2}{2R^2}\cos 2\varphi\right)=\frac{b}{4\pi}\left[-\ln\left(x^2+y^2\right)+\frac{x^2-y^2}{R^2}\right]. \quad (9)$$

The first terms in all the parentheses are components of the logarithm of complex variable $z = x + iy$, and represent own field of the dislocation [22]. The second terms are expressed by components of the quadratic function $z^2/2R^2$, and represent so-called "image forces". In general, the solution satisfies the condition of elastic equilibrium: $\partial u_x/\partial x + \partial u_y/\partial y = 0$; $\partial u_x/\partial y - \partial u_y/\partial x = 0$ [22, 23].

With including the image forces, the boundary conditions are achieved. They are specific for XRD: $\varepsilon(\boldsymbol{R}) = \varepsilon_{yy}(\boldsymbol{R}) = du_y(\boldsymbol{R})/dy = 0$. This is a result of exclusion of statistical deviations by achieving unambiguity of accounting the strain on the border of circular neighborhood of the dislocation (with radius R). In this finite-differential task, this moment could be significant.

Further parameters and coordinates are practically used in a dimensionless form: $d_0 = b = 1$; $R/d_0 \rightarrow R$; $(x/d_0, y/d_0) \rightarrow (x,y)$.

In the general scheme of further calculations two options have been included: $\boldsymbol{S}\parallel\boldsymbol{b}$ и $\boldsymbol{S}\perp\boldsymbol{b}$. Primarily an analytical expression is obtained for the average strain on base an equation $2n\varepsilon_n = u_{j,n} - u_{j,-n}$. It is done by the difference $u_y(x,y+n) - u_y(x,y-n)$ (8) for the first variation ($S \parallel b \parallel Y$), and by $u_x(x+n,y) - u_x(x-n,y)$ (9) for the second one ($\boldsymbol{S}\perp\boldsymbol{b} \parallel Y$), where (x,y) are the median coordinates of atomic pairs. To display the required distribution, the obtained formulas have been converted onto dependence of the x or y from ε_n. Explicitly, this was feasible for y. Thus, the following formula is obtained for the first variation:

$$y(\zeta_n) = \sqrt{2nx\cot\left[2n\left(\zeta_n + x/R^2\right)\right] - x^2 + n^2}\,, \tag{10}$$

wherein $\zeta_n = 2\pi\varepsilon_n/b$. Being obtained in this way, the formula for the second cause actually differs from the first one by substitution $n \to in$, whereby the cotangent (10) converts onto the hyperbolic form, and the result stays real.

Details of numerical calculations. Numerical calculation of the distribution function is the next step. First of all, values S_n are determined using the formula (10) as yardage of an area limited by fixed values ε_n within the neighborhood ($x^2 + y^2 \le R^2$). The distributions $P_n(\varepsilon_n)$ (7) is further calculated by differentiation:

$$P_n = -dS_n / S_0 d\varepsilon_n \qquad \left[S_n = \int_{-R}^{R} y(x, \varepsilon_n) dx \right]. \tag{11}$$

wherein $S_n(0) \approx \pi R^2$ in fact up to medium n. Differentiation of S_n is substituted onto differences at the interval $\pm \Delta q/2$. Similarly with the manner applied to output the formula (1) [10], the reduced and renormalized functions and coordinates were practically used: $i^{\varepsilon}(h/\varepsilon_o) = \varepsilon_o I^{\varepsilon}(h)$; $f_n(q) = \varepsilon_o P_n(\varepsilon)$, wherein $q = \varepsilon/\varepsilon_o$, $H = 1$. Analytical and empirical relationships were represented by rows with such increments: $\Delta q = 0{,}02$; $\Delta x/R = 0{,}002$; $\Delta 2n/R = 0{,}02$.

Further according to (7) and the followed transformations, the numerical calculation of the Fourier coefficients (F_n) for the functions $f_n(q)$ is carried out:

$$F_n = \Delta q \left\{ f_n(0) + 2\sum_{i=1}^{i_{\max}} f_n(q_i) \cos\left[2\pi q_i (2kn/R)\right] \right\}. \tag{12}$$

The calculation results are shown in Fig. 1 for the variation $\boldsymbol{S} \| \boldsymbol{b}$.

