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ACCOUNTING OF THE ELASTICITY MODULES ANISOTROPY IN HSP METALS FOR X-RAY INVESTIGATIONS OF DISLOCATION STRUCTURE

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A calculation of X-ray diffraction on the dislocation structure of polycrystalline materials with the biaxial anisotropy of the crystal lattice has been carried out. The task was reduced to definition of the field of lattice distortion in this neighborhood applied to edge dislocations of the «c» type in condition of anisotropy of elastic modules of a crystal. As a result of general solution of this task, a parameter of spatial anisotropy of the distortion field was defined from elastic modules and further included into tensors of transformation of both initial isotropic model of this field and its coordinates. According to this principle a modified mathematical model of the field of elastic atomic displacements in the neighborhood of an edge dislocation has been built. The final result shows that this anisotropy entirely reflects onto dislocation specific parameters of distortion that can be obtained by an XRD method for determination dislocation distributions and density. It is noted that for hcp metals widely used, accounting of this anisotropy would be reduced to small corrections of parameters.
KEYWORDS: X-ray analysis, diffraction, distortion, dislocations, dislocations density, elastic modules, anisotropy, hcp metals

УРАХУВАННЯ АНІЗОТРОПІЇ ЕЛАСТИЧНИХ МОДУЛІВ У ГЩУ-МЕТАЛАХ ПРИ РЕНТГЕНІВСЬКІМ ДОСЛІДЖЕННІ ДИСЛОКАЦІЙНОЇ СТРУКТУРИ

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Проведено розрахунок рентгенівської дифракції на дислокаційній структурі полікристалічних матеріалів в умовах двоосної анізотропії кристалічної решітки. Задачу зведено до визначення статистичного розподілу деформацій пружно-анізотропної кристалічної решітки в околиці крайових дислокацій типу «с». За модулями пружності шляхом пошуку загального рішення такої задачі визначено параметр просторової анізотропії поля деформацій, який далі введено до складу тензорів перетворення початкової ізотропної моделі цього поля і його координат. За таким принципом побудовано модифіковану математичну модель поля атомних зсувів кристалічної решітки в околиці крайової дислокації. Остаточний результат виражається в тому, що така анізотропія цілком і повністю відображається на характерних параметрах дислокаційних мікродеформацій, що можуть визначатися рентгенівським методом та служити для розрахунку розподілу дислокацій і їх щільності. Відзначається, що для ГЩУ-металів, широко використовуваних в техніці, урахування такої анізотропії зводиться до невеликих корекцій дислокаційних параметрів.
КЛЮЧОВІ СЛОВА: рентгеноструктурний аналіз, дифракція, мікродеформації, дислокації, щільність дислокацій, модулі пружності, анізотропія, ГЩУ-метали

УЧЁТ АНИЗОТРОПИИ МОДУЛЕЙ УПРУГОСТИ ГПУ-МЕТАЛЛОВ ПРИ РЕНТГЕНОВСКОМ ИССЛЕДОВАНИИ ДИСЛОКАЦИОННОЙ СТРУКТУРЫ

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Проведен расчёт рентгеновской дифракции на дислокационной структуре поликристаллического материала в условиях двуосной анизотропии кристаллической решётки. Задача сведена к определению статистического распределения искажений упруго-анизотропной кристаллической решётки в окрестности краевых дислокаций типа «*c*». По модулям упругости путём поиска общего решения такой задачи определён параметр пространственной анизотропии поля искажений, введенный далее в состав тензоров преобразования исходной изотропной модели этого поля и его координат. По такому принципу построена модифицированная математическая модель поля атомных смещений кристаллической решётки в окрестности краевой дислокации. Окончательный результат выражается в том, что такая анизотропия целиком и полностью отображается на характерных параметрах дислокационных искажений, определяемых рентгеновским методом, по которым рассчитывается распределение дислокаций и их плотность. Отмечается, что для ГПУ-металлов, широко используемых в технике, учёт такой анизотропии сводится к небольшим поправкам к дислокационным параметрам.
КЛЮЧЕВЫЕ СЛОВА: рентгеноструктурный анализ, дифракция, искажения кристаллической решётки, дислокации, плотность дислокаций, модули упругости, анизотропия, ГПУ-металлы

