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Dislocation energy and Peierls stress: a rigorous calculation from the lattice theory*

Wang Shao-Feng(王少峰)†

Institute for Structure and Function, Chongqing University, Chongqing 400044, *China*

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In the classical Peierls–Nabarro (P-N) theory of dislocation, there is a long-standing contradiction that the stable configuration of dislocation has maximum energy rather than minimum energy. In this paper, the dislocation energy is calculated rigorously in the context of the full lattice theory. It is found that besides the misfit energy considered in the classical P-N theory, there is an extra elastic strain energy that is also associated with the discreteness of lattice. The contradiction can be automatically removed provided that the elastic strain energy associated with the discreteness is taken into account. This elastic strain energy is very important because its magnitude is larger than the misfit energy, its sign is opposite to the misfit energy. Since the elastic strain energy and misfit energy associated with discreteness cancel each other, and the width of dislocation becomes wide in the lattice theory, the Peierls energy, which measures the height of the effective potential barrier, becomes much smaller than that given in the classical P-N theory. The results calculated here agree with experimental data. Furthermore, based on the results obtained, a useful formula of the Peierls stress is proposed to fully include the discreteness effects.

Keywords: dislocation energy, Peierls stress, lattice theory
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1. Introduction

For the dislocation theory, a fundamental problem is the dislocation mobility that is directly related to the plastic property of materials. Due to discreteness of lattice, a dislocation cannot move unless the applied stress exceeds a critical value. This critical value of the stress is generally named as Peierls stress or Peierls–Nabarro (P-N) stress. Even though the Peierls stress can be obtained for real materials through numerical calculations, such as atomistic simulation or electron-density functional technique, our knowledge on the relation between Peierls stress and lattice characteristics mainly comes from the analytical or semi-analytical results given in the P-N formalism.[1−7] In the classical P-N theory, the Peierls stress was obtained by calculating the misfit energy associated with the discreteness of lattice. There are continuous efforts to improve the understanding of the misfit energy and Peierls stress.[4,5,8,9] However, a long-standing contradiction that the stable configuration of dislocation has maximum energy rather than minimum energy has not been settled in the research on the subject. The contradiction must be removed to make the dislocation theory self-consistent. The issue of where the contradiction results from and how to remove it must be addressed thoroughly.

In this paper, the dislocation energy is calculated rigorously in the context of the lattice theory that has been presented recently.[10−12] It is found that the dislocation energy can be divided into two parts: one part is independent of the discreteness of the lattice and divergent for an infinite lattice; another part is associated with the discreteness of the lattice. The part associated with discreteness consists of misfit energy and elastic strain energy. The misfit energy comes from the interaction between the half-crystals. The elastic strain energy[13] comes from deformation of the half-crystals. The change of the elastic strain energy with the position of the dislocation has been mentioned before. But it is generally considered to be negligible. In the classical P-N theory, the elastic strain energy is a constant since the half-crystals were simplified as elastic continuum. Thus, as the dislocation moves through the crystal, the entire variation of the energy is only attributed to the change in the misfit energy. Actu-

*Project supported by the National Natural Science Foundation of China (Grant No 10274057).
†E-mail: sfwang@cqu.edu.cn

ally, in the classical P-N theory the relation between the energy and the position of the dislocation is obtained in such an ad hoc way[8] that it is not clear how to incorporate the elastic strain energy associated with discreteness. In the lattice theory of dislocation, the discreteness of crystals is considered completely. One can clearly calculate the elastic strain energy as well as the misfit energy associated with discreteness. The results calculated show that if only the misfit energy is considered, one recovers the result given in the classical P-N theory. But, in this case the stable configuration of the dislocation has a maximum energy rather than a minimum energy. This is a serious contradiction that should not exist in a self-consistent theory. Fortunately, it is found that if both the misfit and elastic strain energies are taken into account, the stable configuration of dislocation takes a minimum energy, and so the contradiction is naturally removed. In contrast to the traditional opinion, the elastic strain energy associated with the discreteness is larger than the misfit energy in magnitude. The contribution of the elastic strain energy is opposite to that of the misfit energy. While the elastic strain energy makes the dislocation energy increase, the misfit energy makes the dislocation energy decrease. Because the elastic and misfit energies cancel each other, the total energy associated with discreteness is much smaller than that given in the classical P-N theory. As a consequence, the Peierls stress will be greatly lowered in the lattice theory. This conclusion provides a qualitative explanation to the fact that theoretical prediction in the classical P-N theory is frequently much larger than the experimental data.

