SPLITTING OF DISLOCATIONS IN THE PEIERLS-NABARRO MODEL

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A numerical method of solution of the Peierls-Nabarro integro-differential eqation for a given force law $\tau(f)$ is proposed. The solution, i.e., the disregistry $f(x)$ or the dislocation density $\varrho(x) = \mathrm{d}f/\mathrm{d}x$ is found in a form which describes the splitting of a dislocation into the chosen number of partial dislocations. The method is applied to the study of planar cores of $\frac{1}{2}\langle 111\rangle$ dislocation in b.c.c. metals on $\{112\}$ and on $\{110\}$ planes. The force laws $\tau(f)$ are derived from the dependence of the stacking fault energy γ on disregistry f; the $\gamma(f)$ curves calculated by Vítek (1969) for α-Fe for two different interatomic potentials are used. In all cases, the solution is well represented by splitting into three partials.

1. INTRODUCTION

1.1. Peierls-Nabarro model

The Peierls-Nabarro model [1, 2] can be considered as an elastic model of the dislocation core, assumed to be planar along the slip plane. The periodic structure of the crystal along the slip plane is taken into account as a periodic force interaction between the surfaces of two elastic half spaces A, B (Fig. 1).

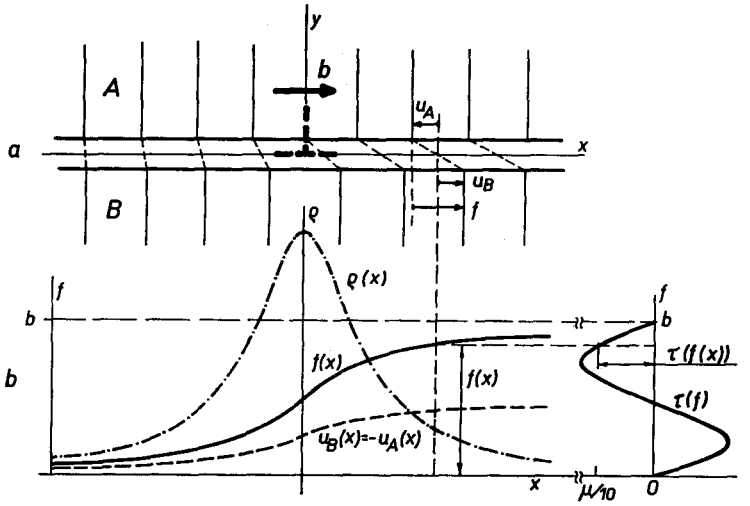

Fig. 1. a) Peierls-Nabarro model of an edge dislocation; b) schematic course of the force law $\tau(f)$, disregistry $f(x)$ and dislocation density $\varrho(x)$ for one dislocation with complete Burgers vector $\boldsymbol{b}$.

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Assume an edge dislocation parallel to the z axis with the Burgers vector $\boldsymbol{b}$ parallel to the x axis. The force (shear traction) τ in the x direction which the half space A exerts on a unit area of the surface of B at the place where the relative displacement of the two surfaces in the x direction is $f(x)$, is taken as a periodic function of f with the period b,

$$\tau = \tau(f) . \tag{1}$$

This relation is called the force law and f the disregistry. Note that f is introduced as the local displacement of the B half space with respect to the A half space, $f(x) = u_B(x) - u_A(x)$ (this definition of disregistry slightly differs from that of the relative displacement ϕ used e.g. in [1, 2]).

The disregistry for one dislocation must fulfil the boundary conditions at $x = \pm\infty$,

$$\lim_{x \to -\infty} f(x) = 0 , \quad \lim_{x \to +\infty} f(x) = b \tag{2}$$

and τ the conditions

$$\tau = 0 \quad \text{for} \quad f = 0 , \quad f = b . \tag{3}$$

The condition of equilibrium leads to a relation between $\tau(f)$ and $f(x)$ called the Peierls-Nabarro (P.N.) integro-differential equation [1, 2],

$$\frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{1}{x-t} \frac{\mathrm{d}f(t)}{\mathrm{d}t} \, \mathrm{d}t = \tau(f) , \tag{4}$$

where μ is the shear modulus and ν the Poisson ratio (isotropic continuum in A, B is assumed); the integral should be understood as the Cauchy principal value.

1.2. Solutions $f(x)$ for given force laws $\tau(f)$

In the original papers [1, 2], the force law $\tau(f)$ was assumed to be given and was chosen in a very special form

$$\tau = -\frac{\mu b}{2\pi d} \sin\left(\frac{2\pi}{b} f\right) \tag{5}$$

called the sine force law; d is the distance between the neighbouring slip planes. In this special case, the solution of (4) was easily found as

$$f(x) = \frac{b}{\pi} \tan^{-1} \frac{x}{\xi} + \frac{b}{2} . \tag{6}$$

The parameter

$$\xi = d/[2(1-\nu)] \tag{7}$$

characterizes the dislocation width. The solution of the P.N. model can be completed if $f(x)$ is known (for a review see e.g. [3, 4, 5]).

