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The discrete correction of the core structure for the ⟨100⟩{010} edge dislocation in bcc Fe*

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Abstract

The core structure of the ⟨100⟩{010} edge dislocations in body-centered cubic (bcc) crystal Fe has been investigated by the modified Peierls–Nabarro (P–N) equation which includes the discrete correction. An analytical expression of the dislocation solution of the dislocation equation has been obtained by using the truncation approximation. It is found that the dislocation width is nearly doubled by the discrete effects and the agreement between the theoretical prediction and the numerical simulation is improved remarkably.

1. Introduction

It is widely accepted that defects such as dislocations play a key role in determining the mechanical properties of materials [1, 2]. A great deal of work has focused on studies of the core structure of dislocation because the dislocation core is significant to many phenomena and is the key to understand the dislocation properties [3, 4]. It is generally believed that besides the numerical calculation the P–N theory is the best for determining the dislocation core [1]. However, there are still some fundamental issues that need to be clarified in the P–N theory itself. One of the important issues is the lattice discrete effects. In the P–N theory, the crystal was treated approximately as an elastic continuum body and so the discrete effects were underestimated [5]. In particular, displacement varies so rapidly at the dislocation core that the Peierls equation should be modified in the region.

In this paper, the lattice discrete effect is taken into account in calculating the core structure of the ⟨100⟩{010} edge dislocation in bcc Fe. The contribution of the lattice effect can be described by a term proportional to the second order derivative of the displacement field. The new dislocation equation with the lattice discrete correction is referred to as the modified P–N equation. The results calculated from the modified P–N equation are compared with those obtained from the classical P–N equation and the numerical simulations. It is found that the core width is greatly broadened by the discrete effects, and our results agree well with the data from the numerical simulations. Therefore, in order to arrive at a precise prediction, it is necessary to include the lattice discrete correction and use the modified P–N equation in calculating the dislocation core structure.

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2. The modified P–N equation

The dislocation core structure in the bcc Fe attracts much attention of researchers because the dislocations in bcc Fe are various. The most simple type of dislocation is the ⟨100⟩{010} edge dislocation. Bullough and Perrin [6] and Gehlen *et al* [7] studied the ⟨100⟩{010} edge dislocation of bcc Fe based on the atomic simulations using the Johnson potential. Both their results show that the dislocation core is very narrow with a radius of between 1.25b and 1.65b (b is the Burgers vector). Chen *et al* established the core structure of the ⟨100⟩{010} edge dislocation by using the molecular dynamics simulation and the radius of the dislocation core they calculated is 1.67b [8]. In theory, Yan *et al* discussed the dislocation based on the P–N model by taking into account the generalized-stacking-fault (GSF) energy [9]. The effective core radius (half width) they calculated is between 0.85b and 0.93b. Obviously, the core radius they calculated is much smaller than those in numerical simulations. The reason may be that the lattice discrete effects were ignored incorrectly.

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The modified P–N equation due to the lattice discrete correction has been obtained firstly using the solvable models and derived later in a model-independent way [10]. In a strict way, the discrete effects are represented in the modified P–N equation by a second-differential term and an integral term with the integrand including the third-differential. However, the integral term is less important than the second-differential term. In fact, the discrete effects can be effectively represented by the second-differential term provided that the new coefficient is determined in a self-consistent way. For the ⟨100⟩{010} edge dislocation in bcc crystal Fe, which is shown in figure 1, the modified P–N equation containing the discrete correction takes the following form:

$$-\beta\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2}-\frac{\mu}{\pi(1-\nu)}\int_{-\infty}^{\infty}\frac{\frac{\mathrm{d}u^x}{\mathrm{d}x}|_{x=x'}}{x'-x}\,\mathrm{d}x'=f(u^x) \qquad (1)$$

where u^x is the relative displacements of the bilateral misfit planes along the slip direction ⟨100⟩, f is the nonlinear interaction that can be calculated from GSF energy, ν and μ are Poisson's ratio and shear modulus, respectively, β is a new parameter describing the lattice discrete effects.

The physical implication of the left-hand of the modified P–N equation can be understood in the following way. When the crystal is viewed as a set of planes parallel to the misfit plane, the misfit plane itself plays a distinct role compared with other planes. To see this more clearly, let us imagine a crystal with zero shear modulus. For such a crystal, the internal planes have no effects on the misfit plane on which the displacement field u is defined. The contribution comes only from the interaction among the atoms on the misfit plane. In this case, the integral term disappears and the second-differential term remains only in equation (1). Therefore, one can conclude that the second-differential term originates mainly from the interaction among the atoms on the misfit plane, while the integral term originates mainly from the interaction between the atoms on the misfit plane and atoms in the interior. In the long wavelength approximation, the force in a unit area attributed to the interaction of the atoms on the misfit plane is given by

$$\frac{mc_s^2}{a^2}\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2}, \qquad (2)$$

where the symmetry of the dislocation has been used, c_s is the wavevelocity of the misfit plane which is uncoupled from the other planes, m is the atom mass, a is the lattice constant. Therefore, it is reasonable to expected that

$$\beta\propto\frac{mc_s^2}{a^2}. \qquad (3)$$

Although the ratio may be dependent of the crystal structure, but considering the approximation accuracy in the dislocation calculation, it is assumed to be a constant. From the solvable model, it is known that the ratio constant equals 3/4.

