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Non-planar dislocation cores

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THE models of dislocations in crystals are reviewed from the point of view of continuum models of a discrete lattice. Special attention is paid to the Peierls-Nabarro model, which takes into account the discrete crystal structure along one slip plane. The Peierls-Nabarro model is then generalized to describe a screw dislocation with its core extended along three slip planes. As an example, the structure of the core of a 1/2 [111] screw dislocation in α-Fe extended along three {110} planes is studied. The possibility application of the proposed model in the study of sessile-glissile transformations of screw dislocations in b.c.c. metals under an external stress is finally discussed.

Modele dyslokacji w kryształach są rozważane z punktu widzenia kontynualnych modeli sieci dyskretnej ze zwróceniem szczególnej uwagi na model Peierlsa-Nabarro, który uwzględnia dyskretną strukturę kryształu wzdłuż płaszczyzny poślizgu. Model Peierlsa-Nabarro został następnie uogólniony do opisu dyslokacji śrubowej z jej jądrem rozciągniętym wzdłuż trzech płaszczyzn poślizgu. Jako przykład zbadano strukturę jądra dla dyslokacji śrubowej 1/2 [111] w α-Fe rozciągniętej wzdłuż trzech płaszczyzn {110}. W zakończeniu przedyskutowano możliwość zastosowania zaproponowanego modelu do badania transformacji typu "sessile-glissile" śrubowych dyslokacji w metalach o strukturze krystalicznej b.c.c. pod działaniem naprężeń zewnętrznych.

Модели дислокаций в кристаллах рассматриваются с точки зрения континуальных моделей дискретной решетки, с обращением особенного внимания на модель Пейерлса-Набарро, которая учитывает дискретную структуру кристалла вдоль плоскости скольжения. Модель Пейерлса-Набарро затем обобщена на описание винтовой дислокации с ее ядром растянутым вдоль трех плоскостей скольжения. Как пример исследована структура ядра для винтовой дислокаций 1/2 [111] в α-Fe растянутой вдоль трех плоскостей {110}. В заключению обсуждена возможность применения предложений модели для исследования преобразования типа „sessile-glissile'' винтовых дислокаций в металлах с кристаллической структурой под действием внешних напряжений.

1. Introduction

PLASTIC deformation of body centered cubic (b.c.c.) metals at low temperatures ($T < 0.2T_m$ where T_m is the melting temperature in K) is now generally believed to proceed from special properties of screw dislocation cores (for a review see [1, 2, 3]). The Burgers vector of active dislocations is $\mathbf{b} = 1/2 \langle 111 \rangle$ and thus the screw dislocations lie along the $\langle 111 \rangle$ directions, which are the axes of the three-fold symmetry of the lattice. Therefore, a screw dislocation core in its lowest energy state assumes a three-fold symmetry configuration so that the screw dislocation is sessile. It can move only if the core has been transformed by external stress (usually with help of thermal activation) into a planar glissile configuration. To conclude, the screw dislocations are, at a low temperature, much less mobile than the edge or mixed dislocations which have planar cores. The screw dislocations are thus responsible, on the one hand, for a strong increase of the flow stress with decreasing temperature and, on the other hand, for a complicated slip geometry in b.c.c. metals [1, 2, 3].

The first proposals for a theoretical explanation of the process of sessile-glissile transformations were based on a simplified idea of dislocation splitting into singular partials in non-planar and planar configurations [1]. A detailed description of the structure of screw dislocation cores in b.c.c. metals can be based on atomistic models, especially on a computer simulation of the lattice with a dislocation (see review [4]). Recently, the Peierls-Nabarro (P.N.) model has been applied in describing dislocations with planar cores, edge dislocations in particular, in b.c.c. metals [5, 6].

It will be the attempt of this paper to generalize the P.N. model to describe screw dislocations with non-planar cores.

The present dislocation models will first be discussed from the point of view of continuum models of a discrete lattice. Moreover, the incorporation of a non-linear material law and of the lattice periodicity into the continuum treatment of the P.N. model will be stressed. After obtaining a general formulation of the P.N. model for the dislocation core extended along three slip planes, preliminary results will be given on the structure of screw dislocations in α-Fe with the core extended along three planes of the $\{110\}$ type without external stress. Finally, the possibility of applying the generalized P.N. model to a detailed study of sessile-glissile transformations of screw dislocations will be discussed.

