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An improvement of the Peierls equation by taking into account the lattice effects*

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An improvement of the Peierls equation has been made by including the lattice effects. By using the non-trivially gluing mechanism for the simple cubic lattice, in which atoms interact with its first and second nearest neighbours through a central force, the dislocation equation has been derived rigorously for the isotropic case. In the slowly varying approximation, the Peierls equation with the improvement by including the lattice effects has been obtained explicitly. The new equation can be used to substitute for the old one in theoretical investigations of dislocations. The major change of the predicted dislocation structure is in the core region. The width of the dislocation given by using the new equation is about three times that given by the classical Peierls–Nabarro theory for the simple cubic lattice.

Keywords: dislocation, Peierls equation, lattice effect
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1. Introduction

The core structure of a dislocation is of importance because it determines the mobility of the dislocation. The core structure can be addressed successfully for an actual crystal through a numerical calculation such as atomistic simulation or electron-density functional technique. However, the limitation of numerical results is obvious. The understanding of the dislocation should not rely on the numerical calculations only. A rationally physical model and analytical theory can reveal general relation between the dislocation structure and crystal characteristics and provide a deep insight to the problems.

Theoretically, the dislocation was first studied in the frame of elastic continuum theory.[1] On the basis of the results from the elastic continuum theory, a significant theory was presented by Peierls and later elucidated and extended by Nabarro.[2,3] In the Peierls–Nabarro (P-N) theory, the width of a dislocation and the Peierls stress—the critical stress required for making a dislocation move through the crystal—were meaningfully related to the crystal characteristics. Even though there are arguments about the drawbacks and limitations, in particular, the accuracy of the predictions, the fundamental concepts and the methods originating from the P-N theory still play a unique role in the discussion of dislocation up to now.[4−12]

In the P-N theory, the crystal with a dislocation is first cut into two parts along the glide plane, and then glued together in a non-trivial way. The dislocation is produced through nonlinear interaction between two parts. This profound idea gives us a way to deal with topological defects. However, there exist drawbacks in the P-N model. The most serious drawback is that the half-infinite crystals resulting from cutting was approximated as an elastic continuum body. Since the discreteness effect was underestimated in the continuum approximation especially at the dislocation core where displacement varies abruptly, the width of the dislocation obtained from the P-N model is usually much narrower than that observed experimentally. And the Peierls stress predicted is generally considered only valuable qualitatively.

Recently, the discreteness effects have been incorporated into the P-N theory in a way in which the integrations are replaced by the discrete sums.[5] However, in order to improve the P-N theory by including lattice effects adequately, it is necessary to relax the continuum approximation at the beginning. Unfor-

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tunately, when the discreteness of the lattice is fully considered, the problem to be solved will be very hard, and the advantages in conceptual and calculating simplicity will be weakened greatly. A good way to deal with the issue is to look for an improvement of the Peierls equation while including the lattice effect.

In this paper, a model of the simple cubic (SC) crystal of atoms interacting with their first and second nearest neighbours through a central force is considered. By using the non-trivially gluing mechanism, the dislocation equation has been derived rigorously for the isotropic case. Since the deformation associated with the dislocation varies slowly, it is reasonable to change the discrete equation into the integro-differential equation. The expanding series in terms of derivatives of the displacement field is obtained. If only the leading term is kept, one recovers the Peierls equation. If higher-order terms are kept also, one obtains the improvement of the Peierls equation with modification by discrete lattice effect. The improved equation is discussed briefly. One can see that the major change in the predicted dislocation is in the core structure. The width of the dislocation is much wider than that in the classical P-N theory. As a consequence, one can expect that the Peierls stress should decrease greatly.

2. Model and the cohesive law

The crystal with dislocation 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

$$H = H_{\rm a} + H_{\rm b} + H_{\rm int},$$

where $H_{\rm a}(H_{\rm b})$ is the Hamiltonian of the half-infinite crystal above (below) the glide plane, $H_{\rm int}$ stands for the interaction between the two half crystals concerned (Fig.1). In the classical P-N model, each half-infinite crystal is approximated as an isotropic elastic-continuum. Here the continuum approximation is relaxed, the discreteness of lattice is fully considered. In order to emphasize the elementary physics and clarify the key issues in an unquestionable way, a relatively simple model — the dislocation in a SC lattice is investigated, where the SC lattice is assumed to be harmonic one in which the atom interacts with its first and second nearest neighbours through a central force. The Hamiltonian is

$$\begin{aligned} H_0 =& \frac{\alpha}{2}\sum_R [(u^x_{R+a_1} - u^x_R)^2 \\ &+ (u^y_{R+a_2} - u^y_R)^2 + (u^z_{R+a_3} - u^z_R)^2] \\ &+ \frac{\beta}{4}\sum_R [(u^x_{R+a_1+a_2} - u^x_R + u^y_{R+a_1+a_2} - u^y_R)^2 \\ &+ (u^x_{R+a_1+a_3} - u^x_R + u^z_{R+a_1+a_3} - u^z_R)^2 \\ &+ (u^x_{R+a_1-a_2} - u^x_R - u^y_{R+a_1-a_2} + u^y_R)^2 \\ &+ (u^x_{R+a_1-a_3} - u^x_R - u^z_{R+a_1-a_3} + u^z_R)^2 \\ &+ (u^y_{R+a_2+a_3} - u^y_R + u^z_{R+a_2+a_3} - u^z_R)^2 \\ &+ (u^y_{R+a_2-a_3} - u^y_R - u^z_{R+a_2+a_3} + u^z_R)^2], \end{aligned} \tag{1}$$

where α and β are the harmonic interaction constants between the nearest neighbouring pair and the second nearest neighbouring pairs respectively, $\boldsymbol{u}_R$ is the displacement field.