2. A brief discussion on the dislocation energy and Peierls stress

Due to the periodicity of crystal, the dislocation energy changes periodically as the dislocation moves through the lattice

$$E(x+b) = E(x),$$

where coordinates is chosen so that the x-axes is parallel to the glide direction, b is period of the lattice in the gliding direction. As a periodic function, the dislocation energy can be expanded in the Fourier series. Generally, the series is truncated to be

$$E(x) = E_0 + \frac{1}{2}E_{\rm p}\cos\frac{2\pi x}{b}, \qquad (1)$$

where E_0 is a constant that diverges for an infinite lattice, $E_{\rm p}$ is referred to as Peierls energy. The Peierls energy $E_{\rm p}$ originates from the discreteness of lattice. The magnitude of $E_{\rm p}$ represents the height of barrier that blocks the dislocation moving. The Peierls stress $\sigma_{\rm p}$ is given by[8]

$$\sigma_{\rm p} = \max\left|\frac{1}{b}\frac{{\rm d}E_{\rm p}(x)}{{\rm d}x}\right|.$$

Within the approximation of Eq.(1), one has

$$\sigma_{\rm p} = \frac{\pi|E_{\rm p}|}{b^2}.$$

For a free crystal there are two equilibrium configurations of dislocation. One of them has minimum energy $E_{\rm min} = E_0 - |E_{\rm p}|/2$, the other has maximum energy $E_{\rm max} = E_0 + |E_{\rm p}|/2$. The dislocation changes its configuration continuously from one to the other while travelling through the crystal under the applied stress. Therefore, the energy of the moving dislocation oscillates between the minimum and maximum energies. A static dislocation with minimum energy is stable, and so can be observed in experiments. It is the convention to choose the center of the stable configuration to be the origin of the coordinate, $x = 0$. As soon as this convention is used, the energy $E_{\rm p}$ in Eq.(1) must be negative to guarantee the energy function Eq.(1) takes minimum at the origin, $E(x=0) = E_0 + E_{\rm p}/2 = E_{\rm min}$. The energy $E_{\rm p}$ will be calculated explicitly below for the two-dimensional triangular lattice. The calculated results show that the contribution of misfit energy to the $E_{\rm p}$ is positive, the contribution of elastic strain energy to the $E_{\rm p}$ is negative, and the sum of them is always negative as required in a self-consistent theory. Therefore, if the misfit energy is considered only, there will be a contradiction that stable dislocation has a maximum energy rather than a minimum energy. If the both misfit and elastic energy associated with discreteness are taken into account, there will exist no contradiction.

The crystal with dislocation in it can be viewed as two half-infinite crystals glued together along the glide plane in a nontrivial way. The Hamiltonian is composed of three terms

$$H = H_{\rm above} + H_{\rm below} + H_{\rm int},$$

where $H_{\rm above}(H_{\rm below})$ is the Hamiltonian of the half-infinite crystal above (below) the glide plane, $H_{\rm int}$ stands for the interaction between two half crystals concerned. Usually, each half-infinite crystal is approximated as a harmonic one in which atoms interact

with a harmonic force. In order to obtain a compact $H_{\rm int}$, it is generally assumed that for an individual atom in a given half-crystal the other half-crystal looks like a perfect crystal just having slipped globally in a certain way. That is to say, every atom on the border feels the same periodic potential ϕ except for a phase factor. In this approximation, the interaction energy can be written as

$$H_{\rm int} = \sum_{\boldsymbol{R}} \phi[\boldsymbol{u}_{\rm above}(\boldsymbol{R}) - \boldsymbol{u}_{\rm below}(\boldsymbol{R})], \qquad (2)$$

where $\mathbf{u}_{\rm above}$ ($\mathbf{u}_{\rm below}$) is the displacement of atoms on the border of the half-infinite crystal above (below) the glide plane, the summation runs over either of two borders. Obviously, neither the treatment of the nonlinear region as a thin strip only including border atoms, nor the way of description of the interaction as a local one is a realistic one. However, it has an advantage in yielding analytical results and revealing fundamental relations. The periodic potential ϕ can be expanded in the Fourier series. If two leading terms is kept only and the elastic limit is required to be recovered, one has

$$\begin{aligned}&\phi(u^x_{\rm above} - u^x_{\rm below})\\ =&\frac{\mu b^3}{4\pi^2 d}\left[1 + \cos\frac{2\pi(u^x_{\rm above} - u^x_{\rm below})}{b}\right],\end{aligned} \qquad (3)$$

where μ is the shear module, d is the spacing between the two borders. Note that the numerical factor is $1/4$, instead of $1/8$ given frequently in the classical Peierls theory where the summation runs over both upper and lower borders. The potential obtained is in the sinusoidal-force law

$$f^x(u^x) = \frac{\mu b^2}{2\pi d}\sin\left(\frac{4\pi u^x}{b}\right), \qquad (4)$$

where $u^x_{\rm above} = -u^x_{\rm below} = u^x$ has been used.