2. Dislocation models and material laws

For a practical description, the distorted crystal around a dislocation is often conventionally divided into two parts. The thin region along the dislocation line having a diameter equal to a few interatomic distances, where the crystal structure is heavily distorted, is called the dislocation core while the outer part is considered as an elastically deformed crystal or continuum.

Three types of models have been developed to describe the properties of dislocations (see e.g. [7]):

1. *Continuum models*, i.e., the dislocation is imagined in a continuum which can be elastic, isotropic or anisotropic, linear or non-linear, homogeneous or non-homogeneous, even visco-elastic; the dislocation can be treated with a singular dislocation line or with hollow core. The concept of a continuous distribution of infinitesimal dislocations can also be accepted. The material properties are fully characterized by the properties (usually elastic) of the chosen continuum and only some geometrical characteristics of the dislocation in the crystal lattice are taken into account, especially the Burgers vector of the dislocation and the form of the dislocation line. The surprising success of this model lies in the fact that the stress field of a dislocation decreases slowly at the distance r from the dislocation line as $1/r$ so that the main part of the dislocation energy is stored as

an elastic energy in a relatively large crystal region and only a small part of energy is stored in the core region. This model is, therefore, suitable for describing the mutual interactions of dislocations and their interaction with some other lattice defects in terms of stresses, energies, etc.

2. *Atomistic models*, which respect the discrete structure of the crystal. However, the number of atoms which has to be considered is so large that deeper physical theories, e.g. quantum mechanics, can be used only for some very special considerations and the atomistic models are usually developed as mechanistic models. The atomic lattice is represented by a lattice of mass points and the material properties are given by interatomic forces usually represented by central pairwise potentials between the mass points (see, e.g., [4]). These models can give information on the detailed structure of the dislocation core and on the dislocation properties which depend sensitively on the core structure, e.g. on the dislocation mobility in the lattice. The present atomistic models are based on a computer simulation of a crystal block with a dislocation. The essential weak point of these models is that they are based on a limited knowledge of the interatomic potentials [8].

3. *Intermediate models*, which combine the two previous models: on the one hand, they respect the discrete structure of the core at least to some extent, and, on the other hand, they take into consideration the connexion of the core region with the outer crystal represented by a continuum. This approach is, in fact, often respected in the above mentioned models. For example, a correction is usually added to the elastic energy of a dislocation in continuum based on a crude atomistic estimation of the core energy. In a computer simulation of a block of atoms with a dislocation, the boundary condition is usually taken from a solution of a dislocation in an anisotropic continuum. In intermediate models, the material properties are given not only by the elastic constants but also by interatomic potentials in the core region or at least by some other quantities, taking into account the properties of the discrete core region in some simplified way. A typical model of this type is the P.N. model.

3. Comments on the Peierls-Nabarro model of a dislocation with a planar core

The P.N. model [9, 10] is a special intermediate dislocation model formed in a body having the following properties:

The body is assumed to consist of two elastic half spaces A and B (Fig. 1) with additional mutual force interaction between the two adjacent surfaces; this interaction is thought to be due to the atomic interaction between the atoms on the upper and on the lower face. For a relative tangential displacement $f(x)$ (called disregistry) of the faces A and B, $f(x) = u_B(x, -a/2) - u_A(x, a/2)$, the shear stress component τ_{xy} at the faces, $\tau_{xy}(x, -a/2) = \tau_{xy}(x, a/2) = \tau(f(x))$, where $\tau(f)$ is due to the mutual interaction between the atoms. However, τ is taken in the continuum approximation as a continuous function of f, i.e., as an interaction between the points of the faces. Therefore, $\tau(f)$ represents the additional material property of the model (besides the shear modulus μ and the Poisson ratio ν of the isotropic half spaces A, B) and is usually called the force

