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2009 J. Phys. A: Math. Theor. 42 025208

(http://iopscience.iop.org/1751-8121/42/2/025208)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 025208 (9pp) doi:10.1088/1751-8113/42/2/025208

A unified dislocation equation from lattice statics

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Received 30 July 2008, in final form 22 September 2008
Published 4 December 2008
Online at stacks.iop.org/JPhysA/42/025208

Abstract

A unified equation is presented for dislocations on the basis of lattice statics and symmetry principles. The equation satisfied by the displacement field defined on the two-dimensional misfit-plane can be applied to curved dislocations as well as straight dislocations. The correction for discreteness, which is important for the core structure, is included in the equation and related to the acoustic phonon velocity and lattice geometry structure. The dislocation equation of the new theory can be viewed as a kind of unification of the Peierls–Nabarro and Frenkel–Kontorva models of dislocations.

PACS numbers: 45.05.+x, 61.72.Bb

1. Introduction

Dislocation is a kind of topological defect in solids. The plastic deformation of solids is controlled in part by dislocation mobility, and the dislocation mobility is strongly affected by the core structure of the dislocation [1]. Hence, a key issue of dislocation is the core structure. The most famous theory of dislocations is the Peierls–Nabarro (P–N) theory that can predict the core width and the Peierls stress analytically [2, 3]. In order to investigate dislocations with both edge and screw components like the partial dislocation in the FCC lattice, the classical P–N theory has been extended to be a so-called 2D model in which the displacement is described by a two-dimensional vector [4–7]. The 2D model can be applied to straight dislocations, but cannot be applied to curved dislocations. Actually, there has been no true 2D model until now because the two components of the displacement are defined on a one-dimensional line.

In the P–N theory, the fundamental equation was derived through the balance between the nonlinear interaction from the misfit gluing and the linear interaction from the deformation. The linear interaction was obtained by an assumption that the crystal can be approximated as an elastic continuum. So the P–N theory is a hybridization of discreteness and continuum. Recently, the author has derived a dislocation equation from lattice statics that can recover

the Peierls equation when the effects of lattice discreteness are neglected [8]. However, in analogy to the original Peierls equation, the dislocation equation previously obtained by the author cannot easily be applied to the complex dislocations and needs to be generalized.

In this paper, a unified equation is derived on the basis of lattice statics and symmetry principles for the dislocation. The unified equation satisfied by the displacement field defined on the two-dimensional misfit plane is a true two-dimensional (2D) model that can be used to deal with curved dislocations as well as straight dislocations. When a straight dislocation line is considered, the old 2D equation is recovered as a special case. Furthermore, the discrete effect of the lattice, which is important to the core of dislocation, has been incorporated in a self-consistent way. The coefficients relevant to the discrete effects have been related to the acoustic phonon velocity and the lattice geometry.

2. Reduced dynamical matrix (RDM) for the surface of a half-infinite lattice

The main idea of the P–N theory is that the dislocation is created by gluing two half-infinite crystal. If the crystal with a dislocation is cut into two parts along the glide plane, each individual part is a regular crystal with the cut plane as its surface. Due to nonlinear interactions, the dislocation can be produced when the two parts are glued together non-trivially. In order to obtain the dislocation equation that only relates to the displacement of the atoms on the misfit plane, one needs to first solve the balance problem for a half-infinite crystal acted on by external forces on the surface. The problem can be formally solved by using the concept of the compensating force [8].

In the harmonic approximation, the force felt by an atom in an infinite lattice can be written as $-Du$, where D is the dynamical matrix and u is the displacement field. For the atoms in the half-infinite part above the cut plane, the force attributed to the atoms in the upper half can be obtained by extracting the contribution of the low half from the total force

$$-Du - (-\Gamma u),$$

where $-\Gamma u$ is the force from the atoms in the lower half. In the equilibrium, the external force f is balanced by the internal force

$$Du - \Gamma u = f. \tag{1}$$

This is the balance equation of the half-infinite crystal. The solution of equation (1) can be written as

$$u = G(1 - \Gamma G)^{-1} f, \tag{2}$$

where G is Green's function defined by

$$DG = 1.$$

When the force f imposed on the surface and only the displacements of the atoms on the surface are of interest, equation (2) gives the relation between the imposed force and the displacements of the atoms on the surface. It is helpful to introduce the reduced dynamical matrix (RDM) Λ,

$$\Lambda^{-1} = G(1 - \Gamma G)^{-1}, \tag{3}$$

and rewrite equation (2) as

$$\Lambda u = f,$$

or explicitly

$$\sum_{\mathbf{R}'} \sum_{j} \Lambda_{ij}(\mathbf{R} - \mathbf{R}') u_j(\mathbf{R}') = f_i(\mathbf{R}). \tag{4}$$