A numerical method of solution of the P.N. equation (4) for more complicated force laws was given in [6, 7]. The force laws were derived from the stacking fault energies $\gamma(f)$ (calculated in [8] for b.c.c. metals from an atomic model) with the help of the relation [5]

$$\tau(f) = -\mathrm{d}\gamma(f)/\mathrm{d}f\,. \tag{8}$$

The solutions $f(x)$ corresponding to $\tau(f)$ were found by a numerical iterative method.

1.3. Dislocation density $\varrho(x)$ and dislocation splitting

Another interpretation can be given to the P.N. model [9]. The cut along the slip plane can be taken as an equilibrium continuous distribution of infinitesimal dislocations with the Burgers vector density ϱ,

$$\varrho(x) = \mathrm{d}f/\mathrm{d}x\,, \tag{9}$$

so that the Burgers vector of dislocations between x and $x + \mathrm{d}x$ is $\mathrm{d}b = \varrho(x)\,\mathrm{d}x$ and

$$\int_{-\infty}^{\infty} \varrho(x)\,\mathrm{d}x = b\,. \tag{10}$$

While the solution (6) corresponding to the sine force law leads to one maximum on the $\varrho(x)$ curve, the numerical solutions in [6, 7] for more realistic force laws in b.c.c. metals lead to a higher number of maxima or at least to subsidiary humps on the $\varrho(x)$ curves. This result can be interpreted as dislocation splitting. Its quantative description requires the determination of the positions and of the Burgers vectors of the partial dislocations; one way will be proposed in this paper.

1.4. Force laws $\tau(f)$ corresponding to chosen disregistry $f(x)$

A pair of functions, $f(x)$ and $\tau(f)$, which is a solution of equation (4) can also be obtained in the following way: if $f(x)$ is chosen then the left side of eq. (4) gives, after integration, a function of x, $T(x)$, which can be expressed as $T(g(f)) = \tau(f)$ if the inverse function $x = g(f)$ exists.

This method was used in [10, 11, 12] where the dislocation splitting was studied. The function $f(x)$ was taken as a sum of two solutions of type (6) corresponding to the sine force law. However, the force law $\tau(f)$ corresponding to the total disregistry f differs from the sine law because the P.N. equation (4) is not linear.

Another function $f(x)$ was chosen in [13] to describe one non-split dislocation with a wider core,

$$f(x) = \frac{b}{\pi}\left[1 - (c-1)\frac{\partial}{\partial c}\right]\tan^{-1}\frac{x}{c\xi} \tag{11}$$

and the corresponding $\tau(f)$ was found. The influence of the parameter c on the form of the $\tau(f)$ curves and on the dislocation width was studied in [13]; the case $c = 1$ corresponds to the sine force law.

Note that the functions $\eta(t) = -\mu[2(1-\nu)]^{-1}\,\mathrm{d}f(t)/\mathrm{d}t$ and $T(x)$ are connected by the Hilbert transform, $T(x) = (1/\pi)\int_{-\infty}^{\infty}\eta(t)/(t-x)\,\mathrm{d}t$, so that the tables and some properties of the Hilbert transform can be helpful in finding the pair $f(x)$ and $T(x)$.

This method of determination of the pair of functions f and τ is rather formal: the force law $\tau(f)$ corresponding to the chosen disregistry $f(x)$ need not have physical significance.

1.5. Dislocation splitting corresponding to a given force law $\tau(f)$

In this paper, a method will be proposed which enables to find, to the given force law $\tau(f)$, the corresponding disregistry $f(x)$ (or the dislocation density $\varrho(x)$) in the form which directly determines the dislocation splitting, i.e., the positions and Burgers vectors of the partial dislocations. The sought disregistry $f(x)$ will be assumed in the form of a sum of terms of type (11) describing the individual partials, with a sufficient number of free constants. These constants will be determined from the P.N. equation (4) even for complicated given force laws $\tau(f)$.

The numerical results will be given for b.c.c. metals for which the solution of the P.N. equation has already been studied in [6, 7] using another numerical method so that a comparison of the results of both methods will be possible.

The results will be compared with the previous ideas on the splitting of dislocations in b.c.c. metals, especially with the so called generalized splitting [14] as well as with some recent atomic models of the dislocation cores.

2. APPROXIMATE SOLUTION OF THE PEIERLS-NABARRO EQUATION FOR A GIVEN FORCE LAW

2.1. Solution corresponding to a combination of partial dislocations

Assume that the force law $\tau = \tau_0(f)$ is given. An approximate solution $f(x)$ of the P.N. equation (4) for one dislocation having the complete Burgers vector b can be obtained in the following way.