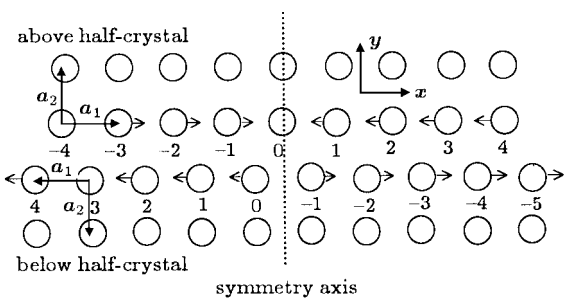


Fig.1. The reference configuration of the atoms and the coordinates defined by a pair of orthogonal unit vectors x and y (the z-axis perpendicular to the paper plane is not plotted). The lattice is divided into an upper part and a lower part. The lattice vector is defined locally for the different part. The displacement given in the text is relative to the position in this figure.

In the continuum approximation, the Hamiltonian becomes

$$\begin{aligned} H_0 =& \int {\rm d}V \Big[\frac{\alpha+2\beta}{2a}(e^2_{xx} + e^2_{yy} + e^2_{zz}) \\ &+ \frac{2\beta}{a}(e^2_{xy} + e^2_{xz} + e^2_{yz}) \\ &+ \frac{\beta}{a}(e_{xx}e_{yy} + e_{xx}e_{zz} + e_{yy}e_{zz})\Big], \end{aligned} \tag{2}$$

where a is the lattice constant, and

$$e_{xx} = \frac{\partial u^x}{\partial x}, \quad e_{xy} = \frac{1}{2}\left(\frac{\partial u^x}{\partial y} + \frac{\partial u^y}{\partial x}\right), \cdots,$$

are strains. The non-zero elements of the stiffness matrix are

$$c_{11} = \frac{\alpha+2\beta}{a}, \quad c_{12} = c_{44} = \frac{\beta}{a}.$$

The equilibrium equation of the lattice subjected to a

given external force $\boldsymbol{f}$ is

$$\begin{aligned}
&\frac{\alpha}{a}\nabla^2 u^x + \frac{2\beta}{a}\frac{\partial}{\partial x}\nabla\cdot\boldsymbol{u} \\
&+\frac{\beta-\alpha}{a}\left(\frac{\partial^2 u^x}{\partial y^2}+\frac{\partial^2 u^x}{\partial z^2}\right)+\frac{f^x}{a^3}=0, \\
&\frac{\alpha}{a}\nabla^2 u^y + \frac{2\beta}{a}\frac{\partial}{\partial y}\nabla\cdot\boldsymbol{u} \\
&+\frac{\beta-\alpha}{a}\left(\frac{\partial^2 u^y}{\partial x^2}+\frac{\partial^2 u^y}{\partial z^2}\right)+\frac{f^y}{a^3}=0, \\
&\frac{\alpha}{a}\nabla^2 u^z + \frac{2\beta}{a}\frac{\partial}{\partial z}\nabla\cdot\boldsymbol{u} \\
&+\frac{\beta-\alpha}{a}\left(\frac{\partial^2 u^z}{\partial x^2}+\frac{\partial^2 u^z}{\partial y^2}\right)+\frac{f^z}{a^3}=0. \qquad (3)
\end{aligned}$$

For $\alpha=\beta$, the SC lattice becomes isotropic one, and the equilibrium equation can be written as

$$\frac{\alpha}{a}\nabla^2\boldsymbol{u}+\frac{2\alpha}{a}\nabla(\nabla\cdot\boldsymbol{u})+\frac{1}{a^3}\boldsymbol{f}=0. \qquad (4)$$

Comparing with standard equation of an isotropic continuum, one has the shear modulus $\mu=\alpha/a$, Poisson ratio $\nu=1/4$, and Young modulus $E=5\alpha/(2a)$.

The cohesive interaction that glues the two half-crystals together is a crucial point in the dislocation theory. The sinusoidal-force law initially put forward in the Frenkel and Kontorova (F-K) model,[13] and used in the P-N theory had successfully described the interaction in a simple way. A more accurate description is suggested to relate the interaction to the generalized stacking-fault energy which can be obtained from first-principle density-functional calculation.[6,7,14] In the point view of lattice theory, a useful effective-interaction can be given in the following way. Because only small distortion occurs in the case of dislocation, for the atoms in a given half-crystal the dominative part of the potential from the other half-crystal is the same as that produced by a perfect crystal. This leads to the periodic potential approximation first used in the F-K model. On the other hand, the displacement takes place bilaterally, obviously it is not enough to obtain the interaction by applying the periodic potential of the perfect crystal trivially. In order to incorporate the relative displacement and maintain the simplicity, a helpful idea is to introduce the phase shift concept, i.e. the difference of the potential felt by different atoms is just a phase factor which is determined by the atom position relative to the crystal on the other side. For the SC lattice, the phase factor of the atom ℓ on the border of the upper half-crystal (Fig.1) is given through the middle point of a pair of neighbouring atoms on the lower side, hence the potential felt by the atom ℓ is

$$\phi=\phi[\boldsymbol{u}^a_\ell-\frac{1}{2}(\boldsymbol{u}^b_{-\ell}+\boldsymbol{u}^b_{-\ell-1})],$$

where ϕ is the potential given by the perfect half-crystal and can be obtained from the stacking-fault energy. In this way, the interaction Hamiltonian is proportional to the summation of the potential of the atoms on the border, i.e.

$$\sum_\ell \phi\left[\boldsymbol{u}^a_\ell-\frac{1}{2}(\boldsymbol{u}^b_{-\ell}+\boldsymbol{u}^b_{-\ell-1})\right].$$

This effective interaction is general enough in the lattice discussion of dislocation.