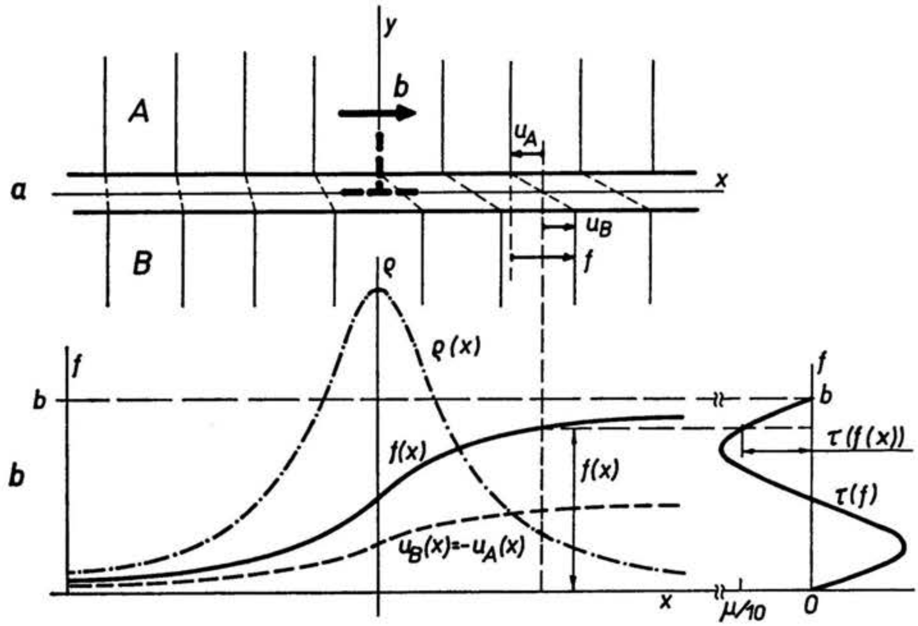

FIG. 1. a. Peierls-Nabarro model of an edge dislocation with a planar core; b. schematic course of the force law $\tau(f)$, disregistry $f(x)$ and dislocation density $\varrho(x)$.

law. The form of the force law in a given material also depends on the position of the crystallographic plane chosen for the xz plane. So as to be consistent with the assumed crystal structure, the force law $\tau(f)$ must fulfil the following conditions:

(i) $\tau(f)$ must be a periodic function of f with the period b equal to the crystal lattice period in the x direction, $\tau(f) = \tau(f+b)$;

(ii) at points where $f = 0$ also $\tau(0) = 0$;

(iii) for small f ($|f| \ll b$), the force law must be consistent with Hooke's law, $\lim_{f\to 0} [\partial\tau(f)/\partial f] = -\mu/a$, if e.g. a tetragonal lattice with the lattice parameters a, b is considered.

As a material law the force law $\tau(f)$ represents the resistance of the lattice against generally large relative tangential displacements f concentrated between two neighbouring atomic planes and, therefore, can be deduced from the interatomic potentials. The method of calculation was proposed by VÍTEK [11]. For the homogeneous disregistry $\mathbf{f}$ along a chosen plane, the increase $\gamma(\mathbf{f})$ of the energy of the crystal per unit area of the interface is calculated by using the interatomic potentials; γ is called the generalized stacking fault energy and the surface representing the plot of γ over the plane of disregistries $\mathbf{f}$ is called the γ-surface. The force law for a given direction in the plane can then be calculated as $\tau(f) = -d\gamma/df$.

For a non-zero disregistry $f(x)$ and without external forces, the body will be in equilibrium if the shear stresses $\tau_{xy}(x)$ at the interface, which are caused by the elastic response of the two half spaces is equal to the force law $\tau(f(x))$. This condition can be expressed in the form of the P.N. equation [9, 10]

$$\frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{df(t)/dt}{x-t} dt = \tau(f(x)), \tag{3.1}$$

where the integral should be understood as the Cauchy principal value.

An edge dislocation parallel to the z axis and with the Burgers vector **b** in the x direction (i.e., with the slip plane xz) is formed in the body if the disregistry fulfills the boundary conditions

$$\lim_{x\to-\infty} f(x) = 0, \quad \lim_{x\to\infty} f(x) = b. \tag{3.2}$$

The problem of dislocation can then be solved in two steps. First, for a given force law $\tau(f)$, the P.N. equation (3.1) represents an integro-differential equation for disregistry $f(x)$, which has to be solved with the boundary conditions (3.2). Note that the Eq. (3.1) is non-linear because of the periodic force law $\tau(f)$. Secondly, when the disregistry $f(x)$ is known, other properties of the dislocation within the P.N. model can be studied. For example, the stresses in the half spaces A, B can be found for given mixed boundary conconditions $u_A(x, a/2) = -\frac{1}{2} f(x)$, $\tau_{xyA}(x, a/2) = \tau(f(x))$ and $u_B(x, -a/2) = \frac{1}{2} f(x)$, $\tau_{xyB}(x, -a/2) = \tau(f(x))$, for a plain strain problem in the linear theory of elasticity. The displacements in the y direction and all the stress components cross the interface continuously.

An intuitive interpretation can be given to the P.N. model: the cut along the slip plane can be taken as a continuous distribution of infinitesimal dislocations with the dislocation density $\varrho(x) = df(x)/dx$ so that the Burgers vector of dislocations between t and $t+dt$ is $db = \varrho(t)dt$.