The velocity c_s can be well expressed in terms of the bulk wavevelocity. It is observed that when the transverse wave propagates in the bulk crystal along a plane like (010), the velocity mainly depends on the coupling between the planes. So the coupling between planes can be removed by an operation of subtraction. In the present case, it is found

$$c_s^2\approx c_\mathrm{l}^2-c_\mathrm{t}^2, \qquad (4)$$

where c_l and c_t are the longitudinal and transverse wavevelocities. The velocities c_l and c_t can be expressed by the elastic constants [11]

$$c_\mathrm{l}^2=\frac{2\mu(1-\nu)}{\rho(1-2\nu)}, \qquad c_\mathrm{t}^2=\frac{\mu}{\rho},$$

where $\rho=\frac{m}{\Omega}$ is the mass density, $\Omega=\frac{a^3}{2}$ is the volume of the primitive cell. It is easy to obtain from equations (3) and (4)

$$\beta=\frac{3\mu\Omega}{4(1-2\nu)}, \qquad (5)$$

where isotropy has been assumed.

In the classical P–N model, the right-hand of equation (1) is given by the sinusoidal force law. The sinusoidal force law is a rough approximation for the real materials. A modification of the sinusoidal force law has been discussed in [12]

$$f=-\frac{\partial\gamma}{\partial u^x}, \qquad (6)$$

$$\gamma=\frac{\mu a^2}{2\pi^2 d}\sin^2\frac{\pi u^x}{a}\left(1+\Delta\sin^2\frac{\pi u^x}{a}\right), \qquad (7)$$

where $d=a/2$ is the spacing between the misfit planes, dimensionless parameter Δ describes the higher order correction in the Fourier series of the misfit energy. If $\Delta=0$, one recovers the sinusoidal force law. For the ⟨100⟩{010} edge dislocation in bcc Fe, Δ can be determined by the fitting of the GSF energy calculated numerically. The first-principles calculations of the GSF energy have been done in the spin-polarized local density approximation (LSDA) and the spin-polarized generalized gradient approximation (SGGA) [9].

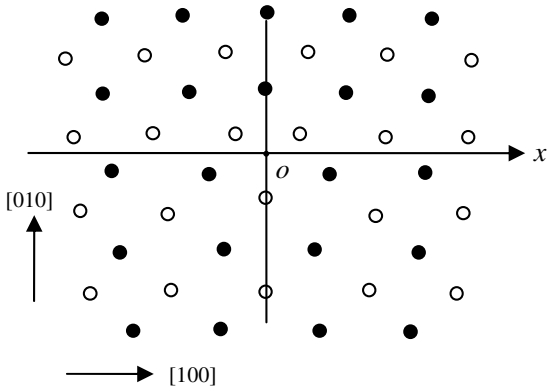

Figure 1. The configuration of the ⟨100⟩{010} edge dislocation in bcc Fe. The atoms represented by the solid circles and the empty circles are the vertex angle atoms and the body-centered atoms of bcc Fe. The horizontal line represented the cut plane which divides the lattice into an upper part and a lower part, the vertical line is the symmetry center. The cut plane is also the slip plane and the dislocation slips along the direction ⟨100⟩. The coordinate origin is at the center of the dislocation.