In the following discussion, the coordinate system is chosen in such a way that the dislocation line is taken to be the z-axis, the x-axis is parallel to the glide direction, and the y-axis is perpendicular to the dislocation line and glide direction (Fig.1). Usually, the relative displacement component parallel to the y-axis is small for the dislocation, we expand ϕ into power series

$$\phi(\boldsymbol{r})=\phi|_{y=d}+\frac{\partial\phi}{\partial y}|_{y=d}(y-d)+\frac{1}{2}\frac{\partial\phi^2}{\partial y^2}|_{y=d}(y-d)^2,$$

where d is the spacing between glide planes. The second term on the right hand side of the equation, which describes the force felt by a atom moving along the straight line $y=d$ and vanishes at the equilibrium point, can be neglected for simplicity. The first term is a periodic function $\phi(x+a)=\phi(x)$. If the periodic potential $\phi(x)$ is expanded in a triangular series, and only the non-trivial leading term is kept, one has the potential of the sinusoidal-force law

$$\phi(x)=\frac{\mu a^4}{4\pi^2 d}\left(1+\cos\frac{2\pi x}{a}\right), \qquad (5)$$

where as done frequently, the coefficient has been determined by the condition that elastic limit should be recovered. Remember that x in Eq.(5) is the relative displacement.

3. Half-infinite problem related to the dislocation equation

The deformation problem related to the edge dislocation in a simple cubic lattice is a quasi two-dimensional problem. There is no displacement in the direction parallel to the dislocation line

$$u^z = 0,$$

and the displacements of the atoms are uniform along the dislocation line

$$u^x_{R+a_3} = u^x_R, \quad u^y_{R+a_3} = u^y_R.$$

In this case, the Hamiltonian becomes

$$\begin{aligned} H_0 =& \frac{\alpha+\beta}{2}\sum_R[(u^x_{R+a_1}-u^x_R)^2-(u^y_{R+a_2}+u^y_R)^2] \\ &+\frac{\beta}{4}\sum_R[(u^x_{R+a_1+a_2}-u^x_R+u^y_{R+a_1+a_2}-u^y_R)^2 \\ &+(u^x_{R+a_1-a_2}-u^x_R-u^y_{R+a_1-a_2}+u^y_R)^2]. \end{aligned}$$

Note that the nearest neighbour interaction constant is $\alpha+\beta$ in the quasi two-dimensional deformation.

The equilibrium equation can be written as

$$Du_R = f_R \tag{6}$$

where the 2×2 matrix is given by

$$D = \begin{bmatrix} ((\alpha+\beta)\Delta_1+\dfrac{\beta}{2}(\Delta_{12}+\bar{\Delta}_{12}) & \dfrac{\beta}{2}(\Delta_{12}-\bar{\Delta}_{12}) \\ \dfrac{\beta}{2}(\Delta_{12}-\bar{\Delta}_{12}) & (\alpha+\beta)\Delta_2+\dfrac{\beta}{2}(\Delta_{12}+\bar{\Delta}_{12}) \end{bmatrix} \tag{7}$$

with

$$\Delta_1 = 2-T_1-T_1^{-1},$$

$$\Delta_2 = 2-T_2-T_2^{-1},$$

$$\Delta_{12} = 2-T_1T_2-(T_1T_2)^{-1},$$

$$\bar{\Delta}_{12} = 2-T_1T_2^{-1}-(T_1T_2^{-1})^{-1},$$

where T_1 and T_2 are translation operators defined respectively by

$$T_1u_R = u_{R+a_1}, \quad T_2u_R = u_{R+a_2}.$$

For the half-infinite lattice subjected to the force on the border, the boundary equation is

$$\begin{aligned} &\alpha(2u^x_R-u^x_{R-a_1}-u^x_{R+a_1}) \\ &+\frac{\beta}{2}((2u^x_R-u^x_{R+a_1+a_2}-u^x_{R-a_1+a_2} \\ &+u^y_{R-a_1+a_2}-u^y_{R+a_1+a_2}) = f^x_R, \end{aligned}$$

$$\begin{aligned} &\alpha(u^y_R-u^y_{R+a_2}) \\ &+\frac{\beta}{2}((2u^y_R-u^y_{R+a_1+a_2}-u^y_{R-a_1+a_2} \\ &+u^x_{R-a_1+a_2}-u^x_{R+a_1+a_2}) = f^y_R. \end{aligned} \tag{8}$$

A method for obtaining the relation between the displacement of the border atoms and the boundary force was given previously.[8] It is straightforward to apply the method to the SC lattice. The detailed derivation is long and arduous. Here only the main results are presented.

The lattice Green's function defined through

$$\sum_m D_{nm}G_{mn'}(\boldsymbol{R}-\boldsymbol{R}') = \delta_{nn'}\delta_{RR'} \tag{9}$$

reads

$$G_{nn'}(\boldsymbol{R}) = \frac{1}{\Omega^*}\int_{BZ}\mathrm{d}\boldsymbol{k}\tilde{G}_{nn'}(\boldsymbol{k})\mathrm{e}^{-\mathrm{i}k\cdot R},$$

with

$$\tilde{G} = \frac{1}{\Delta}\begin{bmatrix} 2(1-\cos k_ya)+1-\cos k_xa\cos k_ya & -\sin k_xa\sin k_ya \\ -\sin k_xa\sin k_ya & 2(1-\cos k_xa)+1-\cos k_xa\cos k_ya \end{bmatrix}, \tag{10}$$

and

$$\Delta = (-2+\cos k_xa+\cos k_ya)(-2+\cos k_xa+\cos k_ya-2+2\cos k_xa\cos k_ya),$$

where the isotropic condition $\alpha=\beta$ has been used, and for convenience, $\alpha+\beta=2\alpha=1$ has been taken. From the boundary equation, the effective force is

$$F = f+\Gamma u$$

where

$$\Gamma = \begin{bmatrix} \frac{1}{4}(2 - T_1^{-1}T_2^{-1} - T_1T_2^{-1}) & \frac{1}{4}(T_1T_2^{-1} - T_1^{-1}T_2^{-1}) \\ \frac{1}{4}(T_1T_2^{-1} - T_1^{-1}T_2^{-1}) & \frac{1}{2}(1 - T_2^{-1}) + \frac{1}{4}(2 - T_1^{-1}T_2^{-1} - T_1T_2^{-1}) \end{bmatrix}. \tag{11}$$