In previous studies [1-3], a complex of techniques of analysis of the dislocation structure in hcp metals was described. These developments are directed onto solving of problems of X-ray substructural studies of metals used in nuclear reactors: zirconium, titanium and hafnium. A distinctive feature of the methodical basis is to use the most direct approach for calculating the X-ray diffraction on distorted neighborhood of dislocations, especially in relation to the edge dislocations. It is, first of all, the use of physical and mathematical model of elastic-equilibrium displacement

fields of atoms and, on the basis of it, calculation of the distribution of the normal distortion (ε) of crystal lattice within the neighborhood – it is an universal function $f(q)$:

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

wherein $q = \varepsilon/\varepsilon_o$, and $\varepsilon_o = b/\pi R$ is a dislocation parameter of distortion ε; b is the Burgers vector of the edge dislocation; R is the radius of its individual neighborhoods in the vicinity of those with the same type and configuration. At the same time it has been show that, with sufficient accuracy, this distribution directly describes the corresponding intensity of X-ray difraction $i(h)$ under the identification ε with coordinates h what is the relative deviation of the diffraction vector from a site the reciprocal lattice [2].

One of the practical features of the development results associated with the versatility of function $f(q)$ for dislocations of all types and orientations – the differences are reduced onto change of expressions for the distortion parameters: $\varepsilon_o = kb/\pi R$. So, factor k is equal to $\sin^2\beta$ for edge dislocations and $\sin\beta\cdot\cos\beta$ for screw ones, where β is the angle between the main direction of the dislocation line and the diffraction vector (S). This makes it possible to divide the types of dislocations – "a" and "c" ("$c+a$") – in structure of hcp metals during the analysis of a wide number of experimental lines. In this case, the experimental parameter ε_o is divided into components ε_{oa} and ε_{oc} according both to the types of edge dislocations and to 3-time dimension of the object. As a result, the following orientation relationship used [4]:

$$\varepsilon_0(\alpha)=\varepsilon_{0a}\sin^2\alpha+\varepsilon_{0c1}+\varepsilon_{0c2}\cos^2\alpha, \tag{2}$$

wherein α is the angle between the direction of X-ray diffraction and the crystallographic direction [0002]; ε_{oa} is the distortion parameter for the "a"-dislocations of prismatic slip; $\varepsilon_{oc1,2}$ are those for two orthogonal directions of "a"-dislocations along the basal plane.

If the sample is a plate and X-ray measurements undertaken only from its surface, it remains to consider these two parameters are equal. As a result, the density of dislocations (of edge type) defined as a combination of its three partial components ρ_j calculated by three according parameters in formula (2): $\rho_j = \pi\varepsilon_{oj}^2/b_j^2$ [3]. Determination ε_o parameter associated with another practical feature of the method.

This feature is satisfactory accuracy of X-ray profile models simulated by convolution of distribution $f(q)$ with the Gaussian function, where the latter of which shows the effect of random strain in dimension of grains (intergranular strain). Speaking more specifically, by such convolution, as shown, it can be quite accurately modeled the Voigt function, which widely used for approximation of X-ray lines during phase-structural studies. As a result, the parameter ε_o (2) can be determined per the half-width (w_C) of a Voigt function component, which approximate diffraction on distortion by form of the Cauchy function $C(h)$: $\varepsilon_o \approx 1.7w_C$ [1, 3].

The problem is that all methodical calculations actually received only in approach of isotropic elasticity. In particular, it was shown that under these conditions the parameter ε_o for a fixed edge dislocation direction is not depend on orientations of the Burgers vector. It remains unclear how the anisotropy of parameters of crystalline medium elasticity, what is typical for hcp metals and alloys, affects the calculation result. The purpose of this work is to determine the nature and extent of effect of such anisotropy on the function and parameters of distribution of dislocation distortion. It is supposed for this to repeat the entire sequence of calculations including this factor.