In the original papers [9, 10], sine force law was chosen for simplicity, $\tau = -\mu b/ /(2\pi a)\sin(2\pi f/b)$, and the corresponding disregistry $f(x) = (b/\pi)$ arctg$(x/\xi)+b/2$ or dislocation density $\varrho(x) = (b/\pi)\xi/(x^2+\xi^2)$ were easily found; the parameter $\xi = a/(2(1-\nu))$ characterizes the dislocation width.

It should be pointed out that no general theorems on the existence, uniqueness and stability of solution of the P.N. equation with given boundary conditions are known for general force laws. Numerical methods of solution for more complicated force laws have been developed [5, 6] and the details of the structure of cores of edge dislocations in b.c.c. metals were described in terms of dislocation densities $\varrho(x)$; the peaks in $\varrho(x)$ have been interpreted as partial dislocations. An inverse method of solution can also be used [6]: for chosen disregistry $f(x)$ (or density $\varrho(x)$) with some free parameters c_i, the integral in (3.1) can be calculated and, therefore, τ as a function of x is found. Then, the force law $\tau(f)$ can be constructed by eliminating x from the functions $\tau(x)$ and $f(x)$, or a given force law $\tau(f)$ can be approximated by means of the adjustable free parameters c_i. An approximate solution $f(x)$ of (3.1) for a given force law can be found in this way.

Note further that the P.N. equation (3.1) is invariant with respect to an arbitrary displacement: if $f(x)$ is a solution of (3.1) with the boundary conditions (3.2), then,

$f(x+c)$ is also a solution of (3.1) with (3.2) for an arbitrary c. Therefore, within the used quasi-continuum treatment, the dislocation is freely movable and an external stress cannot be incorporated into the Eq. (3.2); otherwise no stable solution would exist. Nevertheless, the P.N. model was used for calculating the P.N. stress, i.e., the external stress necessary to move the dislocation through the lattice [9, 10]. However, the discrete structure of the slip plane had to be taken into account additionally in a rather artificial way. Using the continuous solution $f(x)$ of the P.N. equation, the total interaction energy $W = b \sum_{i=-\infty}^{\infty} \gamma_i(f(x_i))$ of all atomic pairs placed above and below the slip plane at discrete points was calculated. From changes of W with an additional relative homogeneous displacement of the two half spaces, the P.N. barrier and the P.N. stress can be found [10], even for complicated force laws [12].

In the continuum approximation given by the P.N. equation (3.1), the core energy W_0 can be defined as $W_0 = \int_{-\infty}^{\infty} \gamma(f(x))dx$. It can be shown [13] that, for $f(x)$ satisfying the Eq. (3.1), W_0 does not depend on the force law and that $W_0 = \mu b^2/(4\pi)$.

4. Peierls-Nabarro model of a screw dislocation with core extended along three slip planes

For a screw dislocation parallel with the z-axis, the body will be assumed to consist of three elastic isotropic wedge-like sections A, B, C separated by three cuts along the slip planes P_1, P_2, P_3 (Fig. 2). Section C has been divided into two parts and a screw dislocation with the Burgers vector **b** along z has been reduced by a constant relative displacement of C_1 with respect to C_2. All the elastic displacements and the disregistries

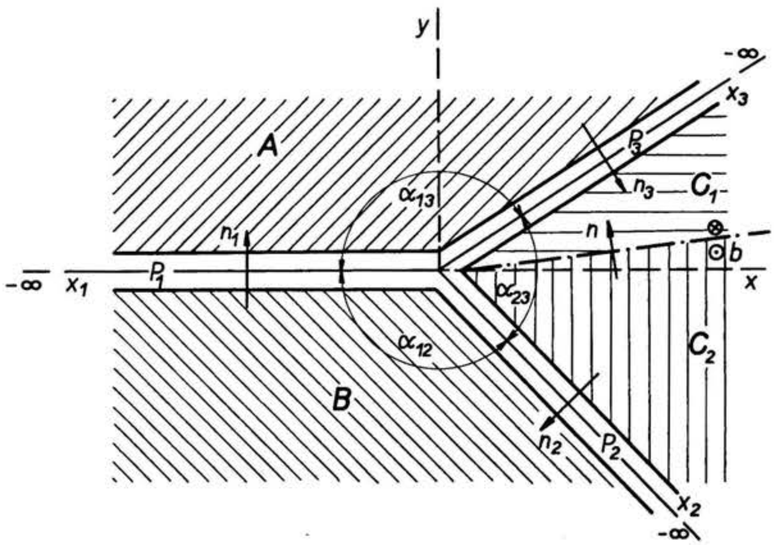

FIG. 2. Peierls-Nabarro model of a screw dislocation with the core extended along three slip planes P_i; all displacements and disregistries are parallel with the z-axis (perpendicular to the figure plane).

f_i across the P_i planes will be in the z-direction. The sign of disregistries is defined in the following way: f_1, f_2, f_3 are the relative displacements of B with respect to A, C_1 with respect to B and A with respect to C_2, respectively.