The equation that relates the displacement of atoms on the border to the force is

$$\sum_{\ell'} \Lambda(\ell - \ell')\boldsymbol{u}(\ell') = \boldsymbol{f}(\ell), \tag{12}$$

where the components of the displacement and the force have been arranged in column matrix respectively

$$\boldsymbol{u}(\ell) = \begin{bmatrix} u^x(\ell) \\ u^y(\ell) \end{bmatrix}, \quad \boldsymbol{f}(\ell) = \begin{bmatrix} f^x(\ell) \\ f^y(\ell) \end{bmatrix};$$

$\Lambda(\ell)$ is a 2×2 matrix

$$\Lambda(\ell) = \begin{bmatrix} \Lambda_{xx}(\ell) & \Lambda_{xy}(\ell) \\ \Lambda_{yx}(\ell) & \Lambda_{yy}(\ell) \end{bmatrix},$$

given by

$$\Lambda(\ell) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}q\tilde{\Lambda}(q)\mathrm{e}^{-\mathrm{i}\ell q}, \tag{13}$$

$$\tilde{\Lambda}(q) = \begin{bmatrix} 1 - \cos q + \frac{\sqrt{3}}{\chi}\sqrt{(1-\cos q)^3(3-\cos q)} & \mathrm{i}\sin q\left[1 - \frac{\sqrt{3}}{\chi}(1-\cos q)\right] \\ -\mathrm{i}\sin q\left[1 - \frac{\sqrt{3}}{\chi}(1-\cos q)\right] & \frac{1}{\chi}\sqrt{(1-\cos q)^3(5+\cos q)} \end{bmatrix} \tag{14}$$

with

$$\chi = \sqrt{(5+\cos q)(3-\cos q)} - \sqrt{3}(1+\cos q)$$

$$-\pi \le q \le \pi.$$

$\tilde{\Lambda}$ is a Hermite matrix

$$\tilde{\Lambda}^{\dagger} = \tilde{\Lambda},$$

and its diagonal elements of matrix Λ are even-function of the order number ℓ

$$\Lambda_{xx}(-\ell) = \Lambda_{xx}(\ell), \qquad \Lambda_{yy}(-\ell) = \Lambda_{xx}(\ell),$$

its non-diagonal elements are odd-function

$$\Lambda_{xy}(-\ell) = -\Lambda_{xy}(\ell), \qquad \Lambda_{yx}(-\ell) = -\Lambda_{yx}(\ell).$$

It is helpful to interpret the $\Lambda(\ell - \ell')\boldsymbol{u}(\ell')$ as a force field produced by the source $\boldsymbol{u}(\ell')$, which is the displacement of the atom ℓ'. If there is an atom located at ℓ, this atom will feel a force $-\Lambda(\ell - \ell')\boldsymbol{u}(\ell')$ given by atom ℓ'. The force field is proportional to the displacement of the source atom, and can be superposed when there exist many source atoms. Due to translation symmetry, the force field is a function of the relative coordinate. Because $\Lambda(0) \neq 0$, there exists a self-interaction that is excluded in the conventional force concept, so it should be careful when the force concept is used.

4. Dislocation equation and the post-continuum approximation

By using the solution of the half-infinite lattice, the dislocation equation that is only related to the atoms on the bilateral borders can be written as

$$\sum_{\ell'} \Lambda(\ell - \ell')\boldsymbol{u}_{\mathrm{a}}(\ell') = \boldsymbol{f}_{\mathrm{a}}(\ell),$$

$$\sum_{\ell'} \Lambda(-\ell + \ell')\boldsymbol{u}_{\mathrm{b}}(-\ell') = \boldsymbol{f}_{\mathrm{b}}(-\ell), \tag{15}$$

where $\boldsymbol{u}_{\mathrm{a}}$ and $\boldsymbol{u}_{\mathrm{b}}$ are displacement fields of the upper border and lower border respectively, $\boldsymbol{f}_{\mathrm{a}}$ and $\boldsymbol{f}_{\mathrm{b}}$ are force fields resulting from the interaction between the upper and lower half-infinite crystals. In order to use the same kernel Λ for the both two half-crystals, it is necessary to use the local lattice vector that is intrinsic to the crystal block (see Fig.1). Obviously, if the upper part rotates 180°, it will change to be the lower part. Therefore, the intrinsic order number differs a minus for the border atoms on the different sides.

For the cohesive law given for the SC lattice in the first section, it is easy to show

$$\boldsymbol{f}_{\mathrm{b}}(-\ell) = -\frac{1}{2}\boldsymbol{f}_{\mathrm{a}}(\ell) - \frac{1}{2}\boldsymbol{f}_{\mathrm{a}}(\ell - 1).$$