3. Calculation for a dislocation in the triangular lattice

Recently, we have developed a method to solve boundary problem of the half-infinite lattice. By virtue of the solution obtained in the boundary problem, a set of dislocation equations have been derived explicitly for the two-dimensional triangular lattice. The dislocation equations are only related to displacements of the atoms on the border. Because the displacement field of a dislocation varies slowly in the space, the discrete dislocation equations can be changed into the following integro–differential equations:[12]

$$\begin{aligned}&-\beta b^2\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2} - \eta_1 b\frac{\mathrm{d}u^y}{\mathrm{d}x} - \frac{\mu b\eta}{\pi}\int_{-\infty}^{\infty}\frac{\frac{\mathrm{d}u^x}{\mathrm{d}x}|_{x=x'}}{x'-x}\mathrm{d}x'\\ &= f^x(x),\end{aligned} \qquad (5)$$

$$\eta_1\frac{\mathrm{d}u^x}{\mathrm{d}x} - \frac{\eta_2}{\pi}\int_{-\infty}^{\infty}\frac{\frac{\mathrm{d}u^y}{\mathrm{d}x}|_{x=x'}}{x'-x}\mathrm{d}x' = 0, \qquad (6)$$

where u^x (u^y) is the displacement parallel (perpendicular) to the glide direction; the force component $f^x(x)$ felt by the border atom located at position x is given by the sinusoidal-force law Eq.(4); β, η, η_1 and η_2 are characteristic parameters of the lattice. Using the Hilbert transformation, from Eq.(6) one has

$$\frac{\mathrm{d}u^y}{\mathrm{d}x} = -\frac{\eta_1}{\pi\eta_2}\int_{-\infty}^{\infty}\frac{\frac{\mathrm{d}u^x}{\mathrm{d}x}|_{x=x'}}{x'-x}\mathrm{d}x'. \qquad (7)$$

Substituting Eq.(7) into Eq.(5), one obtains the modified Peierls equation

$$\begin{aligned}&-\beta b^2\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2} - \frac{\mu b}{\pi(1-\nu)}\int_{-\infty}^{\infty}\frac{\frac{\mathrm{d}u^x}{\mathrm{d}x}|_{x=x'}}{x'-x}\mathrm{d}x'\\ =&f^x(x),\end{aligned} \qquad (8)$$

where the condition that the Peierls equation should be recovered in the slow varying limit has been used, ν is the Poisson ratio

$$\frac{1}{1-\nu} = \eta - \frac{\eta_1^2}{\eta_2}.$$

Equation (8) can be viewed as a generalization of the Peierls equation. In the classical P-N theory, the first term in Eq.(8) was missing due to continuum approximation for the crystal.

It is not easy to thoroughly understand the physical meaning of the parameters appearing in the equations. In particular, the new parameter β originating from the discreteness of the lattice has no correspondence in the elastic continuum theory. In order to understand its implication better, it is needed to study the dislocation equation for different types of lattice. For the case of the triangular lattice in which atoms interacted with the nearest neighbours through central harmonic force[10], the parameters are given by

$$d = \frac{\sqrt{3}}{2}b, \qquad \nu = 1/4,$$

$$\mu = \frac{\alpha d}{2b}, \qquad \beta \simeq \frac{3}{4}\alpha,$$

where α is the harmonic interaction constant.

The dislocation equations (5) and (6) are nonlinear integro-differential equations. It can hardly be solved exactly. In Ref.[11] a systematic method was put forward to obtain approximate solution. By using the method, for arbitrary parameters given in Eqs.(5) and (6) the solution is obtained

$$u^x = \frac{b}{2\pi}\left[\arctan q + \frac{cq}{1+q^2}\right],$$

$$u^y = \frac{(1-2\nu)b}{4\pi(1-\nu)}\left[\ln(1+q^2) - \frac{2c}{1+q^2}\right], \qquad (9)$$

where

$$q = \kappa x, \qquad \kappa = \kappa_0(1-c), \qquad \kappa_0 = \frac{2(1-\nu)}{d},$$

and $c = 1-\epsilon$, ϵ is given by the root of the following algebra equation

$$\frac{\beta b(1-\nu)^2}{\mu d}(16-11\epsilon)\epsilon^2 + \frac{25}{6}\epsilon - 2 = 0.$$