FORMULATION OF THE TASK

To dislocations, oriented in the direction of the axis "c" of hcp crystal (they can be either edge or screw ones), this problem does not concern since they accept the maximum symmetry inherent to hcp crystal lattice. Effect of the anisotropy will thus reduce to dislocations lying in the basal plane. In this case, we consider the edge "c"-component dislocations, in particular "c"-type edge dislocation entirely. It differs from "a"-type ones of prismatic slipping by presence of biaxial anisotropy in orthogonal cross section, i.e. in a prismatic plane of hcp lattice.

In the isotropic-continuum approach of determining of displacement field $\boldsymbol{u}(\boldsymbol{r})$ of atoms, conditions of elastic equilibrium are reduced to equations $div\boldsymbol{u} = |rot\boldsymbol{u}| = 0$. This provide for elastic deformations $\varepsilon_{ij} = \partial u_i/\partial x_j$ the following expressions: $\varepsilon_{ij} = \varepsilon_{ji}$; $\Sigma\varepsilon_{ii} = 0$. In the case of anisotropic elastic parameters one should replace the displacements $\boldsymbol{u}(\boldsymbol{r})$ onto stresses $\boldsymbol{\sigma}(\boldsymbol{r})$: $div\boldsymbol{\sigma} = |rot\boldsymbol{\sigma}| = 0$ [5]. As a result, it is reduced to the expressions – $\sigma_{ij} = \sigma_{ji}$; $\Sigma\sigma_{ii} = 0$, where $i, j = 1; 3$ - designation, respectively, the coordinates x and y where first one varies along the basal plane of the crystal lattice, and the second one does along the "c"-axis.

These conditions are specifically expressed in the following form:

$$\sum\sigma_{ii}=\sigma_{11}+\sigma_{33}=\left(C_{11}\varepsilon_{11}+C_{13}\varepsilon_{33}\right)+\left(C_{33}\varepsilon_{33}+C_{31}\varepsilon_{11}\right)=\left(C_{11}+C_{13}\right)\varepsilon_{11}+\left(C_{13}+C_{33}\right)\varepsilon_{33}=0, \tag{3}$$

$$\sigma_{ij}-\sigma_{ji}=0\ \rightarrow\ C_{44}\left(\varepsilon_{13}-\varepsilon_{31}\right)=0 \tag{4}$$

wherein C_{ij} are the elastic modules with indices corresponding to the accepted notation; C_{44} is the shear modulus.

Thus, it may be noted that in the constancy of mathematical presentation of the conditions of equilibrium, the elastic parameters anisotropy changes their object in limits of linear transformations. As in the original task, let the Burgers vector ***b*** is directed along the "*c*"-axis of crystal cell, i.e. along the *y* (see figure). Then in general, principles of transformation will be reduced to the following:

– according to the equations (4), the condition for shear strain retains the same as for the case of isotropy – $\varepsilon_{31} = \varepsilon_{13}$;
– because of the immutability of the Burgers vector, changing along its direction (*y* or "*c*"-axis) by the anisotropy effect would formally be absent;
– thus, the transformations will only be along the direction *x*, and the corresponding rate would be defined by the ratio between ε_{ii} in the equation (3).

As a result, the recuired field of elastic displacements of atoms – $\boldsymbol{u}(\boldsymbol{r}) = u_x\boldsymbol{i} + u_y\boldsymbol{j}$ ($\boldsymbol{r} = x\boldsymbol{i} + y\boldsymbol{j}$) – can be defined from the solution that obtained in terms of isotropy – $\boldsymbol{u}_0(\boldsymbol{r}_0)$, – by the following transformations:

$$\vec{u}(\vec{r}) = u_x(x,y)\vec{i} + u_y(x,y)\vec{j} = ku_{0x}(\vec{r}_0)\vec{i} + u_{0y}(\vec{r}_0)\vec{j}; \quad \vec{r}_0 = x_0\vec{i} + y_0\vec{j} = kx\vec{i} + y\vec{j}, \tag{5}$$

where the anisotropy appears at $k \neq 1$.