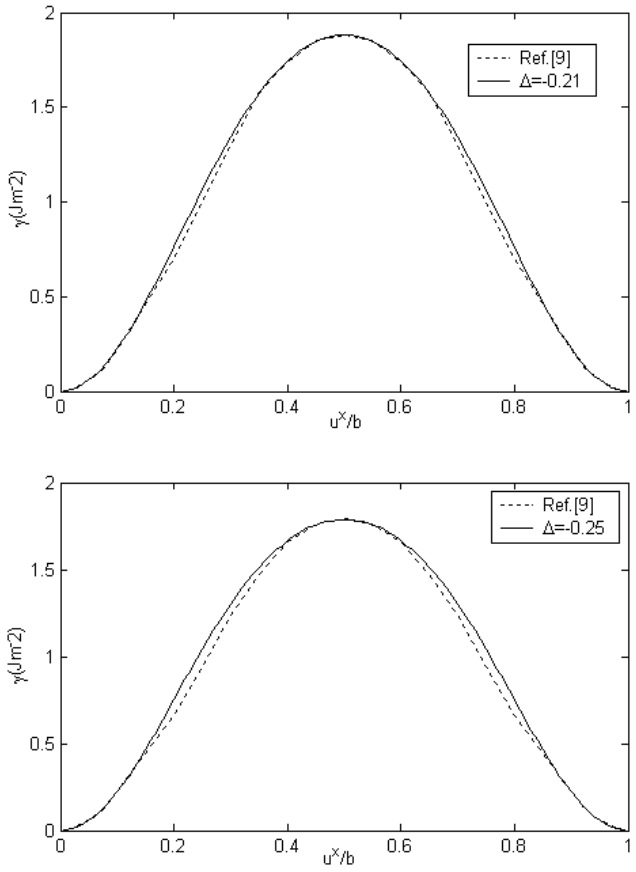

Figure 2. The fitting of the GSF energy. The solid lines and the dotted lines represent the GSF energies used in this paper and calculated in [9], respectively.

From figure 2, one sees that the numerical results can be well described by equation (7) and the parameter Δ is negative and varies in the range from -0.21 to -0.25 when different approximations are used.

The modified P–N equation can be solved by the truncating method given by one of the authors previously [13]. The solution is

$$u^x = \frac{a}{\pi}\left[\arctan p + \frac{(1-\varepsilon)p}{1+p^2}\right] + \frac{a}{2} \tag{8}$$

with

$$p = \kappa x, \qquad \kappa = \frac{2\varepsilon(1-\nu)}{d},$$

and ε is the root of the following algebraic equation

$$\Delta\left(1+\frac{3\varepsilon}{7}\right) - \frac{\varepsilon^2}{\varepsilon_0^2}\left(1-\frac{11\varepsilon}{16}\right) + (1-\varepsilon)^2 = 0, \tag{9}$$

where ε_0 is given by

$$\frac{1}{\varepsilon_0^2} = \frac{8\beta(1-\nu)^2}{\mu d}.$$

This solution is valid as long as the correction Δ is not large. The dimensionless parameter ε_0 only depends on the elastic properties and geometry structure. For the $\langle 100\rangle\{010\}$ edge

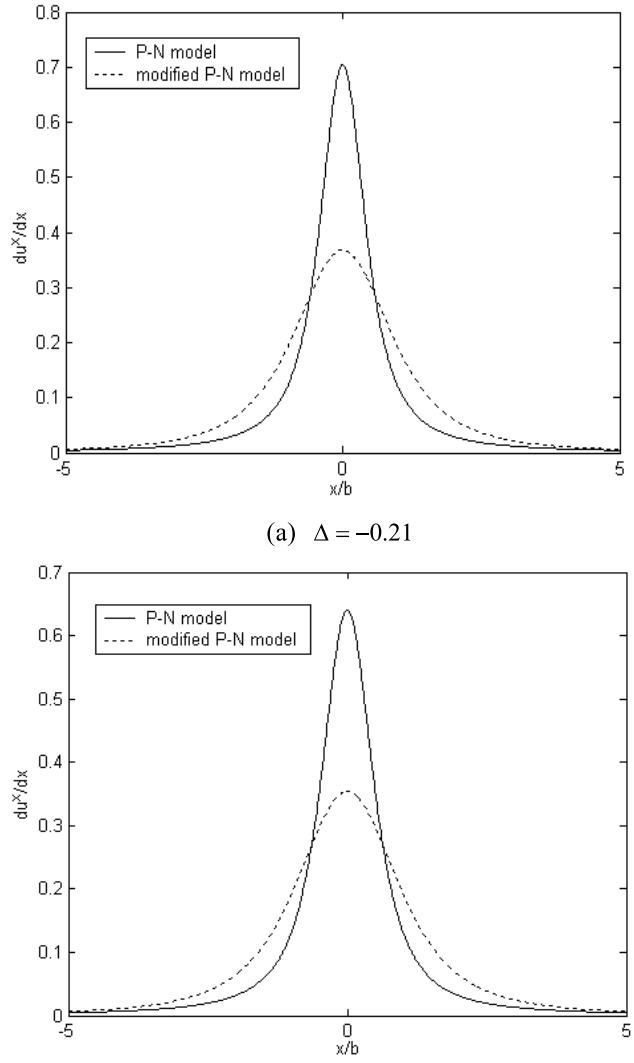

Figure 3. The dislocation densities of the $\langle 100\rangle\{010\}$ edge dislocations in bcc Fe.

dislocation in bcc Fe, $\varepsilon_0 = 0.37$, and $\varepsilon = 0.24$ if $\Delta = -0.21$, $\varepsilon = 0.23$ if $\Delta = -0.25$. The dislocation densities have been plotted for $\Delta = -0.21$ and $\Delta = -0.25$ in figure 3. Obviously, the modified dislocation core is much wider than that given by the P–N equation. In figure 4, the structure factor ε has been plotted as a function of ε_0 and Δ, which is given by equation (9). For the positive Δ, ε increases linearly with ε_0. For negative Δ, ε increases nonlinearly, but slowly.