Because ϵ is usually small, the algebra equation can be solved through iteration. In fact, it is easy to verify that the root can be well approximated by

$$\epsilon = \epsilon_0 - \frac{67}{96}\epsilon_0^2, \qquad \epsilon_0 = \frac{1}{2(1-\nu)}\sqrt{\frac{\mu d}{2\beta b}}, \qquad (10)$$

for $0 < \epsilon_0 < 0.7$. It is worth to point out that the dislocation solution Eq.(9) is a robust one, i.e. the solution almost does not change its form when a different force law is adopted. Like $1/\kappa_0$ in the classical P-N theory, the reciprocal $1/\kappa$ is interpreted as a characteristic width of the dislocation. For the triangular lattice,

$$\kappa_0 = \frac{\sqrt{3}}{b}, \qquad \epsilon_0 = \frac{1}{3}, \qquad c = 0.744, \qquad \kappa \simeq \frac{\kappa_0}{4}.$$

We see that the width of the dislocation is about four times as large as that given in the classical P-N model.

With the dislocation solution, we are ready for calculation of the dislocation energy and Peierls stress. In order to simplify the calculation, a useful theorem is presented in the following.

Theorem. If the Hamiltonian of a many-particle system is homogeneous

$$H(\lambda \boldsymbol{u}_1, \lambda \boldsymbol{u}_2, \cdots) = \lambda^j H(\boldsymbol{u}_1, \boldsymbol{u}_2, \cdots), \qquad (11)$$

then in equilibrium, the interaction potential energy of the system can be obtained by

$$H = \frac{1}{j}\sum_i \boldsymbol{f}_i \cdot \boldsymbol{u}_i, \qquad (12)$$

where $\boldsymbol{u}_i$ is the coordinate of the particle i, $\boldsymbol{f}_i$ is the external force imposed on the particle i.

The proof of the theorem is simple. For the atom i, the internal force from the interaction among the atoms is given by $-\dfrac{\delta H}{\delta \boldsymbol{u}_i}$. In the equilibrium, the internal force must be balanced by the external force $\boldsymbol{f}_i$

$$-\frac{\delta H}{\delta \boldsymbol{u}_i} + \boldsymbol{f}_i = 0.$$

Taking differential for Eq.(11) about λ, and then let $\lambda = 1$, one has the identity

$$H = \frac{1}{j}\sum_i \frac{\delta H}{\delta \boldsymbol{u}_i}\cdot \boldsymbol{u}_i.$$

Using the balance equation, one immediately arrives at the conclusion of the theorem. For the system with the harmonic interaction, one has $j = 2$.

The dislocation energy is obtained by substituting the solution into the Hamiltonian. There are three terms

$$E_{\rm dis} = E_{\rm above} + E_{\rm below} + E_{\rm int},$$

where $E_{\rm above} = H_{\rm above}|_{u\to{\rm solution}}$ ($E_{\rm below} = H_{\rm below}|_{u\to{\rm solution}}$) is the elastic strain energy of the half crystal above (below) the glide plane, $E_{\rm int} = H_{\rm int}|_{u\to{\rm solution}}$ is called the misfit energy. The evaluation of $E_{\rm above}$ and $E_{\rm below}$ can be simplified by using the above theorem where $\boldsymbol{f}_i$ now is the interaction force between two half-infinite crystals, and the summation runs over either border. Besides, it can be easily proven that

$$E_{\rm above} = E_{\rm below}.$$

Thus, the elastic strain energy of the two half-infinite crystals can be written as

$$E_{\rm elastic} = E_{\rm above} + E_{\rm below} = \sum_\ell f^x(u_\ell^x)u_\ell^x,$$

and the total energy of dislocation is given by

$$E_{\rm dis} = \sum_\ell \frac{\mu b^3}{4\pi^2 d}\left[1+\cos\frac{4\pi u_\ell^x}{b}\right] + \sum_\ell \frac{\mu b^2}{2\pi d}u_\ell^x \sin\left(\frac{4\pi u_\ell^x}{b}\right). \qquad (13)$$

The first sum in Eq.(13) represents the misfit energy, the second sum represents the elastic strain energy. Let

$$\theta_\ell = \frac{2\pi u_\ell^x}{b}.$$

After arrangement, one obtains

$$E_{\rm dis} = \frac{\mu b^3}{2\pi^2 d} \sum_{\ell=-\infty}^{\infty} (\theta_\ell \sin\theta_\ell + \cos\theta_\ell)\cos\theta_\ell. \qquad (14)$$