Introducing mass-centre coordinate for a pair of neigh-

bouring atoms on the lower border

$$\boldsymbol{v}(\ell) = \frac{1}{2}\boldsymbol{u}_{\rm b}(-\ell) + \frac{1}{2}\boldsymbol{u}_{\rm b}(-\ell-1),$$

from Eq.(15), one has

$$\begin{aligned}&\sum_{\ell'} \Lambda(-\ell+\ell')\boldsymbol{v}(\ell') \\ &= -\frac{1}{2}\boldsymbol{f}_{\rm a}(\ell) - \frac{1}{4}[\boldsymbol{f}_{\rm a}(\ell+1) + \boldsymbol{f}_{\rm a}(\ell-1)] \\ &\simeq -\boldsymbol{f}_{\rm a}(\ell), \end{aligned} \tag{16}$$

where the approximation $\boldsymbol{f}_{\rm a}(\ell+1)+\boldsymbol{f}_{\rm a}(\ell-1) \simeq 2\boldsymbol{f}_{\rm a}(\ell)$ has been taken in the last step. Within the approximation, it is not difficult to verify that the dislocation equation can be reduced to

$$\begin{aligned} u^x_{\rm a}(\ell) &= -v^x(\ell) = u^x(\ell), \\ u^y_{\rm a}(\ell) &= v^y(\ell) = u^y(\ell), \end{aligned}$$

and the following equations are satisfied by $u^x(\ell)$ and $u^y(\ell)$

$$\begin{aligned}&\sum_{\ell'}[\Lambda_{xx}(\ell-\ell')u^x(\ell') + \Lambda_{xy}(\ell-\ell')u^y(\ell')] = f^x(\ell), \\ &\sum_{\ell'}[\Lambda_{yy}(\ell-\ell')u^y(\ell') - \Lambda_{xy}(\ell-\ell')u^x(\ell')] = 0. \end{aligned} \tag{17}$$

The reduction implies that one has chosen a special solution in such a way that the two points aligned vertically have the same vertical displacement; as for the horizontal displacements, they are equal in magnitude, but opposite in direction.

The simplified equation (17) is a satisfactory one as a suitable starting point in the discussion of dislocation structure. However, the matrix elements of $\Lambda(\ell)$ given by Fourier transformation, Eq.(13), can be hardly calculated rigorously. Furthermore, a discrete equation like Eq.(17) can be hardly solved analytically even though the kernel matrix $\Lambda(\ell)$ has been obtained. Therefore, the dislocation equation should be simplified further for practical use.

Let us write the first diagonal matrix element as

$$\begin{aligned}&\tilde{\Lambda}_{xx}(q) = 1 - \cos q + \tilde{w}, \\ &\tilde{w} = \frac{\sqrt{3}}{\chi}\sqrt{(1-\cos q)^3(3-\cos q)}. \end{aligned} \tag{18}$$

At a first glance, the last term $\tilde{w}$ in Eq.(18) has no analogy with its counterpart of the triangular lattice. Surprisingly, the behaviours of $w(\ell)$ are quite similar to the triangular lattice. As a function of atom position ℓ, $w(\ell)$ has a long tail that falls off slowly, and a short head that oscillates strongly (Fig.2). Based on the observation, a phenomenological treatment was put forward to simplify $w(\ell)$ in Ref.[8]. Unfortunately, it is found that the same treatment cannot bring a desired result for the case of square lattice. It is necessary to look for a new method.

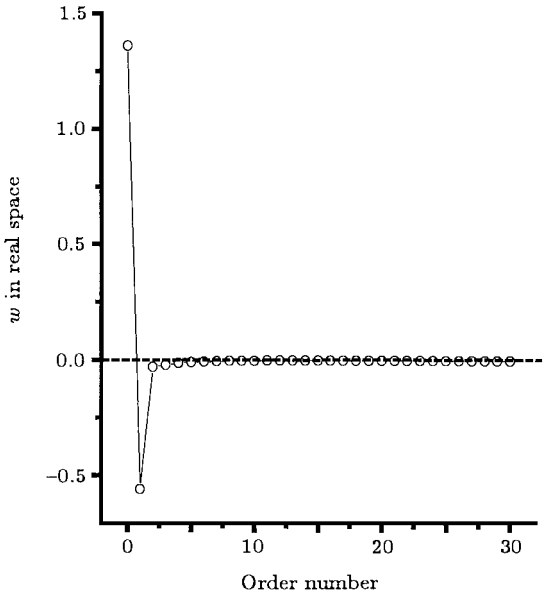


Fig.2. The function $w(\ell)$ calculated numerically through Eq.(13). Its behaviour is analogous to that obtained in the case of the triangular lattice.[8] The analogy strongly indicates that the modification from the discreteness will possess a universal feature.

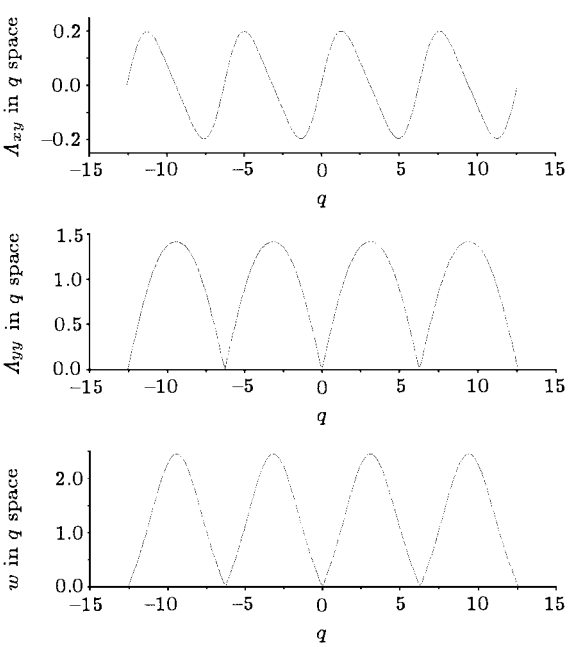


Fig.3. The kernel Λ in the q space. The functions w and Λ_{yy} in the q space should be carefully treated when one expands them in the Fourier series. The functions w and Λ_{yy} are actually periodic functions with a period 4π rather than 2π as it looks at the first glance.