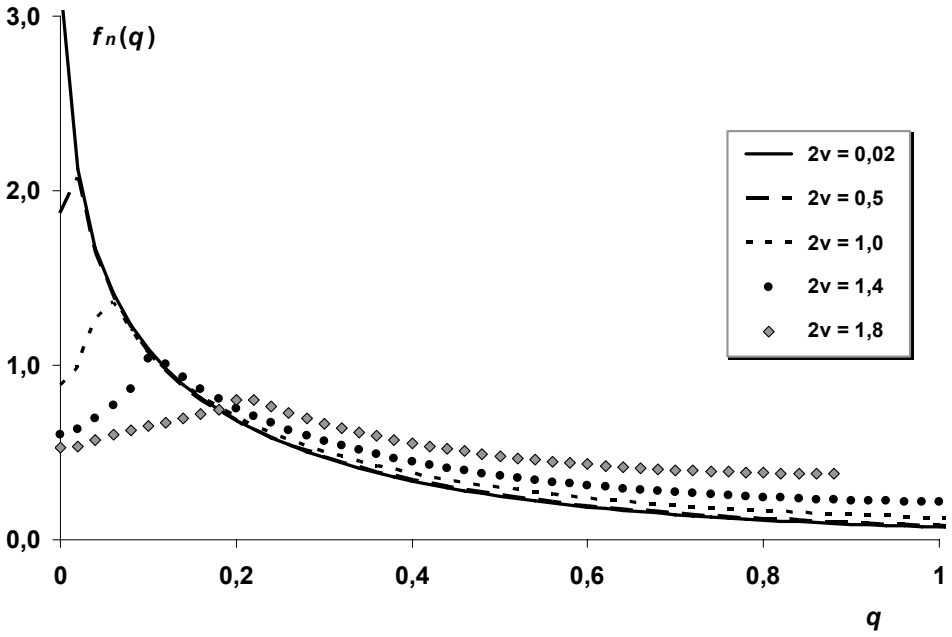

Fig. 1. View of the reduced distributions $f_n(q)$ of strain $\varepsilon = \varepsilon_o q$ calculated for the variation $\boldsymbol{S} \| \boldsymbol{b}$ with different values of $2v = 2kn/R$

Obtained coefficients are included in calculation of the profile $i^{\varepsilon}(h/\varepsilon_o)$:

$$i^{\varepsilon}(q) = \frac{2k}{R}\left\{ F_0 + 2\sum_{2n=1}^{R} F_n \cos\left[2\pi q (2kn/R)\right] \right\}. \tag{13}$$

The scaling factor k was chosen to maximize elimination of inaccuracies in the harmonic approximation – small oscillations and an effect of large-scale periodicity. In particular, by limiting $2n \le R$, the optimal solution was obtained as a function with the period $2q_{\max} = 4$:

$$i_p^{\varepsilon}(q)=\sum_m i^{\varepsilon}(q-2mq_{\max}). \tag{14}$$

Results of calculation of this intensity (14) are shown in Fig. 2 for the variations $\boldsymbol{S}\|\boldsymbol{b}$ и $\boldsymbol{S}\perp\boldsymbol{b}$. Because the function $f_{½}(q)$ ($2n = 1$) occurs identical for both them and moreover coincides with $f(q)$ (1) [10] within the error 0,001, a $f_p(q)$ function as its analogue has been calculated by the same manner (14) and is also shown. A decrement $\Delta i = i^{\varepsilon}_p - f_p$ is also done.