In order to compare our results quantitatively with the results obtained previously, the half width of the $\langle 100\rangle\{010\}$ edge dislocation, defined as the atomic distance over which u^x changes from $a/4$ to $3a/4$, has been calculated. The results are summarized in table 1. It is shown that if the discrete correction is neglected, our results are very close to that obtained by Yan *et al* [9]. However, having taken into account the lattice discrete correction, the corresponding core width is nearly doubled. This indicates that the discrete correction is important. The half width obtained from the modified P–N theory is about 1.5–1.6b, which agrees with 1.25–1.65b [7] and

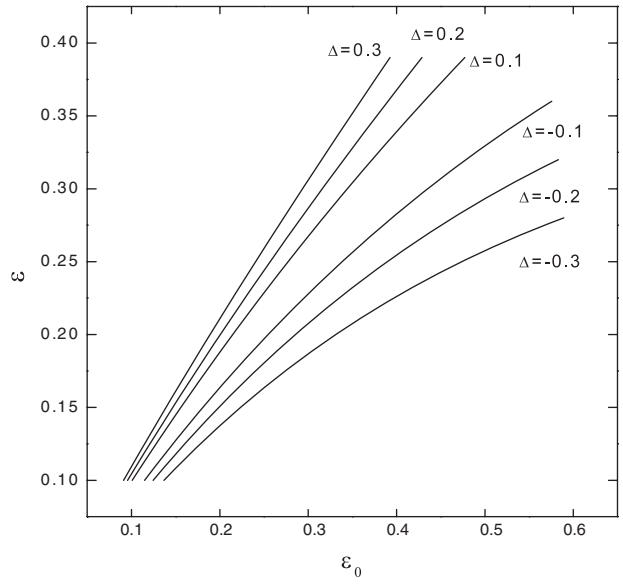

Figure 4. The relations between ε and ε_0 for different Δ.

Table 1. The half width of the dislocation core in units of the Burgers vector $b = a$.

	$\Delta = -0.21$	$\Delta = -0.25$
P–N	0.88, 0.85 [9]	0.94, 0.93 [9]
Modified P–N	1.51	1.57
Numerical simulation	1.25 − 1.65 [7], 1.67 [8]	

1.67b [8] obtained from numerical simulations. This indicates that the modified P–N equation can provide a quantitative prediction with a satisfactory accuracy.

In summary, the core of the ⟨100⟩{010} edge dislocation in bcc Fe has been calculated by using the modified P–N equation which contains the lattice discrete correction. The results agree well with those obtained from numerical simulations. The problem of it being too narrow to fit the numerical results, which exists in the P–N model, has been removed automatically. Therefore, the P–N equation should be modified by taking the lattice correction into account. Although the ⟨100⟩{010} edge dislocation in Fe is a concrete dislocation that is not very active in bcc crystal, our conclusions are valid for other dislocations and are significant for the dislocation theory. A detailed investigation of the influence of the discrete correction on other dislocations like ⟨111⟩{110} will be presented in the future.

References

[1] Hirth J P and Lothe J 1982 *Theory of Dislocations* 2nd edn (New York: Wiley)
[2] Schoeck G 2005 *Mater. Sci. Eng.* A **400** 7–17
[3] Duesbery M S and Richardsom G Y 1991 *CRC Crit. Rev. Solid State Mater. Sci.* **17** 1
[4] Vitek V 1992 *Prog. Mater. Sci.* **36** 1
[5] Peierls R E 1940 *Proc. Phys. Soc.* **52** 23
[6] Bullough R and Perrin R C 1967 *Rept. Theoret. Phys. Div.* Didoct Berks, AERR Harwell, p 175
[7] Gehlen P C, Rosenfield A R and Hahn G T 1968 *Appl. Phys.* **39** 5246
[8] Chen L Q, Wang C Y and Yu T 2006 *Acta Phys. Sin.* **55** 5890
[9] Yan J A, Wang C Y and Wang S Y 2004 *Phys. Rev.* B **70** 174105
[10] Wang S F 2002 *Phys. Rev.* B **65** 094111
Wang S F 2008 *J. Phys. A: Math. Theor.* **41** 015005
[11] Landau L D and Lifshitz E M 1986 *Theory of Elasticity* 3rd edn (Singapore: Butterworth-Heinemann) p 88
[12] Wang S F, Wu X Z and Wang Y F 2007 *Phys. Scr.* **76** 593
[13] Wang S F 2003 *Phys. Lett.* A **313** 408