Let us choose the disregistry in the form

$$(12)\qquad f(x) = \sum_{i=1}^{N} f_i(x) = \sum_{i=1}^{N}\left\{\frac{\alpha_i b}{\pi}\left[1-(c_i-1)\frac{\partial}{\partial c_i}\right]\tan^{-1}\frac{x-x_i}{c_i\xi} + \frac{\alpha_i b}{2}\right\} =$$

$$= \frac{b}{\pi}\sum_{i=1}^{N}\alpha_i\left[\tan^{-1}\frac{x-x_i}{c_i\xi} + (c_i-1)\,\xi\,\frac{x-x_i}{(x-x_i)^2+(c_i\xi)^2}\right] + \frac{b}{2},$$

where ξ is given by eq. (7), N, α_i, c_i, x_i are free constants, N is an integer and

$$0 < \alpha_i \leqq 1\,, \quad \sum_{i=1}^{N} \alpha_i = 1\,, \quad c_i \geqq 1\,. \tag{13}$$

The corresponding dislocation distribution $\varrho(x)$ follows from eq. (9),

$$\varrho(x) = \frac{b}{\pi} \sum_{i=1}^{N} \alpha_i \xi \frac{(x - x_i)^2 + (2c_i - 1)\,(c_i\xi)^2}{[(x - x_i)^2 + (c_i\xi)^2]^2}\,. \tag{14}$$

The disregistry $f(x)$ is chosen as a sum of elementary solutions $f_i(x)$ of the type given by eq. (11) introduced first by Foreman, Jaswon and Wood [13]. These elementary solutions describe here the individual partials which are placed at x_i, have the Burgers vectors $b_i = \alpha_i b$ and dislocation widths characterized by parameters $\xi_i = c_i\xi$.

The functions $f(x)$ and $\varrho(x)$ fulfil the conditions (2) and (10), respectively. The disregistry $f(x)$ in (12) is an increasing function of x, projecting the interval $-\infty \leqq x \leqq +\infty$ on the interval $0 \leqq f \leqq b$ so that the inverse function

$$x = g(f) \tag{15}$$

exists and is given uniquely. As the chosen form of $f(x)$ in (12) is rather complicated, the inverse $g(f)$ has to be calculated numerically.

The function

$$T(x) = \frac{\mu}{2\pi(1 - \nu)} \int_{-\infty}^{\infty} \frac{1}{x - t} \frac{\mathrm{d}f(t)}{\mathrm{d}t}\,\mathrm{d}t \tag{16}$$

can be found by integration using $\mathrm{d}f(t)/\mathrm{d}t = \varrho(t)$ given by eq. (14),

$$T(x) = \frac{\mu b}{\pi d} \sum_{i=1}^{N} \alpha_i (x - x_i)\,\xi \frac{(x - x_i)^2 + c_i(3c_i - 2)\,\xi^2}{[(x - x_i)^2 + (c_i\xi)^2]^2}\,. \tag{17}$$

The corresponding force law $\tau(f)$ follows from eqs. (17) and (15) as

$$\tau(f) = T(g(f))\,. \tag{18}$$

It depends on f, on the given constants μ, ν (through ξ), b, d and on the free constants N, α_i, c_i, x_i.

It fulfils the Hooke's law for the disregistry f close to 0 or b. We have, for $x \to -\infty$, from eq. (12)

$$f_- = (b/\pi) \sum_{i=1}^{N} \alpha_i [-\pi/2 - c_i\xi/x + (c_i - 1)\,\xi/x] + b/2 = -b\xi/(\pi x)$$

and from eq. (17) $T_- = \tau_- = \mu b\xi/(\pi d x)$. In a similar way, for $x \to +\infty$, it is

$$f_+ = (b/\pi) \sum_{i=1}^{N} \alpha_i [\pi/2 - c_i\xi/x + (c_i - 1)\,\xi/x] + b/2 = b - b\xi/(\pi x)$$

and $\tau_+ = \mu b\xi/(\pi dx)$. The Hooke's law follows from these relations,

$$\tau_- = -\mu f_-/d\,, \quad \tau_+ = \mu(b - f_+)/d\,.$$

The pair of functions, $\tau(f)$ and $f(x)$, represents an exact solution of the P.N. equation (4). The solution for the given force law $\tau_0(x)$ can be obtained from the equation

$$T(x, N, \alpha_i, c_i, x_i) = \tau_0(f(x, N, \alpha_i, c_i, x_i))\,. \tag{19}$$

If the constants N, α_i, c_i, x_i can be found in such a way that eq. (19) is fulfilled exactly for all x then $f(x)$ given by eq. (12) represents an exact solution of the P.N. equation corresponding to $\tau_0(f)$. However, for complicated force laws $\tau_0(f)$ given e.g. numerically, the equation (19) can only be solved approximately. Then, the disregistry $f(x)$ for fixed values N, α_i, c_i, x_i is only an approximate solution for $\tau_0(f)$. It also can be interpreted as an exact solution of the P.N. equation for another force law $\tau(f)$ given by eqs. (18), (17) and (15) which slightly differs from the given force law $\tau_0(f)$.