The force laws $\tau_i(f_i)$ can be obtained from the stacking fault energies $\gamma_i(f_i)$ using the relations

(4.1) $$\tau_i(f_i) = -d\gamma_i(f_i)/df_i.$$

The coordinates $x_i < 0$ will be chosen in planes P_i in the directions perpendicular to z. The boundary conditions for the disregistries f_i will be supposed in the form

(4.2) $$f_i(x_i) = \varepsilon_i \quad \text{for} \quad x = -\infty, \quad \sum_{i=1}^{3} f_i(0) = b.$$

The densities $\varrho_i(x_i)$ of the continuous distribution of screw dislocations in the slip planes P_i

(4.3) $$\varrho_i(x_i) = df_i(x)_i/dx_i,$$

are positive and it follows from (4.2) that

(4.4) $$\sum_{i=1}^{3} \int_{-\infty}^{0} \varrho_i(x_i)\,dx_i = b.$$

If an external stress σ_{ij}^E is applied, then the shear stress components σ_i^E in the P_i planes acting in the z direction are

(4.5) $$\begin{aligned} \sigma_1^E &= \sigma_{yz}^E, \\ \sigma_2^E &= \sigma_{yz}^E \cos\alpha_{12} - \sigma_{xz}^E \sin\alpha_{12}, \\ \sigma_3^E &= \sigma_{yz}^E \cos\alpha_{13} + \sigma_{xz}^E \sin\alpha_{13}, \end{aligned}$$

where α_{ij} is the angle between the planes P_i and P_j (Fig. 2).

The condition of equilibrium can now be expressed in the following way: the sum of shear stresses produced by the (still unknown) screw dislocation distributions from all three half planes and of the external shear stress at a general point x_i of plane P_i has to be equal to the value of the force law $\tau_i(f_i(x_i))$. This condition leads to a system of three non-linear integro-differential equations,

(4.6) $$\frac{\mu}{2\pi} \int_{-\infty}^{0} \frac{\varrho_i(t_i)}{x_i - t_i}\,dt_i + \frac{\mu}{2\pi} \int_{-\infty}^{0} \frac{x_i - t_j\cos\alpha_{ij}}{x_i^2 + t_j^2 - 2x_i t_j \cos\alpha_{ij}}\,\varrho_j(t_j)\,dt_j$$
$$+ \frac{\mu}{2\pi} \int_{-\infty}^{0} \frac{x_i - t_k\cos\alpha_{ik}}{x_i^2 + t_k^2 - 2x_i t_k \cos\alpha_{ik}}\,\varrho_k(t_k)\,dt_k + \sigma_i^E = \tau_i\big(f_i(x_i)\big),$$

where $i, j, k = 1, 2, 3$ and $i \neq j \neq k$. The first integral (in the meaning of the Cauchy principal value) corresponds to the original P.N. term and gives the shear stresses from the dislocation distribution in the P_i plane (half plane in our case) at its points x_i, the second and third integral give the shear stresses from the dislocation distributions of P_j and P_k planes acting at the point x_i in plane P_i.

The system of the three equations (4.6) together with the definition (4.3) and the boundary conditions (4.2) represent the generalized P.N. equation for a screw dislocation with the core extended along three planes. In contrast to the planar case, the generalized P.N. equation is no more invariant with respect to a displacement in the slip planes and, therefore, the influence of an external stress can be taken into account. The disregistries $f_i(x_i)$ (or densities $\varrho_i(x_i)$) should be found from (4.6) for given force laws $\tau_i(f_i)$ and external stress σ_i^E. A numerical method of solution has to be used for realistic force laws.