As is done usually, with an addition of dislocation translation, the energy depends on the position of the dislocation.[8] By means of Poisson's summation formula, as a function of the position x, the dislocation energy can be expressed as

$$E_{\rm dis}(x) = \frac{\mu b^2}{2\kappa\pi d} \sum_{n=-\infty}^{\infty} A(n\xi) {\rm e}^{-{\rm i}n(\frac{2\pi x}{b} - {\rm i}\xi)}, \qquad (15)$$

$$A(n\xi) = \frac{{\rm e}^{n\xi}}{\pi} \int_{-\infty}^{\infty} (\theta\sin\theta + \cos\theta)\cos\theta {\rm e}^{{\rm i}n\xi q} {\rm d}q,$$
$$n = 0, \pm 1, \pm 2, \pm 3, \cdots \qquad (16)$$

with

$$\xi = \frac{2\pi}{\kappa b}.$$

$A(0)$ is a divergent constant, $A(n\xi)$ with $n \neq 0$ gives the correction related to the discreteness of the crystal. Because $A(n\xi)$ is generally negligible for $n > 1$, one obtains

$$E_{\rm dis} = \frac{\mu b^2}{2\kappa\pi d} A(0) + \frac{\mu b^2}{\kappa\pi d} A(\xi) {\rm e}^{-\xi} \cos(\frac{2\pi x}{b}). \qquad (17)$$

The dislocation energy given by Eq.(17) possesses the same form as Eq.(1) obtained by a general consideration. The constant energy E_0 and the Peierls energy $E_{\rm p}$ now can be identified to be

$$E_0 = \frac{\mu b^2}{2\kappa\pi d} A(0),$$

$$E_{\rm p} = \frac{2\mu b^2}{\kappa\pi d} A(\xi) {\rm e}^{-\xi}, \qquad (18)$$

and the Peierls stress is given by

$$\frac{\sigma_{\rm p}}{\sigma_{\rm m}} = \frac{4\pi}{\kappa b} |A(\xi)| {\rm e}^{-\xi} = 2\xi |A(\xi)| {\rm e}^{-\xi}, \qquad (19)$$

with

$$\sigma_{\rm m} = \frac{\mu b}{2\pi d}.$$

Similar to the energy, the quantity $A(\xi)$ consists of two parts: one is the misfit part $A_{\rm misfit}$ that results from the interaction between two half-infinite crystals, and another is the elastic part $A_{\rm elastic}$ that results from the deformation of the half-infinite crystals.

Before explicit calculation using the lattice solution, it is instructive to calculate firstly the Peierls energy using old Peierls solution that can be obtained by taking $c = 0$ in the lattice solution Eq.(9). For the old Peierls solution, $\kappa = \kappa_0$, $\theta_\ell = \arctan q_\ell$, $A(\xi)$ can be calculated exactly. The contribution to $E_{\rm P}$ from the misfit energy is

$$E_{\rm P}^{\rm misfit} = \frac{\mu b^2}{\kappa\pi d} {\rm e}^{-\xi}. \qquad (20)$$

If only this part of energy is considered, the resulting Peierls stress is

$$\sigma_{\rm p} = \frac{\mu}{2(1-\nu)} {\rm e}^{-\frac{\pi d}{(1-\nu)b}}, \qquad (21)$$

which agrees with that obtained by Huntington and Wang.[4,5] The contribution to $E_{\rm P}$ from the elastic energy is

$$E_{\rm P}^{\rm elastic} = -\frac{\mu b^2}{2\kappa\pi d} {\rm e}^{-\xi} [e_{\rm c} + \ln(2\xi) - {\rm e}^{2\xi}\Gamma(0, 2\xi)], \qquad (22)$$

where $e_{\rm c} = 0.577215\cdots$ is Euler constant, and function Γ is defined as

$$\Gamma(0, 2\xi) = \int_{2\xi}^{\infty} \frac{{\rm e}^{-t}}{t} {\rm d}t.$$

Γ is small for $\xi \gg 1$. It is easy to see that elastic strain energy associated with discreteness is negative, $E_{\rm P}^{\rm elastic} < 0$, and the misfit energy is positive, $E_{\rm P}^{\rm misfit} > 0$. Furthermore, provided that $\xi > 2.5$, the Peierls energy given by the sum of them is negative:

$$E_{\rm P} = E_{\rm P}^{\rm misfit} + E_{\rm P}^{\rm elastic} < 0.$$

Apparently, for the physically meaningful region, $\nu \sim 1/3$, $d \sim b$, the Peierls energy is always negative. By the way, there is a minimum of the total energy at $\xi = 3.6$, which no longer exists in the lattice theory (Figs.1 and 2). The Peierls stress resulting from $E_{\rm p}$ is given by

$$\frac{\sigma_{\rm p}}{\sigma_{\rm m}} = \frac{4\pi}{\kappa_0 b} \left[1 - \frac{1}{2}\left(e_{\rm c} + \ln\frac{4\pi}{\kappa_0 b}\right)\right] {\rm e}^{-\frac{2\pi}{\kappa_0 b}}, \qquad (23)$$

which is similar to that given in the original Peierls paper.[1]