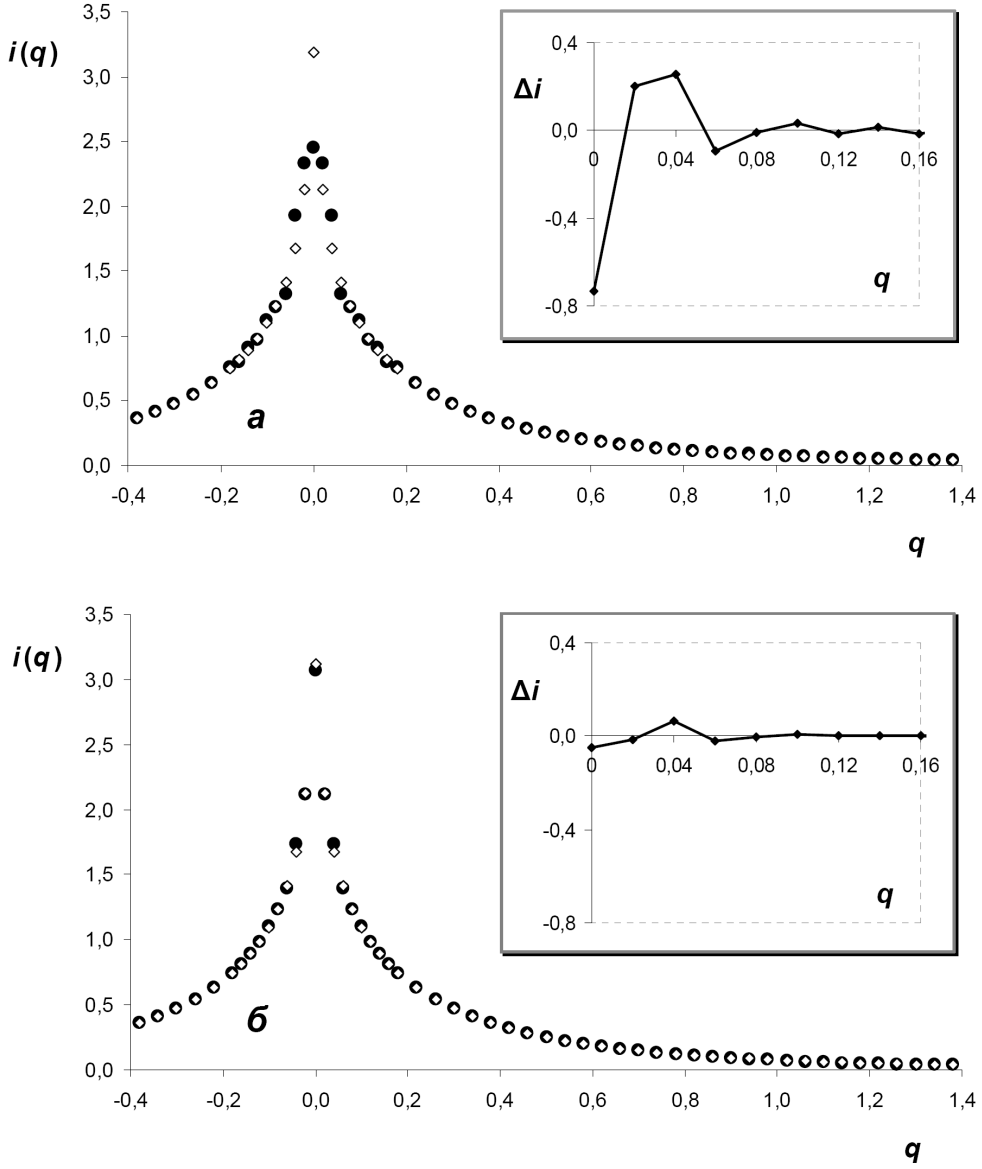

Fig. 2. Representation of the calculation results for the reduced intensity $i^{\varepsilon}(q)$ (●) and the function $f(q)$ (◊) with their inequality Δi for the cases $S\|b$ (*а*) and $\boldsymbol{S}\perp\boldsymbol{b}$ (*б*)

DISCUSSIONS

As follows from the data (Fig. 2), at $h/\varepsilon_o \equiv q > 0.08$ the reduced intensity $i^{\varepsilon}(h/\varepsilon_o)$ is almost identical to its prototype that is the function $f(q)$. This can be explained by similarity of the functions $f_n(q)$ with $f(q)$ (at such q) in a wide range of values $2n$ (Fig. 1).