In this way it is supposed to build a model of the field of atoms displacements in neighborhood of an edge dislocation (of type "*c*") under the elastic anisotropy options. Details of implementation of these options after the transformations (5) will be seen below.

CALCULATION RESULTS AND THEIR ANALYSIS

According to previous calculations [1, 2], the field of atomic displacements $\boldsymbol{u}_0(\boldsymbol{r}_0) = u_{0x}\boldsymbol{i} + u_{0y}\boldsymbol{j}$ in neighborhood of an edge dislocation was defined through assignment, in the initially adopted coordinates (x_0, y_0), a function of complex variable $W(z) = (b/2\pi)[\ln z - z^2/2R_0]$ expressed in this case as follows: $W = -u_{0x} + u_{0y}i$ ($z = x_0 + y_0 i$). Here R_0 is the radius of boundary of the observed neighborhood ($x_0^2 + y_0^2 \le R_0^2$), on which the normal distortion along the survey direction is taken as zero, as dictated by the general principle of constructing the model. Accounting the feature of linear transformations, as assigned by the expressions (5), it is possible to represent the formula for the displacements of atoms in this neighborhood in the following form:

$$u_y = u_{0y} = \frac{b}{2\pi}\left(\arctan\frac{y}{kx} - \frac{kxy}{R_0^2}\right); \qquad u_x = ku_{0x} = -\frac{bk}{4\pi}\left[\ln\left(k^2x^2 + y^2\right) - \frac{k^2x^2 - y^2}{R_0^2}\right]. \tag{6}$$

Along the semiaxis $x > 0$ as a result of these transformations, a slit with width *b* is retained, that related to the 2π-periodicity of the arctangent. According to the formulas (6), a distortion tensor in the plane (x, y) is taken the following form:

$$\varepsilon_{ij} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{yx} & \varepsilon_{yy} \end{pmatrix} = \frac{bk}{2\pi}\left[\frac{1}{k^2x^2 + y^2}\begin{pmatrix} -k^2x & -y \\ -y & x \end{pmatrix} + \frac{1}{R_0^2}\begin{pmatrix} k^2x & -y \\ -y & -x \end{pmatrix}\right]. \tag{7}$$

According to the equation (3), the factor *k* may be determined from the ratio of the diagonal elements of the matrix (7):

$$k = \sqrt{\frac{C_{13} + C_{33}}{C_{11} + C_{13}}}. \tag{8}$$

The following figure shows schematically the distortion of the crystal lattice in the neighborhood of an edge dislocation in the isotropy conditions ($k = 1$) and with the anisotropy coefficient $k = 2$.

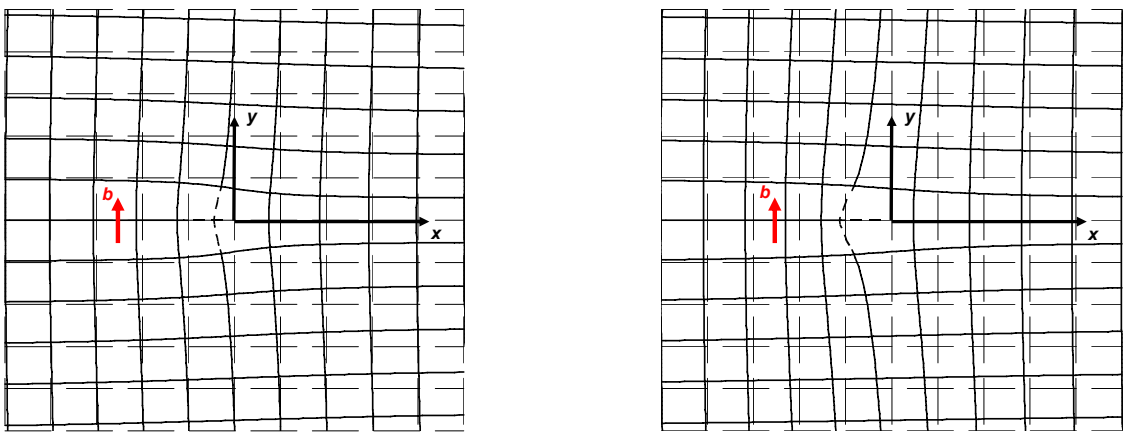

Fig. Illustration of distorted neighborhood of an edge dislocation at both isotropic elastic parameters (left part) and anisotropic those with a factor of $k = 2$ (right part; *b* – Burgers vector).