In the last equation, the atoms on the surface are labeled by two-dimensional lattice vectors $\mathbf{R}$, the components of the displacement are labeled by the subscripts $i = x, y$, $j = x, y$, and translation symmetry has been used.

In wave-vector space ($\mathbf{k}$-space), equation (4) becomes

$$\widetilde{\Lambda}(\mathbf{k})\widetilde{u}(\mathbf{k}) = \widetilde{f}(\mathbf{k}) \tag{5}$$

with

$$u(\mathbf{R}) = \frac{1}{\sigma^*}\int_{BZ} \widetilde{u}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}}\, \mathrm{d}\mathbf{k},$$

$$\Lambda(\mathbf{R}) = \frac{1}{\sigma^*}\int_{BZ} \widetilde{\Lambda}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}}\, \mathrm{d}\mathbf{k},$$

where σ^* is the area of the Brillouin zone of the surface that is a two-dimensional lattice. The RDM $\widetilde{\Lambda}(k)$ should be a Hermitian matrix

$$\widetilde{\Lambda}^{+}(\mathbf{k}) = \widetilde{\Lambda}(\mathbf{k}), \tag{6}$$

and in addition

$$\widetilde{\Lambda}^{*}(\mathbf{k}) = \widetilde{\Lambda}(-\mathbf{k}), \tag{7}$$

the last identity comes from the fact that $\Lambda(\mathbf{R})$ is real. When the matrix $\widetilde{\Lambda}(k)$ is decomposed into the real part and the imaginary part,

$$\widetilde{\Lambda}(\mathbf{k}) = \widetilde{\Lambda}^{r}(\mathbf{k}) + \mathrm{i}\widetilde{\Lambda}^{i}(\mathbf{k}).$$

From equations (6) and (7), it is easy to show that the real part has even parity and the imaginary part has odd parity,

$$\widetilde{\Lambda}^{r}(-\mathbf{k}) = \widetilde{\Lambda}^{r}(\mathbf{k}), \qquad \widetilde{\Lambda}^{i}(-\mathbf{k}) = -\widetilde{\Lambda}^{i}(\mathbf{k}).$$

For a rigid translation of the crystal, the displacement is the same for every atom, that is $u(\mathbf{R}) = u$, and no interaction force will appear,

$$\sum_{\mathbf{R}\prime} \Lambda(\mathbf{R} - \mathbf{R}')u(\mathbf{R}') = \sum_{\mathbf{R}} \Lambda(\mathbf{R})u = 0.$$

This equation is valid for arbitrary vectors u, thus

$$\sum_{\mathbf{R}} \Lambda(\mathbf{R}) = 0,$$

or in k-space

$$\widetilde{\Lambda}(0) = 0, \tag{8}$$

the matrix $\widetilde{\Lambda}$ in k-space vanishes at the center of the Brillouin zone.

3. The RDM with rotation symmetry in the long-wave approximation

In principle, the RDM can be calculated when the dynamical matrix of the solid is given. However, the RDM can be calculated exactly only for a few simplified models. For the case of a dislocation, the displacement field is essentially a slowly-varying field, and so it is unnecessary to calculate the whole RDM. It is enough to consider the long-wavelength approximation in which the discrete effects are included adequately. Besides, since the misfit plane is usually a close-packed plane that is nearly isotropic, it is reasonable to assume that the RDM in the long-wavelength approximation is invariant under the rotation with the axis perpendicular to the misfit plane.