The found $f(x)$ can be taken as a good approximation if the differences between $\tau_0(f)$ and $\tau(f)$ are within the range of errors of determination of $\tau_0(f)$.

A comment on computation will be added. The number N of partials can be best chosen equal to the number of the local minima and humps on the $\tau_0(f)$ curve (a useful property was shown in [6]: a maximum (minimum) on the $\varrho(x)$ curve appears for such x where $\tau(f(x))$ has inflexion, i.e., where $\mathrm{d}^2\tau(f(x))/\mathrm{d}f^2 = 0$, if $\mathrm{d}\tau/\mathrm{d}f > 0$ (if $\mathrm{d}\tau/\mathrm{d}f < 0$)). The method of the least squares has been chosen for the numerical calculation of the free constants. The expression

$$\Delta^2 = |T(x, \alpha_i, c_i, x_i) - \tau_0(f(x, \alpha_i, c_i, x_i))|^2$$

has been minimized by an iteration method for fixed N and the $3N$ constants α_i, c_i, x_i found from the condition $\Delta^2(x) \to 0$.

2.2. Planar cores of $\frac{1}{2}\langle 111\rangle$ dislocations in α-Fe on $\{112\}$ and $\{110\}$ planes

An example will be given for α-Fe for which the γ surfaces, i.e., the dependences of the stacking-fault energy γ on the vector of disregistry $\boldsymbol{f}$ were calculated in [8]. Only a cut of the γ surface parallel to the Burgers vector, i.e., a γ curve is necessary for the P.N. model and the force law $\tau_0 = -\mathrm{d}\gamma/\mathrm{d}f$ can be calculated numerically. As the interatomic forces in iron are not known with sufficient accuracy, the results based on two different interatomic potentials J_0 and J_2 (see [8]) will be used. Figs. 2a, 3a, 4a, 5a give the force laws $\tau_0(f)$ corresponding to the potentials J_0 and J_2 on $\{112\}$ and $\{110\}$ planes, respectively.

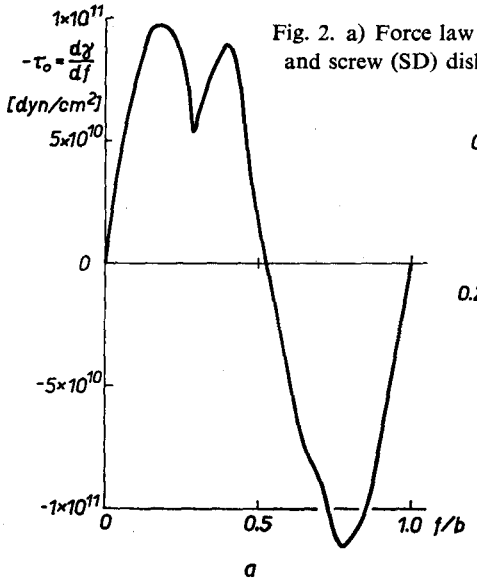
A comment should be added on the sign conventions for the γ surfaces and for dislocations. The normal to the plane xz of the stacking fault (or of dislocation splitting) is chosen in the $+y$ direction and the disregistry f is the relative displacement of the negative (lower) half space with respect to the positive (upper) one (the opposite convention was used for γ surfaces in [8]). The dislocation line is oriented in the $+z$ direction and the FS/RH convention for the sign of the

Burgers vector (see e.g. [5]) is used. Then, an edge dislocation with the Burgers vector in the $+x$ direction has the extra half plane in the upper half space (as shown in Fig. 1) and a screw dislocation with the Burgers vector in the $+z$ direction is right-handed.

Table 1

Orientation of coordinate axes in a b.c.c. crystal for edge or screw dislocation split on $\{112\}$ or $\{110\}$ plane.

xz plane of splitting \ dislocation type	edge, $b = \frac{1}{2}[\bar{1}\bar{1}1]$	screw, $b = \frac{1}{2}[\bar{1}\bar{1}1]$
(112)	$[\bar{1}\bar{1}2]$ y, n, $[\bar{1}\bar{1}1]$ x, b, $[\bar{1}10]$ z	$[\bar{1}\bar{1}2]$ y, n, $[1\bar{1}0]$ x, $[\bar{1}\bar{1}1]$ b, z
(011)	$[011]$ y, n, $[\bar{1}\bar{1}1]$ x, b, $[2\bar{1}\bar{1}]$ z	$[011]$ y, n, $[2\bar{1}\bar{1}]$ x, $[\bar{1}\bar{1}1]$ b, z