It makes sense to introduce a dimensionless quantities system: $s = y/R_0$; $t = kx/R_0$; $q = \varepsilon/\varepsilon_{00}$ ($\varepsilon_{00} = b/\pi R_0$). Then for $\varepsilon = \varepsilon_{il}$ the formula (7) will acquire the following view:

$$q_y = \frac{\varepsilon_{yy}}{\varepsilon_{00}} = \frac{t}{2}\left[\frac{1}{t^2+s^2} - 1\right]; \qquad q_x = \frac{\varepsilon_{xx}}{\varepsilon_{00}} = \frac{k^2 t}{2}\left[\frac{1}{t^2+s^2} - 1\right]. \tag{9}$$

Let us leave out the repetition of the process of calculating the distribution of $f(q)$, referring to the previous results and limiting by formulas (9). It should be noted that in the first formula, the anisotropy coefficient k is really absent. In other words, this formula also relates to a case of isotropy, and the dislocation distortion parameter in this direction, i.e. along the Burgers vector, remains without changes: $\varepsilon_0 = \varepsilon_{00} = b/\pi R$ (where the R is the real radius of the neighborhood border), seeing in this case it would be $R = R_y = R_0$.

If direction of the x-axis is oriented along survey, the dislocation parameter ε_0 is dependent on k. Thus, according to the second equation (9), $\varepsilon_0 = \varepsilon_{00}k^2 = bk/\pi R$, taking account in this case $R = R_x = R_0/k$.

If at last to return to the formula (2), where $\varepsilon_0(\alpha)$ is the dependency has modeled on the basis of experimental data, the value ε_{oc1}, that corresponding to "c"-dislocation lying in the plane of diffraction, may be thus determined with adjusting of following view:

$$\varepsilon_{0c1} = \left(b_c/\pi R_c\right)\left(k\sin^2\alpha + \cos^2\alpha\right), \tag{10}$$

In the adopted orientation of coordinates, for the second orthogonal component "c"-dislocation, x-axis lies in the plane of diffraction. Consequently ε_{xx} distortion do not appear, and thus $\varepsilon_{oc2} = b_c/\pi R_c$.

Table

Elastic modules (GPa) [6] and the anisotropy coefficients k (8) for several HCP metals

Element	C_{11}	C_{13}	C_{33}	k
Be	292.3	14.0	336.4	1.070
Mg	63.5	21.7	66.5	1.017
Ti	162.4	69.0	180.7	1.039
Zr	143.4	65.3	164.8	1.050
Hf	181.1	66.1	196.9	1.032

The Table presents data on the elastic modules of some metals with hcp lattice, and the anisotropy coefficients k calculated by the formula (8). According to these and to formula (10), accounting of the elastic modules anisotropy in this task is reduced to introduction of small adjustments to the formula (2). For the real level of accuracy, these corrections may be considered negligible, especially if to account a real variety of orientations of the grains in materials.

CONCLUSION

In general terms, a principle of accounting the anisotropy of the elastic moduli in calculation the two-dimensional elastic-equilibrium field of atomic displacements in distorted microregions of crystals with hcp lattice has been defined. This principle is reduced to definition of certain anisotropy parameter, which leads to the "biaxial" linear transformation of the displacement field and its coordinates starting from the options of isotropy.

Modified recalculation of the field of elastic atomic displacements and distribution parameters of crystal lattice distortion in neighborhood of an edge dislocation has been carried out using the defined anisotropy parameter.

This anisotropy parameter has been determined for several hcp metals used in nuclear technology. The calculation result shows that accounting the anisotropy in determination both the dislocation distortion parameters of the crystal lattice and dislocation densities is reduced to small corrections, and in many cases such tasks may be confined by the option of isotropy.

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