5. $\frac{1}{2}$ [111] screw dislocation in α-Fe with core extended along three (110) planes without external stress

The atomic structure of the core of a $\frac{1}{2}$ [111] screw dislocation in b.c.c. metals in the low energy state is rather complex. Nevertheless, computer simulations [4] have shown that the relative displacements between the atoms are, to a large extent, concentrated along the $\{110\}$ planes. Therefore, as an approximation within the generalized P.N. model an extension of the core along three $\{110\}$ planes will be considered; this is $\alpha_{ij} = 2\pi/3$. Without external stress, $\sigma_i^E = 0$, the core configuration should follow the three-

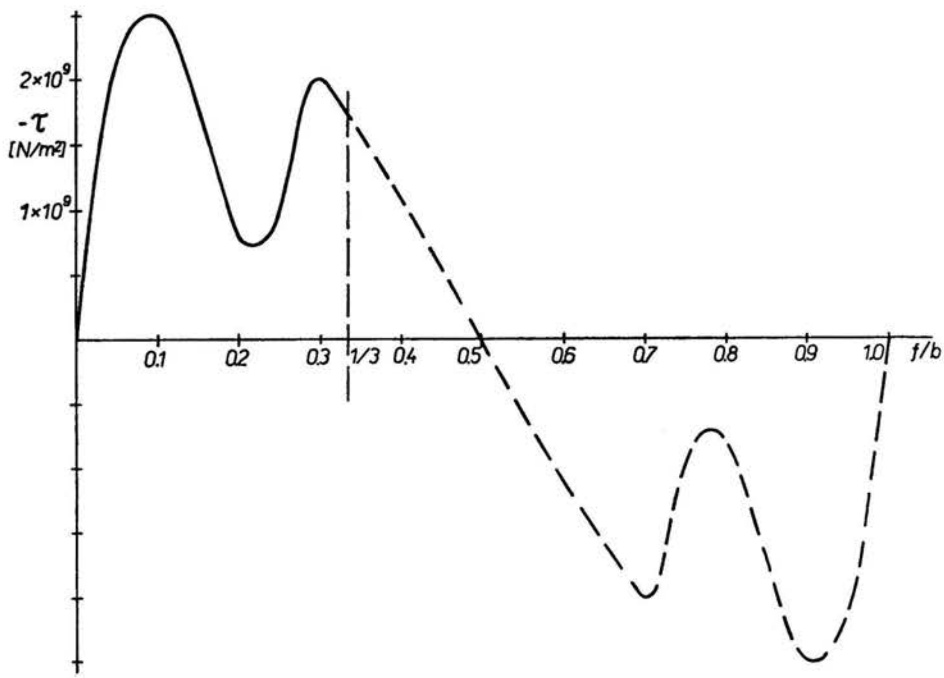

FIG. 3. Force law $\tau(f)$ in α-Fe on $(1\bar{1}0)$ plane in [111] direction based on an atomistic calculation of the γ-surface in [11].

fold crystal symmetry and we can assume that $f_i = f$, $\varrho_i = \varrho$, $\tau_i(f_i) = \tau(f)$ and the system of the three equations (4.6) reduces to one:

$$\frac{\mu}{2\pi}\int_{-\infty}^{0}\varrho(t)\left[\frac{1}{x-t}+\frac{2x+t}{x^2+t^2+xt}\right]dt = \tau(f(t)) \tag{5.1}$$

with the conditions

$$f(-\infty) = 0, \quad f(0) = b/3, \quad \varrho(x) = df/dx. \tag{5.2}$$

The force law $\tau(f)$ for a $(1\bar{1}0)$ plane in the [111] direction based on a γ-surface calculated for α-Fe in [11] is shown in Fig. 3. Using a numerical method of solution based on an inverse method, the corresponding disregistry $f(x)$ was found [14]. Figure 4 shows