As shown in Fig.3, the function $\tilde{w}(q)$ varies continuously, but its differential has a break for $q = 2n\pi$, $n = 0, \pm 1, \pm 2 \cdots$. In addition, $\tilde{w}$ is a periodic even-function,

$$\tilde{w}(-q) = \tilde{w}(q), \qquad \tilde{w}(q + 2\pi) = \tilde{w}(q).$$

Let us expand function $\tilde{w}(q)$ in the Fourier series

$$\begin{aligned}\tilde{w}(q) =& \sum_{n=1}^{\infty} b_n \sin\left(\frac{2n+1}{2}q\right) \\ =& 2.215 \sin\left(\frac{q}{2}\right) - 0.235 \sin\left(\frac{3q}{2}\right) + \cdots, \\ & 0 \le q \le 2\pi, \end{aligned} \tag{19}$$

$$b_n = \frac{1}{\pi}\int_0^{2\pi} \tilde{w}(q) \sin\left(\frac{2n+1}{2}q\right) \mathrm{d}q.$$

Attention should be paid to the fact that $\tilde{w}(q)$ given by Eq.(19) is an odd-function, not an even-function. The equality holds when the variable q is confined to the interval $0 \le q \le 2\pi$. By using Eq.(19), one has

$$\begin{aligned} w(\ell) =& \frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{w}(q) \mathrm{e}^{-\mathrm{i}\ell q} \mathrm{d}q \\ =& \frac{1}{\pi}\int_0^{\pi} \tilde{w}(q) cos(\ell q) \mathrm{d}q \\ =& \frac{1}{2\pi}\sum_{n=1}^{\infty} \frac{(2n+1)b_n}{\left(\frac{2n+1}{2}\right)^2 - \ell^2}, \end{aligned} \tag{20}$$

and

$$\begin{aligned} & \sum_{\ell'} w(\ell - \ell')u(\ell') \\ =& \frac{1}{2\pi}\sum_{\ell'}\sum_{n=1}^{\infty} \frac{(2n+1)b_n}{\left(\frac{2n+1}{2}\right)^2 - (\ell - \ell')^2} u(\ell') \\ =& \frac{-1}{2\pi}\sum_{n=1}^{\infty} b_n \sum_{\ell'} \left[\frac{u(\ell')}{\ell - \ell' - \frac{2n+1}{2}} - \frac{u(\ell')}{\ell - \ell' + \frac{2n+1}{2}}\right] \\ =& \frac{-1}{2\pi}\sum_{n=1}^{\infty} b_n \sum_{\sigma} \frac{u\left(\sigma + \frac{2n+1}{2}\right) - u\left(\sigma - \frac{2n+1}{2}\right)}{\sigma - \ell}, \end{aligned}$$

where σ in the last sum runs over the half-integers. For the case of dislocation, the displacement field varies smoothly and slowly. One can extend function u analytically and expand in the power series, i.e.

$$\begin{aligned} & u(\sigma + \frac{2n+1}{2}) - u(\sigma - \frac{2n+1}{2}) \\ =& \sum_{j=0}^{\infty} \frac{2}{(2j+1)!} \frac{\mathrm{d}^{2j+1}u(\sigma)}{\mathrm{d}\sigma^{2j+1}} \left(\frac{2n+1}{2}\right)^{2j+1}. \end{aligned}$$

In addition, from Eq.(19), it is easy to obtain an identity

$$\sum_{n=1}^{\infty} \left(\frac{2n+1}{2}\right)^{2j+1} b_n = (-1)^j \tilde{w}^{(2j+1)}(0),$$

where

$$\tilde{w}^{(2j+1)}(0) = \frac{\mathrm{d}^{2j+1}\tilde{w}(q)}{\mathrm{d}q^{2j+1}}|_{q=0}$$

is the $(2j+1)$-order derivative at the origin. By virtue of the identity, one can arrive at

$$\begin{aligned} \sum_{\ell'} w(\ell - \ell')u(\ell') =& \frac{-1}{\pi}\sum_{\sigma} \frac{1}{\sigma - \ell}\sum_{j=0}^{\infty} \frac{(-1)^j \tilde{w}^{(2j+1)}(0)}{(2j+1)!} \frac{\mathrm{d}^{2j+1}u(\sigma)}{\mathrm{d}\sigma^{2j+1}} \\ =& \frac{-1}{\pi}\int_{-\infty}^{+\infty} \frac{\mathrm{d}x'}{x' - x}\left[\frac{a}{1!}\tilde{w}^{(1)}(0)\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{a^3}{3!}\tilde{w}^{(3)}(0)\frac{\mathrm{d}^3u}{\mathrm{d}x^3} + \cdots\right]|_{x=x'}, \end{aligned} \tag{21}$$

where $x = \ell a$, a is the lattice constant, the sum over σ has been changed into integral in the last expression.

The same thing can be done for another diagonal element Λ_{yy},

$$\tilde{\Lambda}_{yy}(q) = 1.4456 \sin\left(\frac{q}{2}\right) + 0.0265 \sin\left(\frac{3q}{2}\right) + \cdots, \qquad 0 \le q \le 2\pi,$$

$$\Lambda_{yy}(\ell - \ell')u(\ell') = \frac{-1}{\pi}\int_{-\infty}^{+\infty} \frac{\mathrm{d}x'}{x' - x}\left[\frac{a}{1!}\tilde{\Lambda}_{yy}^{(1)}(0)\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{a^3}{3!}\tilde{\Lambda}_{yy}^{(3)}(0)\frac{\mathrm{d}^3u}{\mathrm{d}x^3} + \cdots]|_{x=x'}. \tag{22}$$

The non-diagonal element Λ_{xy} can be handled in the same way,

$$\begin{aligned}\tilde{\Lambda}_{xy}(q) =& \sum_{n=1}^{\infty} b_n^{xy} \sin(nq) \\ =& \mathrm{i}[0.1912\sin(q) + 0.0287\sin(2q) + \cdots], \\ \Lambda_{xy}(\ell) =& \frac{\mathrm{i}}{2}\sum_{n=1}^{\infty} b_n^{xy}(\delta_{\ell+n} - \delta_{\ell-n}), \\ & - \mathrm{i}\sum_{\ell'} \Lambda_{xy}(\ell-\ell')u(\ell') \\ =& \frac{1}{2}\sum_{n=1}^{\infty} b_n^{xy}[u(\ell+n) - u(\ell-n)] \\ =& \frac{a}{1!}\tilde{\Lambda}_{xy}^{(1)}(0)\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{a^3}{3!}\tilde{\Lambda}_{xy}^{(3)}(0)\frac{\mathrm{d}^3u}{\mathrm{d}x^3} + \cdots \end{aligned} \tag{23}$$

Unlike the diagonal elements, the non-diagonal is a smooth periodic-function. Its differential has no break. As a result, there is no integration appearing in the expression.