In the classical P-N theory, the Peierls solution describes the stable configuration of the dislocation located statically at the origin. So its energy must be minimum. If the dislocation moves under an applied stress, the energy of the dislocation should increase. However, as shown above, if the misfit energy is considered only, $E_{\rm P}$ will be positive, and the energy of dislocation decreases as the dislocation leaves the origin. The energy of the stable configuration of the dislocation is a maximum rather than a minimum. This

serious contradiction existed a long time in the classical P-N theory. Now, it is clear that the contradiction results from neglecting the elastic strain energy associated with discreteness. If the elastic strain energy as well as the misfit energy associated with discreteness is taken into account, the contradiction will be naturally removed. In fact, the magnitudes of the elastic strain energy and the misfit energy are in the same order, neither of them can be neglected.

To confirm the assertion reached from the old Peierls solution, let us investigate the energy of the dislocation solution in the lattice theory. For the lattice solution Eq.(9), it is hard to have an analytical expression as simple as Eq.(23). Because the integrand oscillates rapidly and decays slowly, it is even not easy to evaluate numerically. By observing that the parameter c in the solutions varies in the region $0 < c < 1$, $A(\xi)$ can be calculated by the method of power-series expansion. In order to gain sufficient accuracy, one has to keep high-order terms in the power series. The calculating process is long and arduous. It is omitted here. The final result is very long:

$$A = A_{\text{elastic}} + A_{\text{misfit}}, \tag{24}$$

$$A_{\text{elastic}} = \sum_{n=1}^{7} \left(t_n J_n + \frac{1}{2} s_n L_n \right),$$

$$A_{\text{misfit}} = \frac{1}{2} \sum_{n=1}^{6} m_n L_n,$$

where

$$J_1 = -\frac{1}{2}[(e_{\text{c}} + \ln 2\xi) - \mathrm{e}^{2\xi}\Gamma(0, 2\xi)],$$

$$J_n = K_{n-1} - \frac{\xi}{4(n-1)}[(e_{\text{c}} + \ln 2\xi)L_{n-1}(\xi) + \mathrm{e}^{2\xi}\Gamma(0, 2\xi)L_{n-1}(-\xi)], \quad n = 2, 3, 4, \cdots$$

$$L_1 = 1,$$

$$L_2 = \frac{1}{2}(1 + \xi),$$

$$L_3 = \frac{1}{8}(3 + 3\xi + \xi^2),$$

$$L_4 = \frac{1}{48}(15 + 15\xi + 6\xi^2 + \xi^3),$$

$$L_5 = \frac{1}{384}(105 + 105\xi + 45\xi^2 + 10\xi^3 + \xi^4),$$

$$L_6 = \frac{1}{3840}(945 + 945\xi + 420\xi^2 + 105\xi^3 + 15\xi^4 + \xi^5),$$

$$L_7 = \frac{1}{46080}(103951 + 10395\xi + 4725\xi^2 + 1260\xi^3 + 210\xi^4 + 21\xi^5 + \xi^6),$$

$$K_1 = \frac{1}{4}(1 + \xi),$$

$$K_2 = \frac{1}{32}(3 + 3\xi + 3\xi^2),$$

$$K_3 = \frac{1}{576}(30 + 30\xi + 39\xi^2 + 11\xi^3),$$

$$K_4 = \frac{1}{9216}(315 + 315\xi + 435\xi^2 + 150\xi^3 + 25\xi^4),$$

$$K_5 = \frac{1}{460800}(11340 + 11340\xi + 16065\xi^2 + 5985\xi^3 + 1430\xi^4 + 137\xi^5),$$

Table 1. Coefficients in the expression of $A(\xi)$.

n	t_n	s_n	m_n
1	$1-c$	$2c\,(1-c)$	$2\,(1-c)^2$
2	$2c\left(1-c+\frac{c^2}{3}\right)$	$c\left(-2+6c-4c^2+\frac{4c^3}{3}\right)$	$2c\left(2-3c+\frac{4}{3}c^2-\frac{c^3}{3}\right)$
3	$2c^2\left(1-c+\frac{c^2}{3}-\frac{c^3}{15}\right)$	$4c^2\left(-1+2c-\frac{4c^2}{3}+\frac{c^3}{3}-\frac{c^4}{15}\right)$	$4c^2\left(1-\frac{4}{3}c+\frac{2c^2}{3}-\frac{2c^3}{15}\right)$
4	$\frac{4}{3}c^3\left(1-c+\frac{2c^2}{5}\right)$	$4c^3\left(-1+\frac{5}{3}c-c^2+\frac{c^3}{3}\right)$	$2c^3\left(\frac{4}{3}-\frac{5}{3}c+\frac{4c^2}{5}\right)$
5	$\frac{2}{3}c^4\,(1-c)$	$4c^4\left(-\frac{2}{3}+c-\frac{3}{5}c^2\right)$	$4c^4\left(\frac{1}{3}-\frac{2}{5}c\right)$
6	$\frac{4}{15}c^5$	$4c^5\left(-\frac{1}{3}+\frac{7}{15}c\right)$	$\frac{8}{15}c^5$
7	0	$-\frac{8}{15}c^6$	0