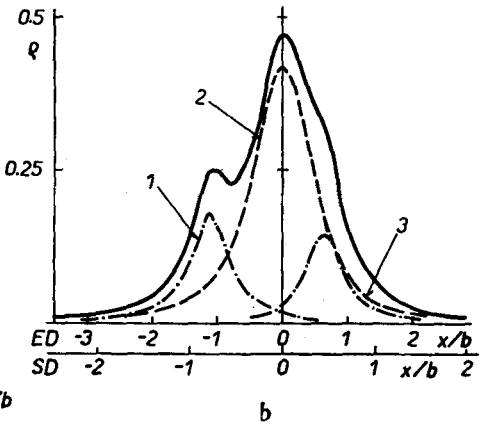


Fig. 2. a) Force law $\tau_0(f)$; b) dislocation density $\varrho(x)$ for edge (ED) and screw (SD) dislocation in α-Fe on $\{112\}$ plane (potential J_0).

An example of the corresponding choice of the coordinate axis in a b.c.c. crystal is shown in Table 1 for four cases which will be studied: $\frac{1}{2}\langle 111\rangle$ edge and screw dislocations split on $\{112\}$ and $\{110\}$ planes.

The shapes of the $\tau_0(f)$ curves suggest that satisfactory results can be obtained for $N = 3$ in all four cases. The results of computation are shown in Table 2 and in Figs. 2b, 3b, 4b, 5b for the values of the constants $b = 2{\cdot}476 \times 10^{-8}$ cm, $\mu = 5{\cdot}767 \times 10^{11}$ dyn/cm^2, $\nu = 0{\cdot}333$, $d = 1{\cdot}167 \times 10^{-8}$ cm for the $\{112\}$ planes and $d = 2{\cdot}022 \times 10^{-8}$ cm for the $\{110\}$ planes.

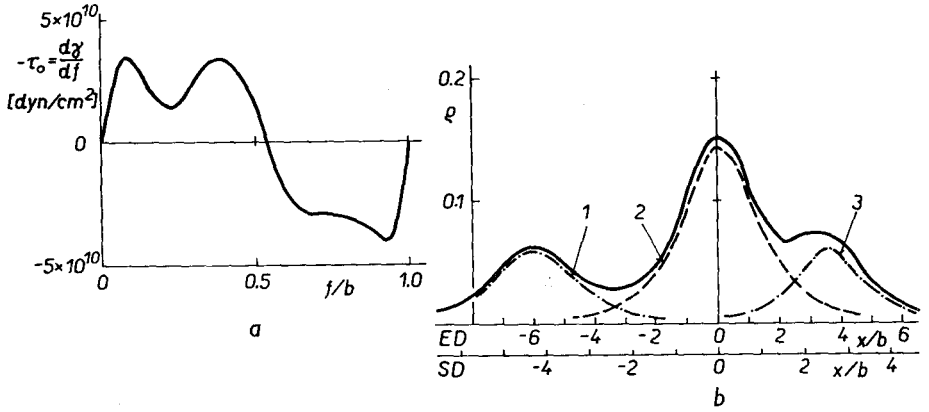


Fig. 3. a) Force law $\tau_0(f)$; b) dislocation density $\varrho(x)$ for ED and SD in α-Fe on $\{112\}$ plane (potential J_2).

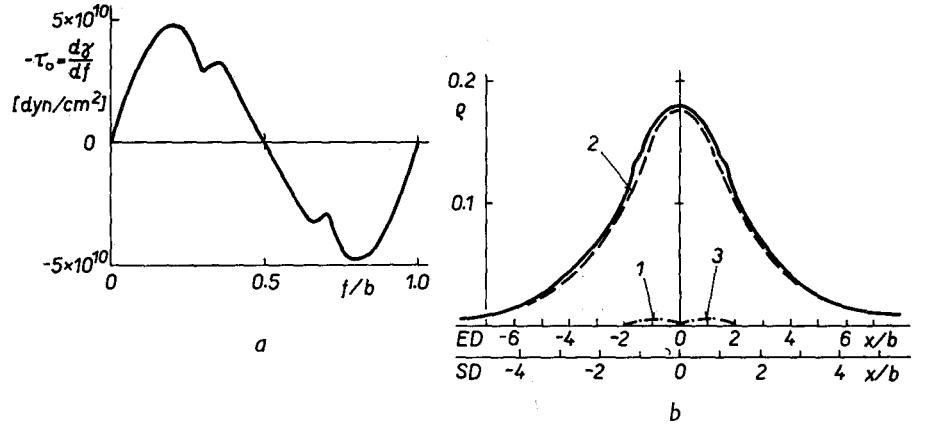


Fig. 4. a) Force law $\tau_0(f)$; b) dislocation density $\varrho(x)$ for ED and SD in α-Fe on $\{110\}$ plane (potential J_0).