By using Eqs.(21–23), the dislocation equation can be changed into an integro-differential equation after a reasonable truncation. If the high-order derivatives are kept, one has the post-continuum approximation that is beyond the elastic continuum theory.

For the SC lattice, some useful coefficients are

$$\tilde{w}^{(1)}(0) = \frac{3}{4}, \qquad \tilde{w}^{(3)}(0) = \frac{9}{16},$$

$$\tilde{\Lambda}_{xy}^{(1)}(0) = \frac{\mathrm{i}}{4}, \qquad \tilde{\Lambda}_{xy}^{(3)}(0) = -\frac{7\mathrm{i}}{16},$$

$$\tilde{\Lambda}_{yy}^{(1)}(0) = \frac{3}{4}, \qquad \tilde{\Lambda}_{yy}^{(3)}(0) = -\frac{3}{16}.$$

5. Generalized Peierls equation and the dislocation solution

From the results given above, one can obtain a generalization of the Peierls equation. Generally the vertical displacement u^y of a dislocation varies more slowly than the parallel displacement u^x. Keeping the derivative terms lower than second-order for u^y, lower than fourth-order for u^x, Eq.(17) becomes

$$\begin{aligned} & -\frac{a^2}{2}\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2} + \mathrm{i}a\tilde{\Lambda}_{xy}^{(1)}(0)\frac{\mathrm{d}u^y}{\mathrm{d}x} - \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\frac{a}{1!}\tilde{w}^{(1)}(0)\frac{\mathrm{d}u^x}{\mathrm{d}x} - \frac{a^3}{3!}\tilde{w}^{(3)}(0)\frac{\mathrm{d}^3u^x}{\mathrm{d}x^3}\right]\Bigg|_{x=x'} = f^x, \\ & -\mathrm{i}a\tilde{\Lambda}_{xy}^{(1)}(0)\frac{\mathrm{d}u^x}{\mathrm{d}x} + \frac{\mathrm{i}a^3}{3!}\tilde{\Lambda}_{xy}^{(3)}(0)\frac{\mathrm{d}^3u^x}{\mathrm{d}x^3} - \frac{a\tilde{\Lambda}_{yy}^{(1)}(0)}{\pi}\int_{-\infty}^{+\infty}\frac{\left.\dfrac{\mathrm{d}u^y}{\mathrm{d}x}\right|_{x=x'}}{x'-x}\mathrm{d}x' = 0. \end{aligned} \tag{24}$$

By using the Hilbert transformation,

$$g(x) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{h(x')\mathrm{d}x'}{x'-x},$$

$$h(x) = -\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{g(x')\mathrm{d}x'}{x'-x},$$

the second equation of Eq.(24) can be changed into

$$\begin{aligned}\frac{\mathrm{d}u^y}{\mathrm{d}x} =& \frac{\mathrm{i}\tilde{\Lambda}_{xy}^{(1)}(0)}{\pi\tilde{\Lambda}_{yy}^{(1)}(0)}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x} \\ & \times\left[\frac{\mathrm{d}u^x}{\mathrm{d}x} - \frac{a^2}{3!}\frac{\tilde{\Lambda}_{xy}^{(3)}(0)}{\tilde{\Lambda}_{xy}^{(1)}(0)}\frac{\mathrm{d}^3u^x}{\mathrm{d}x^3}\right]\Bigg|_{x=x'}. \end{aligned} \tag{25}$$

Substituting this expression into the first equation of Eq.(24), one obtains

$$\begin{aligned} & -\frac{a^2}{2}\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2} - \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x} \\ & \times\left[a\gamma_1\frac{\mathrm{d}u^x}{\mathrm{d}x} - a^3\gamma_3\frac{\mathrm{d}^3u^x}{\mathrm{d}x^3}\right]\Bigg|_{x=x'} = f^x \end{aligned} \tag{26}$$

with

$$\gamma_1 = \tilde{w}^{(1)}(0) + \frac{[\tilde{\Lambda}_{xy}^{(1)}(0)]^2}{\tilde{\Lambda}_{yy}^{(1)}(0)},$$

$$\gamma_3 = \frac{1}{3!}\left[\tilde{w}^{(3)}(0) + \frac{\tilde{\Lambda}_{xy}^{(1)}(0)\tilde{\Lambda}_{xy}^{(3)}(0)}{\tilde{\Lambda}_{yy}^{(1)}(0)}\right].$$

For the SC lattice,

$$\gamma_1 = \frac{2}{3}, \qquad \gamma_3 = \frac{17}{144}.$$

If only the first-order derivative is kept, one recovers the result given in the elastic continuum theory. Through comparison, it can be recognized that

$$\gamma_1 = \frac{\mu a}{1-\nu}.$$

From the results given in the first section, $\nu = 1/4$, $\mu = \alpha/a$, and remembering that $2\alpha = 1$, one can see

that this relation holds exactly. Now, it is ready to write down

$$\begin{aligned}&-\alpha\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2}-\frac{\mu}{\pi(1-\nu)}\\&\times\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left(\frac{\mathrm{d}u^x}{\mathrm{d}x}-\gamma a^2\frac{\mathrm{d}^3u^x}{\mathrm{d}x^3}\right)\Big|_{x=x'}\\&=\frac{\mu a}{2\pi d}\sin\left(\frac{4\pi u^x}{a}\right),\end{aligned}\tag{27}$$

where α has been retrieved, d is the spacing between the upper and lower half-crystals, and

$$\gamma=\frac{\gamma_3}{\gamma_1}.$$

This equation can be reasonably viewed as a natural generalization of the classical Peierls equation. It can be applied generally as long as the coefficients α and γ are determined properly. The coefficients may take different value for different lattice, but the form of the equation will remain invariant. The new terms arise from the effects of lattice discreteness. They are important for the core structure of dislocation, and so the Peierls stress which is sensitive to the core structure.