coefficients $t_{\rm n}, s_{\rm n}$ and $m_{\rm n}$ are given in Table 1. Indeed, this is not a useful expression in practice. However, after several failures in attempting to make improvement, we have to accept this uncomfortable expression. Its correctness has been confirmed by numerical calculation. Substituting $A(\xi)$ into Eq.(18), one obtains the Peierls energy

$$\frac{E_{\rm p}}{\phi_{\rm m}} = 2\xi A(\xi)\mathrm{e}^{-\xi}, \tag{25}$$

where

$$\phi_{\rm m} = \frac{\mu b^3}{2\pi^2 d}$$

is the amplitude of the pair interaction potential given by Eq.(3). The expression of the Peierls energy in units of $\phi_{\rm m}$ is the same as the Peierls stress in units of $\sigma_{\rm m}$ apart from a minus sign. The Peierls energy $E_{\rm p}/\phi_{\rm m}$ as a function of dimensionless variables ϵ_0 and $\kappa_0 b$ is shown In Figs.1 and 2 typically. Bearing an analogy to the case of the old Peierls solution, the part of energy from elastic deformation is negative and the part of energy from misfit gluing is positive. As expected for a self-consistent physical theory, the Peierls energy $E_{\rm P}$ is negative, and so the stable configuration of dislocations has a minimum energy.

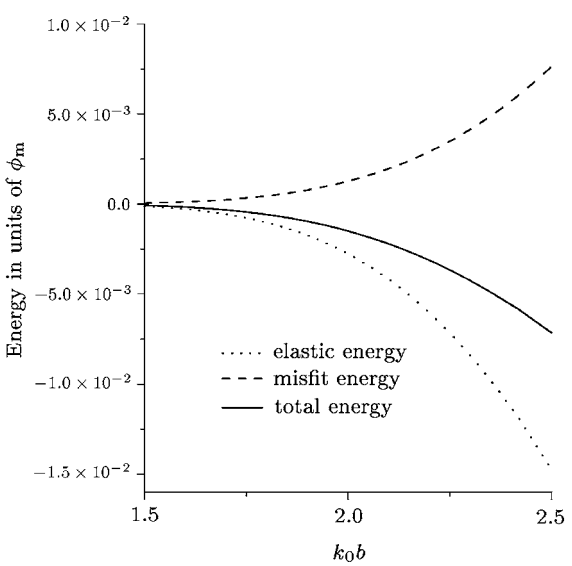


Fig.1. The misfit energy, elastic strain energy and Peierls energy as functions of $\kappa_0 b$, $\epsilon_0 = 0.3$, $\phi_{\rm m} = (\mu b^3)/(2\pi^2 d)$.

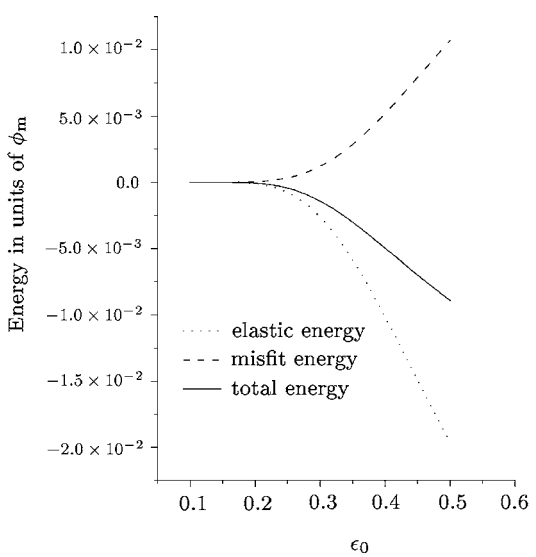


Fig.2. The Peierls energy as a function of ϵ_0, $\kappa_0 b = 2.0$. The energy $E_{\rm p}$ falls off rapidly as ϵ_0 or $\kappa_0 b$ decreases.

4. Discussion and summary

The dislocation equations (8) and dislocation solution (9) acquire a universal form that can be viewed as a natural generalization of the Peierls's one. The parameters in the dislocation equation may take different value for different lattice, but the form of equation will not change greatly. Therefore, it is reasonable to believe that the results obtained from the triangular lattice can be general as long as the physics mechanism does not change.