The $\varrho(x)$ curves are shown in the figures instead of the $f(x)$ curves; their positions have been fixed so that the absolute maxima on $\varrho(x)$ appear at $x = 0$. Beside the resulting $\varrho(x)$ curves showing the total continuous distribution of dislocations, also

the $\varrho_i(x)$ curves corresponding to the three partial dislocations (it is $\varrho(x) = \sum_{i=1}^{N} \varrho_i(x)$) are given. The positions x_i, Burgers vectors b_i ($b_i = \alpha_i b$) and characteristic widths $c_i\xi$ of these partials follow from Table 2.

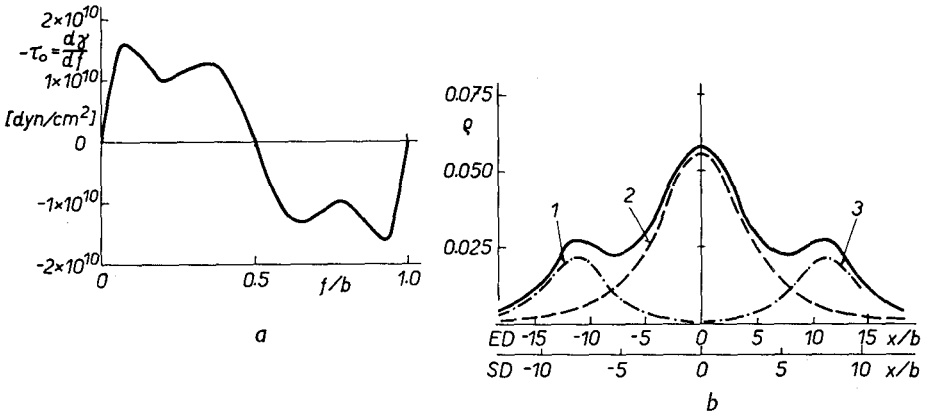


Fig. 5. a) Force law $\tau_0(f)$; b) dislocation density $\varrho(x)$ for ED and SD in α-Fe on $\{110\}$ plane (potential J_2).

Table 2

Splitting of $\frac{1}{2}\langle 111\rangle$ dislocation in the P.N. model in α-Fe (E... edge dislocation, S ... screw dislocation).

Plane	Potential	α_1	E x_1/b	S x_1/b	c_1	α_2	E x_2/b	S x_2/b	c_2	α_3	E x_3/b	S x_3/b	c_3
$\{112\}$	J_0	0·201	− 1·12	−0·75	1·00	0·637	0·00	0·00	2·08	0·162	0·64	0·43	1·00
$\{112\}$	J_2	0·252	− 6·36	−4·24	7·00	0·539	0·00	0·00	6·20	0·209	3·61	2·41	5·84
$\{110\}$	J_0	0·007	− 1·01	−0·67	1·92	0·986	0·00	0·00	5·21	0·007	1·01	0·67	1·92
$\{110\}$	J_2	0·180	−11·06	−7·38	7·98	0·640	0·00	0·00	11·30	0·180	11·06	7·38	7·98

The splittings on the $\{110\}$ planes are symmetrical, those on the $\{112\}$ planes are asymmetrical: a more pronounced local maximum on the $\varrho(x)$ curve appears on the "twinning side" of the dislocation.

The term "twinning side" is connected with a simplified splitting proposed originally on $\{112\}$ planes, $\frac{1}{2}\langle 111\rangle = \frac{1}{6}\langle 111\rangle + \frac{1}{3}\langle 111\rangle$ (see e.g. [3]). If the stacking fault between the two partials has to correspond to an elementary twin, the sequence of the partials is uniquely given and cannot be interchanged. The side of the dislocation with the $\frac{1}{6}\langle 111\rangle$ partial can be called the twinning side. The dislocation moves in the "twinning direction" if the twinning partial $\frac{1}{6}\langle 111\rangle$ moves first and an elementary twin is formed (which is then cancelled by motion of the second, $\frac{1}{3}\langle 111\rangle$ partial). This motion of a dislocation can be expected to take place at lower stresses than the motion in the opposite, "antitwinning direction".

The left side of the dislocation in Fig. 2b and 3b can be called the twinning side because the disregistry $\boldsymbol{f} = \frac{1}{6}[\bar{1}\bar{1}1]$ forms an elementary twin. This can be checked from the following crystallographic rule for twinning on $\{112\}$ planes: if $\boldsymbol{n} = \langle a, a', c\rangle$, where $a = \pm 1$, $a' = \pm 1$, $c = \pm 2$ is, for a given sequence of a, a', c, the normal to the $\{a, a', c\}$ plane then the disregistry $\boldsymbol{f}_{TW} = \frac{1}{6}\langle a, a', -c/2\rangle$ with the same sequence of a, a', c (defined as relative displacement of the negative with respect to the positive part) forms an elementary twin. We have, for $\boldsymbol{n} = [\bar{1}\bar{1}2]$, indeed $\boldsymbol{f}_{TW} = \frac{1}{6}[\bar{1}\bar{1}1]$.