Mismatches Δi with their decaying oscillation occur at small q (<0,08), and may be attributed to both the effects of discrete nature of numerical series at Fourier approximation and unavoidable deviations in compliance the calculation conditions. In particular, relatively increased level of the mismatch for option $S\|b$ as considered is due to irregularities of the trigonometric cotangent (10) and, due to this, was concerned with the forced inclusion of additional restrictions.

Being restricted by small values of strain, those discrepancies thus arise in the boundary (interdislocation) field of the environment. On the other hand, it is clear that the boundary condition accepted from previous calculations [10] and realized by input into formulas (8) and (9) additional terms do not remains adequate for this task at higher values of $2n$.

Obviously, irregular behavior of the functions $f_n(q)$ with small q (Fig. 1) may be explained by this. Thus, these two cases are interconnected.

By input of such conditions it was provided to eliminate the ambiguities in the same manner as the previous calculations were carried out. This is operation with unambiguous dependencies, and the own elastic fields of dislocations are those. Even the strain distributions near the dislocation core are statistical here only on the form of representation, but not in nature. So averaged distortions equaled to zero on limits is the immediate condition of such unambiguity. Whatever the numerical simulation of it and its accuracy, true result must also ensure the regularity at small q both the functions P_n and f_n, and the diffraction profile $i(q)$ what would built. Likeness between $i(q)$ и $f(q)$ must follow here from this in addition to large-scale similarity.

CONCLUSION

So, for a pattern of X-ray diffraction profile on the neighborhood of an edge dislocation, which is based on its mathematical similarity with a statistical strain distribution within this neighborhood, an accuracy test has been carried out by a modified calculation. To calculate the distributions, the point values of distortions were averaged in the intervals between the atoms pairs of diffraction.

When the calculation results were compared with the diffraction of its prototype [10], their practical coincidence on almost the entire region of strain is revealed. The numerical differences and damped oscillations are detected in the narrow area of low strain. Harmonic nature of the differences is associated with the result of the application of Fourier transformations, and their main reason is done with the inadequate expression of boundary conditions for this task.

From this it follows that the prototype of diffraction on a neighborhood of an edge dislocation, i.e. the statistical distribution of point values of strain in this neighborhood, has a satisfactory accuracy as the solution of the stated methodological task.

In particular, at the option of crystallographic isotropy, this also concern to definition the parameter of dislocation distortion (ε_o), precisely speaking – its components corresponding to the types and configurations of dislocations. It is worth mentioning [10] that these components form this parameter by a linear combination – with coefficients that comprise angles β of deviation the main directions of dislocation lines from the diffraction vector. For edge dislocations such coefficient is $\sin^2\beta$, for screw ones – $\sin\beta\cos\beta$. The dislocation density of each component (j) can be estimated using the formula $\rho_j = \pi\varepsilon_{oj}^2 / b_j^2$ [10].

Crystallographic anisotropy of materials can only affect the internal parameters (ε_{oj}) of the distribution $f(q)$. If the edge dislocations directs along any axis of the crystallographic basis, such anisotropy will most appear in a direction perpendicular to the Burgers vector. At this, for their density calculated from the real parameters using the original formulas, the relative change will determined by dividing it per the ratio of the elastic modules $(c_{22}+c_{12})/(c_{11}+c_{12})$, where the indices $(_{11})$ correspond to this direction. For the metals of the titanium subgroup (except for beryllium) the changes do not exceed 10%.

As general considerations, nonuniformity of distribution of dislocations may be the main reason of practical inaccuracy at calculation of their density by both the techniques [10]. This has logical connected with a fact that the moderate level of such nonuniformity in deformed hafnium [14] is a reason of achieving accordance between obtained XRD and TEM data on it. Sharp irregularity of the distribution of strain ($f(q)$) at low q can give significant inaccuracy concerned with higher level of it. At such cases, most adequate results can be obtained from analysis of tails of the diffraction.

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