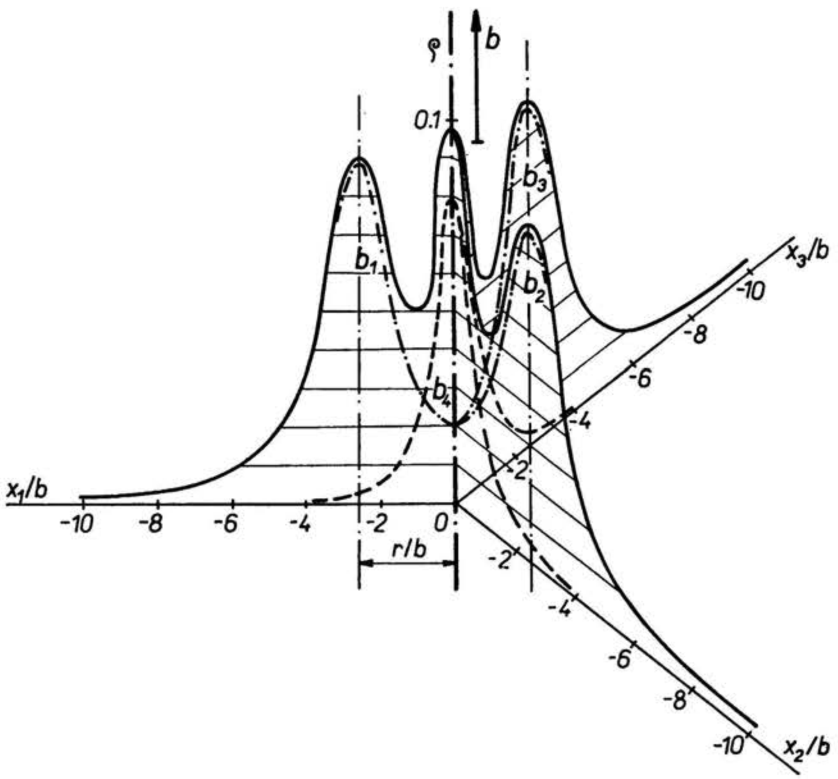

FIG. 4. Dislocation densities $\varrho(x)$ in the dislocation core of a screw dislocation in α-Fe extended along three {110} planes. Calculation was based on the generalized P.N. equation (5.1).

the corresponding dislocation densities $\varrho(x)$ on three {110} planes. For comparison, the dislocation distribution found from the original P.N. equation (3.1) describing the planar core (for a slightly different force law) is shown in Fig. 5. For the low energy configuration with a three-fold symmetry, only that part of the force law $\tau(f)$ for f between 0 and $b/3$ has been used.

The result can be interpreted in terms of a generalized dislocation splitting [15] if the peaks in the dislocation density are identified with partial dislocations. There are three

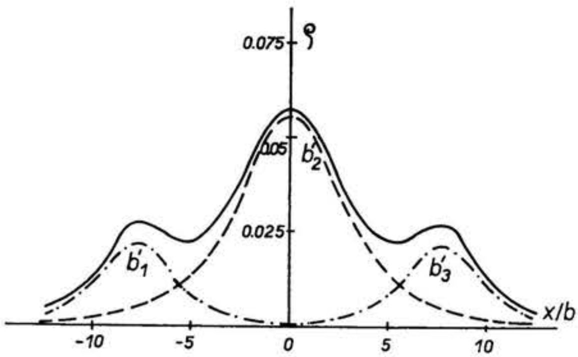

FIG. 5. Dislocation densities $\varrho(x)$ on one (110) plane resulting from the P.N. equation (3.1) for a planar core of a screw dislocation in α-Fe (after [6]).

partials which are placed symmetrically on three $\{110\}$ planes (with the values of the Burgers vectors $b_1 = b_2 = b_3 \approx 0.272b$) connected by generalized stacking faults with the fourth middle partial (with $b \approx 0.184b$). The distance between the middle and side partials (the width of splitting) is $r \approx 2.5b$.

It can be shown that the core energy of the symmetrical configuration without external stress is $W_s = 3 \int\limits_{-\infty}^{0} \gamma\big(f(x)\big)\,dx = \mu b^2/(4\pi)$, independently of the form of the force law; therefore, it is equal to the core energy of the planar configuration, within the continuum treatment.

In Fig. 5 the planar configuration with three partials represents a stable solution of the original P.N. equation (3.1) for a planar core, however, it has, with the same core energy, a higher elastic energy than the three-fold configuration. Therefore, the three-fold symmetry configuration will appear in a b.c.c. crystal without an external stress field and the planar configuration will be formed only under external stress.

6. Discussion

The P.N. equation has been generalized for the case of a screw dislocation with the core extended along three planes. The splitting of screw dislocations on two planes has also been considered by different authors for b.c.c. [1, 4] and h.c.p. metals [16]. The corresponding P.N. model can be considered as a special case of the presented one: for the core extended along two half planes only, the third integral in (4.6) has to be left out and the system reduces to two equations for $i, j = 1, 2$ and $i \neq j$. The model can also be generalized for an extension of the core along more than three planes, in analogy to the models of dislocation splitting in [15].

The proposed generalization maintains the basic simplification of the P.N. model: it treats the body as an elastic continuum with the exception of three (instead of one) slip planes where the non-linear behaviour and the lattice periodicity are considered with the aid of additional continuous materials laws — the force laws. It is, therefore, suitable for the study of screw dislocations with cores extended along three half planes, especially for screw dislocations in b.c.c. metals.