Therefore, the twinning disregistry (for the sign convention used) is in the $+x$ direction, however, the twinning direction of dislocation motion is in the $-x$ direction, in which the twinning partial leads.

The value of the Burgers vector of the partial on the left side in Fig. 2b is $b_1 = \alpha_1 b = 0{\cdot}201b < \frac{1}{3}b$, in Fig. 3b it is $b_1 = 0{\cdot}252b < \frac{1}{3}b$. The analogy of this partial and $\frac{1}{6}[\bar{1}\bar{1}1]$ twinning partial dislocation is not complete, nevertheless, the motion in the twinning direction can be expected to be easier than motion in the antitwinning direction.

The results for edge dislocations are denoted by index E. The solution for screw dislocation can be obtained, as shown by Eshelby [9], from that for edge dislocation if x is replaced by $x' = (1 - \nu)\, x$ (screw dislocations are narrower than edge dislocations). The results for screw dislocations are denoted by index S in Table 2 and by changed scale on the x axis in Figs. 2b–5b. Note that the displacements of the screw dislocation and also the disregistry $f(x)$ are in the z direction.

The total curves $\varrho(x)$ are in good agreement with the corresponding $\varrho(x)$ curves obtained by another numerical method in papers [6, 7] where, however, the decomposition into the partials has not been studied.

The obtained solution, $f(x)$ or $\varrho(x)$, can be taken as an exact solution (within the accuracy of the numerical calculation) of the P.N. equation for the changed force laws $\tau(f)$. These force laws have been calculated from eq. (18) as a final verification of the results and it has been shown that they differ only slightly from the given force laws $\tau_0(f)$ shown in Figs. 2a–5a.

3. DISCUSSION

3.1. Method of solution

Our treatment is fully based on the classical P.N. model and has, therefore, all its disadvantages (a continuum model of a dislocation with an artificially added periodic interaction across the planar core) and advantages (a model mathematically simpler than the three-dimensional atomic models). The main contribution is in the numerical method of finding a solution $f(x)$ for a given, arbitrarily complicated force law $\tau_0(f)$. The method is based on generalization and combination of two previous approaches:

(i) individual partials are characterized by functions $f_i(x)$ of type proposed in [13] for single dislocations ("F.J.W. functions");

(ii) the disregistry $f(x)$ of the complete dislocation is taken as a sum of functions $f_i(x)$ characterizing the individual partials, as done previously in [11, 12, 10] for two partials and for simpler forms of $f_i(x)$ ($\tan^{-1}$ type functions).

The principle of the method is to express $f(x)$ as a function of a number of free parameters and to find the values of these parameters so that the P.N. equation is approximately fulfilled for the given force law $\tau_0(f)$. The main advantage of the method is a direct physical interpretation: the found parameters characterize the N partials into which the dislocation is split: $\alpha_i b$ is the Burgers vector, $c_i\xi$ the width and x_i the position of the i-partial. The comparison with another method of numerical solution [6, 7] has shown a good accuracy of the method used.

3.2. Force law

The force law $\tau_0(f)$ cannot be obtained from experiments. The only direct experimental values available are for small f and for f close to b where $\tau_0(f)$ has to fulfil the Hooke's law.

The only way which has been used for estimation of $\tau_0(f)$ is based on the knowledge of energies γ of the generalized stacking faults [8]. The derived values of τ_0 cannot, however, be taken for definitive for two main reasons:

(i) the interatomic potentials necessary for calculation of $\gamma(\boldsymbol{f})$ are not known with sufficient accuracy, especially for b.c.c. metals. Therefore, different model interatomic potentials were used in [8] and it was shown that they lead to different numerical values of $\gamma(\boldsymbol{f})$, however, to approximately the same shapes of the γ surface. Analogously, also the calculated force laws $\tau_0(f)$ can be expected to have correct shapes, however, inaccurate numerical values;

(ii) the used values $\tau_0 = -\mathrm{d}\gamma/\mathrm{d}f$ correspond to the forces per unit area between two half crystals displaced relatively in the $\boldsymbol{b}$ direction by constant f, with relaxation only in the direction perpendicular to the stacking fault plane. However, the disregistry f varies in the slip plane of a dislocation in the P.N. model. While the above definition of τ_0 can be taken as a good approximation at places where f varies slowly, it can only give a rough estimation of the force law at places where f varies quickly, i.e., especially in the core of narrow dislocations (see also discussion in [7]).