The expressions obtained above are too complicated to apply practically. Simplification must be made. It is found that for the physically interesting range of the parameters, the Peierls stress obtained in the lattice theory can be well approximated by

$$\frac{\sigma_{\rm p}}{\sigma_{\rm m}} = 4\pi {\rm e}^{-\pi(s_{\rm e}+s_{\rm c})} \tag{26}$$

with

$$s_{\rm e} = \frac{d}{(1-\nu)b}, \qquad s_{\rm c} = \sqrt{\frac{2\beta d}{\mu b}}.$$

The relations between the parameters $s_{\rm e}$, $s_{\rm c}$ and $\kappa_0 b$, ϵ_0 are

$$s_{\rm e} = \frac{2}{\kappa_0 b}, \qquad s_{\rm c} = \frac{1}{\kappa_0 b \epsilon_0}.$$

For the understanding of the physical implication of Eq.(26), it is crucial to observe that the parameter $s_{\rm e}$ uniquely determines the asymptotic behaviour far from the core of the dislocation, and the parameter $s_{\rm c}$ only has effect on the core structure. With the same $s_{\rm e}$ but different $s_{\rm c}$, the dislocation will take the same asymptotic behaviour but different core structure. Therefore, $s_{\rm c}$ can be rationally referred to as the core structure factor, and $s_{\rm e}$ can be referred to as the elastic structure factor. The Peierls stress is controlled by the core structure factor as well as the elastic structure factor.

The width of a dislocation can be measured in experiments or evaluated through numerical simulation. Its specific value depends on the way of data fitting. The lattice solution, Eq.(9), which is simple and robust, is a good candidate to be used in data fitting. The width given in this way has a relation with the core structure factor and elastic structure factor, as follows:

$$\frac{1}{\kappa} = s_{\rm c} b \left(1 + \frac{67 s_{\rm e}}{192 s_{\rm c}}\right) \sim s_{\rm c} b. \tag{27}$$

Because the misfit energy and elastic strain energy associated with discreteness cancel each other, and the width of dislocation becomes wide in the lattice theory, the Peierls stress given here is much smaller than in the classical P-N theory. For the triangular lattice, substituting the parameters given above, one obtains $\sigma_{\rm p} \simeq 4 \times 10^{-4}\mu$ for the lattice theory, $\sigma_{\rm p} \simeq 7 \times 10^{-3}\mu$ for the classical P-N theory. If only the misfit energy is considered in the classical P-N theory, one obtains $\sigma_{\rm p} \simeq 4 \times 10^{-2}\mu$. It is interesting to have simple estimation of the Peierls stress for the metal copper based on the results obtained here. For copper, the glide plane is the closest-packed plane, the spacing between the planes is $d = a/\sqrt{3}$ (a is the lattice constant), the magnitude of the Burger's vector of a partial dislocation is $b = a/\sqrt{6}$, the Poisson's ratio is $\nu \simeq 1/3$ and so the elastic factor is $s_{\rm e} \simeq 2$. As for the core structure factor, roughly using the results of the triangular lattice, $\beta \simeq 3\alpha/4$, $\mu \simeq \dfrac{\alpha d}{2b}$, one has $s_{\rm c} \simeq \sqrt{3}$. The resulting Peierls stress is $\sigma_{\rm p} \simeq 10^{-4}\sigma_{\rm m} \simeq 10^{-5}\mu$. It is close to the experimental value $5 \times 10^{-6}\mu$.[14] Considering the approximation used here, the theoretical prediction is in agreement with the experimental data.

In summary, based on the lattice theory of dislocation, an unquestionable calculation of the dislocation energy is presented. The results show that the elastic strain energy associated with the discreteness of lattice is quite important. It is this part of the energy that makes the stable configuration of the dislocation have a minimum energy, and removes the contradiction existing in the classical P-N theory. Furthermore, a simple formula of the Peierls stress is proposed to include the effect of the core structure that is strongly related to the lattice discreteness. The theoretical prediction for the Peierls stress is fairly improved in the calculation. Although such an investigation cannot provide an accurate prediction for real materials in comparison with the numerical calculation like the molecular dynamical simulation and the electron density-functional calculation, it can provide a transparent physics picture and a deep insight to the problem.

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[13] The elastic strain energy includes a constant part and a variable part associated with the discreteness of lattice. Because the constant part has no effect on the dislocation mobility, here, the elastic strain energy refers to the second part. One should not confuse the total elastic strain energy and the variable part associated with discreteness

[14] Young F W 1968 *Dislocation Dynamics* (New York: McGraw-Hill) p 313