To give an example, the equilibrium configuration of a $\frac{1}{2}$ [111] screw dislocation with its core extended along three $\{110\}$ planes without external stress has been found in Sect. 5 for a realistic force law based on atomistic calculations. The interpretation in terms of the density of a continuous distribution of dislocations can be considered as a generalization of the previous models of a sessile splitting of a screw dislocation in b.c.c. metals into four singular partials [1]. This is consistent with recent fully atomistic models showing the concentration of relative interatomic displacements into three $\{110\}$ planes [4].

An advantage of the proposed generalization of the P.N. model on more slip planes is the possibility of studying the effect of the external stress σ_i^E. On the analogy of the previous models of dislocation splitting into singular partials [1, 15], the following behaviour is expected: for small external stress, a stable solution should exist with an asymmetric distribution of dislocation densities $\varrho_i(x_i)$ representing an intermediate stage of transition from the three-fold symmetry configuration into the planar one. The solution should cease to hold for critical values of $\sigma_i^E = T_i$: the corresponding external stress T_i can then be called the critical stress for the sessile-glissile transformation of the screw dislocation at $0K$ (i.e., without thermal activation). As the core energies W_s and W_0 are equal, the energy barrier for the sessile-glissile transformation is due to the difference in elastic energies of the glissile and sessile configurations. Therefore, the critical stress T_i has no direct relation to the P.N. stress given by the lattice periodicity. Nevertheless, this stress is connected with the lattice symmetry described in a quasi-continuum approach and can be called the generalized P.N. stress. The results of a numerical study of the sessile-glissile transformation of a screw dislocation in α-Fe under increasing external stress within the proposed generalized P.N. model will be published later [17].

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References

1. F. KROUPA, V. VÍTEK, *Slip and the conception of splitting of dislocations in* b.c.c. *metals*, Canad. J. Phys., **45**, 945–971, 1967.
2. J. W. CHRISTAN, *Plastic deformation of* b.c.c. *metals*, Proc. of Second Internat. Conf. on the Strength of Metals and Alloys, AMS, Asilomar 1970, 29–70.
3. B. ŠESTÁK, *Geometrie der Gleitung in kubisch-raumzentrierten Metallen*, in Reinststoffe in Wissenschaft und Technik, Akademie Verlag, 221–262, Berlin 1972.
4. V. VÍTEK, *Theory of the core structures of dislocations in body centered cubic metals*, Crystal Lattice Defects, **5**, 1–34, 1974.
5. L. LEJČEK, *Peierls-Nabarro model of planar dislocation cores in* b.c.c. *crystals*, Czech. J. Phys., B **22**, 802–812, 1972.
6. F. KROUPA, L. LEJČEK, *Splitting of dislocations in the Peierls-Nabarro model*, Czech. J. Phys., B **22**, 813–825, 1972.
7. F. R. N. NABARRO, *Theory of crystal dislocations*, Clarendon Press, Oxford 1967.
8. *Interatomic potentials and simulation of lattice defects* (Editors P. C. GEHLEN, J. R. BEELER, R. I. JAFFEE), Plenum Press, New York 1972.

9. R. E. PEIERLS, *The size of a dislocation*, Proc. Phys. Soc., A **52**, 34–38, 1940.
10. F. R. N. NABARRO, *Dislocations in a simple cubic lattice*, Proc. Phys. Soc., A **59**, 256–272, 1947.
11. V. VÍTEK, *Intrinsic stacking faults in body centered cubic crystals*, Phil. Mag., **18**, 773–786, 1968.
12. L. LEJČEK, *Peierls-Nabarro barrier and stress of* 1/2 [111] *edge dislocation in* α-Fe, Czech. J. Phys., B **23**, 56–61, 1973.
13. A. H. COTTRELL, *Theory of crystal dislocation*, Blackie and Son, London 1964.
14. L. LEJČEK, F. KROUPA, *Peierls-Nabarro model of non-planar screw dislocation cores*, Czech. J. Phys. B, **26**, 528–537, 1976.
15. V. VÍTEK, F. KROUPA, *Generalized splitting of dislocations*, Phil. Mag., **19**, 265–284, 1969.
16. M. ŠOB, *Sessile splittings of screw dislocations in* h.c.p. *metals*, Phys. Stat. Sol. (a), **24**, K131–K136, 1974.
17. L. LEJČEK, F. KROUPA, *The effect of stress on the screw dislocation core in* b.c.c. *metals*, Czech. J. Phys. B, to be published.

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