Therefore, the shapes of the theoretical force laws $\tau_0(f)$ should be taken as more reliable than their numerical values. From this point of view and in spite of the fact that the P.N. equation has been solved with a good accuracy, the calculated $f(x)$ dependences have to be taken only as an approximation for the studied crystal. Again, the shapes of the $f(x)$ and $\varrho(x)$ curves can be taken as more reliable than their numerical values. These shapes are sufficiently described by the number, positions and Burgers vectors of the partial dislocations.

3.3. Planar dislocation splitting in α-Fe

The stacking fault energies in b.c.c. metals seem to be very high so that, if the dislocations are split, the width of splitting is small and the partial dislocations overlap. In this case, the dislocation splitting can only be taken as a rough description of the dislocation core.

Different splittings of dislocations in b.c.c. metals have been proposed (for a review see e.g. [15]) based on the classical concept of singular partial dislocations connected by ribbons of stable stacking faults. However, stable stacking faults do not seem to exist in b.c.c. metals [8, 16]. This led to the proposal of the so called generalized splitting of dislocations in b.c.c. metals in [14]. The dislocation is assumed to be split into N singular partials generally with irrational Burgers vectors connected by ribbons of generalized, i.e., in general case instable stacking faults with constant disregistries. This model leads to the P.N. model for $N \to \infty$ [17].

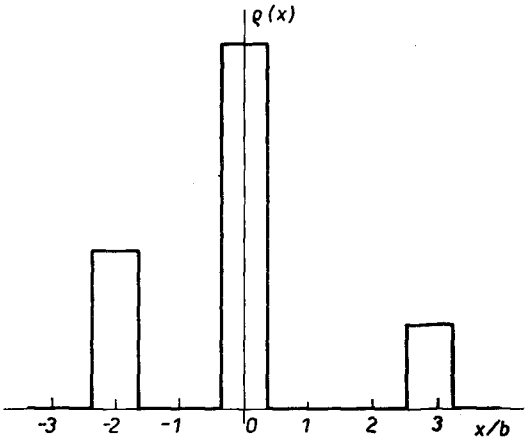


Fig. 6. Schematic generalized splitting of $\frac{1}{2}\langle 111\rangle$ edge dislocation on $\{112\}$ plane into 3 singular partials for γ surface based on potential J_0 (according to [14]) — an analogy of Fig. 2b.

The distribution of the dislocation density $\varrho(x)$ corresponding to the generalized splitting of an edge dislocation in α-Fe on $\{112\}$ plane from [14] is shown schematically in Fig. 6. It was proposed for the γ surface based on the J_0 potential and can be compared with $\varrho(x)$ in Fig. 2. Both splittings propose the same number of partials, $N = 3$, and approximately the same Burgers vectors ($\alpha_1 = 0{\cdot}20$, $\alpha_2 = 0{\cdot}64$, $\alpha_3 = 0{\cdot}16$ in Fig. 2, $\alpha_1 = 0{\cdot}26$, $\alpha_2 = 0{\cdot}60$, $\alpha_3 = 0{\cdot}14$ in Fig. 6), however, the widths of splitting in Fig. 6 are larger than in Fig. 2. If relaxation is allowed in Fig. 6, e.g., as further splitting of the partial dislocations then for $N \to \infty$ the $\varrho(x)$ curve should approach to that in Fig. 2.

It is seen from the comparison with the P.N. model that the concept of generalized splitting in [14] represents a better description of the dislocation core in b.c.c. metals than the classical splitting. However, its main simplification is in the assumption of constant disregistry between the singular partials. The above treatment of the P.N. model can be considered as a further step in generalization of the concept of dislocation splitting: the individual partials are taken as non singular dislocations of finite widths which mutually overlap.

The resulting $\varrho(x)$ curves are in good agreement with the planar cores calculated for edge dislocations in α-Fe from a three-dimensional atomic model using the same interatomic potentials J_0 and J_2, as discussed already in [7]. The present treatment can be, therefore, used to give an interpretation of the atomic model in terms of dislocation splitting.

The minimum energy splitting of $\frac{1}{2}\langle 111\rangle$ screw dislocation should have the threefold symmetry. The proposed planar cores of screw dislocation correspond to a metastable splitting with a higher energy which can be stabilized in an external stress field, transforming the dislocation from the sessile splitting into a glissile one.

The comparison of results obtained with different interatomic potentials, J_0 and J_2, i.e., with different force laws, on $\{112\}$ plane (Fig. 2, 3) and on $\{110\}$ plane (Fig. 4, 5) shows general similarities in the shape of the dislocation densities and in splitting into three partials, however, differences between the Burgers vectors of corresponding partials and differences in the distances between the partials, i.e., in the widths of splitting. These differences show the sensitivity of the results to the changes in the force law. A further improvement of the P.N. model for specific crystals depends mainly on the development of reliable interatomic potentials.

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