The first term in the generalized equation also appears in the case of triangular lattice with different coefficient.[8] It results from the boundary effect. In the continuum approximation, one cannot clearly separate an individual lattice plane from the body of crystal, so the term associated with the boundary effects does not manifests itself. In the full lattice version, the border plane can be clearly identified, so it appears explicitly. Because the boundary plane divides the lattice into two separate parts, and is equally shared by both parts, thus the interaction is half the full interaction. Therefore, the coefficient α in the front of the second order derivative can be given an universal interpretation. It is an effective tensile constant of the glide plane decoupled from the other planes. Obviously, the coefficient α depends on the lattice characteristic, in particular, the glide plane characteristics. Generally, it is hard to relate the coefficient to the characteristic parameters given within continuum approximation. However, a relation between the coefficient α, Young's modulus E and bulk modulus B can be obtained for the SC lattice. The tensile force caused by the strain in glide direction is characterized by stiffness c_{11}. The couple between the planes is characterized by stiffness c_{12}. The tensile constant ignoring the couple should be $c_{11}-c_{12}$. Therefore, the coefficient α can be identified as

$$\alpha=\frac{d}{2}(c_{11}-c_{12}),\tag{28}$$

where d is the spacing of the planes. The Young's modulus and bulk modulus in terms of stiffness matrix elements are

$$E=c_{11}-\frac{2c_{12}^2}{c_{11}+c_{12}},\quad B=\frac{1}{3}(c_{11}+2c_{12}).$$

So one has

$$\alpha=E\left(\frac{3Bd}{9B-E}\right).\tag{29}$$

For the isotropic case, Eq.(29) degenerates into

$$\alpha=\mu d.$$

This expression agrees with our previously result where $d=a$ in the SC lattice.

The coefficient γ is also lattice dependent. Unfortunately, its implication is not as clear as α. One needs to investigate more different type of lattice to reveal the physical origin. However, it is usually small and sometimes negligible.

There are arguments on the applicability and accuracy of the sinusoidal force law.[6,12,15] Apparently, our results is independent of what the cohesive law is adopted. The sinusoidal force law is the first-order approximation of any force (cohesive) law used for actual crystal. The main qualitative features, or even quantitative behaviours can be predicted theoretically by using the sinusoidal force law.

A method for obtaining dislocation solution of Eq.(27) has been developed by introducing a new family of orthogonalized polynomials.[9] The solution takes the form

$$u^x=\frac{a}{2\pi}\left(\arctan p+\frac{cp}{1+p^2}\right)\tag{30}$$

with

$$p=\kappa x,\quad \kappa=\kappa_0(1-c),\quad \kappa_0=\frac{2(1-\nu)}{\mathrm{d}},$$

which satisfies the boundary condition

$$u^x|_{x\to\pm\infty}=\pm\frac{a}{4}.\tag{31}$$

Substituting the solution into the generalized Peierls equation, the left hand side becomes

$$\begin{aligned}&\frac{1}{\epsilon_0^2}(1-c)^2(1-c+4cy)y^2\\&+2(1-c)[y+2cy^2+\gamma\kappa_0^2a^2(1-c)^2y^2\\&\times(-2+8y-24cy+48cy^2)],\end{aligned}$$

and the right hand side becomes

$$2y[1 - 2c^2y(1-y)] + 2cy(2y-1),$$

with

$$y = \frac{1}{1+p^2},$$

$$\epsilon_0 = \frac{1}{2(1-\nu)}\sqrt{\frac{\mu d}{\alpha}}.$$

Multiplying y and integrating over the interval $(0,1)$, one obtains an algebraic equation satisfied by $c = 1-\epsilon$,

$$-\kappa_0^2 a^2 \gamma \left(8\epsilon - \frac{43}{4}\right)\epsilon^3 + \left(1 - \frac{11\epsilon}{16}\right)\frac{\epsilon^2}{\epsilon_0^2} - \epsilon^2 + 2\epsilon - 1 = 0.$$

For the SC lattice, the root gives $c = 0.68$.

The dislocation solution Eq.(30) has the same asymptotic behaviour as that given in the classical P-N theory. But the core structure is quite different. The dislocation width $1/\kappa$ from the generalized equation is several times as large as $1/\kappa_0$ given by the Peierls equation. Because the Peierls stress is sensitive to the core structure, it is expected that the accuracy of the prediction of the Peierls stress will be improved remarkably. The dislocation solution Eq.(30) is a robust one. It can be used to fit the data obtained from the experiments or the numerical calculations.

6. Discussion and summary

An improvement of the Peierls equation has been made by including the lattice effects which was ignored before. It is rational to believe that the terms arising from the discreteness effects is universal so that the form of the equation does not depend on the details of the model. In practical applications, what one needs to do is to properly determine the coefficients that newly appear in the equation. Therefore, the new equation can be reasonably used to be substitute for the old one in theoretical investigations of the dislocation. The major change of the predicted dislocation is in the core structure. The width of the dislocation core is much wider than that in the classical P-N theory.

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