Choosing the coordinates with z-axis normal to the misfit plane (x–y plane), under the rotation transformation with the axis perpendicular to the misfit plane, the wave vector $\mathbf{k} = (k_x, k_y)$, the horizontal components of the displacement $(\widetilde{u}_x, \widetilde{u}_y)$, and the force $(\widetilde{f}_x, \widetilde{f}_y)$ transform as a two-dimensional vector, the matrix block

$$\begin{pmatrix} \widetilde{\Lambda}_{xx} & \widetilde{\Lambda}_{xy} \\ \widetilde{\Lambda}_{yx} & \widetilde{\Lambda}_{yy} \end{pmatrix}$$

transforms as two-dimensional tensor, and $(\widetilde{\Lambda}_{xz}, \widetilde{\Lambda}_{yz})$ transforms as a two-dimensional vector, while the vertical components $\widetilde{u}_z$ and $\widetilde{f}_z$, $\widetilde{\Lambda}_{zz}$ transform as a scalar. Therefore, the invariant RDM under the rotation transformation must be

$$\widetilde{\Lambda}_{ij} = a\delta_{ij} + bk_ik_j, \qquad i, j = x, y$$

and

$$\widetilde{\Lambda}_{iz} = ck_i, i = x, y,$$

i.e.,

$$\widetilde{\Lambda} = \begin{pmatrix} a + bk_x^2 & bk_xk_y & ck_x \\ bk_xk_y & a + bk_y^2 & ck_y \\ c^*k_x & c^*k_y & \widetilde{\Lambda}_{zz} \end{pmatrix}, \tag{9}$$

where a, b and c are scalars. From the results given in section 2, one sees that a and b are real while c is pure imaginary. Because $\mathbf{k} = 0$ is a zero point,

$$\widetilde{\Lambda}|_{\mathbf{k}=0} = 0,$$

in the long-wave approximation one has

$$a(k) = a_1k + a_2k^2 + a_3k^3 + \cdots,$$

$$b(k) = \frac{b_{-1}}{k} + b_0 + \cdots,$$

$$c(k) = \mathrm{i}c_0 + \mathrm{i}c_1k + \mathrm{i}c_2k^2 + \cdots,$$

$$\widetilde{\Lambda}_{zz} = \widetilde{\Lambda}_{zz}^{(1)}k + \widetilde{\Lambda}_{zz}^{(2)}k^2 + \widetilde{\Lambda}_{zz}^{(3)}k^3 + \cdots,$$

with

$$k = \sqrt{k_x^2 + k_y^2},$$

where coefficients $a_1, b_{-1}, c_0, \widetilde{\Lambda}_{zz}^{(1)}$, etc are constants which depend on the properties of the crystal concerned. The terms including the root of k^2 represent the long-range interaction attributed to the atoms in the interior of the half crystal. The terms not including the root of k^2 represent the short-range interaction attributed to the atoms on the misfit plane. Because the main contribution to the coupling between the horizontal components and vertical components comes from the interaction among the atoms on the misfit plane, therefore

$$c(k) = \mathrm{i}c_0 + \mathrm{i}c_2k^2 + \cdots,$$

and there are no terms proportional to the root of k^2 in the expression for the scalar c.

In the first-order approximation in which only the leading terms are kept, one recovers the results given in the elastic continuum theory. The correction from the higher-order terms represents the discrete effects of the lattice. In the following, the lowest correction of the discrete effects considered, i.e., only the terms in the $\widetilde{\Lambda}$ with the power of k not larger than two are kept

$$a(k) = a_1k + a_2k^2, \qquad b(k) = \frac{b_{-1}}{k} + b_0, \qquad c(k) = \mathrm{i}c_0, \qquad \widetilde{\Lambda}_{zz} = \widetilde{\Lambda}_{zz}^{(1)}k + \widetilde{\Lambda}_{zz}^{(2)}k^2.$$

4. The equation in the real space

In the long-wave approximation, the displacement field in the real space is extended as a continuous field defined on the misfit plane (x–y plane)

$$u(\mathbf{r}) = \frac{1}{\sigma^*}\int_{BZ} \widetilde{u}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\mathrm{d}\mathbf{k}.$$

The RDM in real space can be expressed in terms of differential operators and integral operators. What one needs to do is determine these operators. The simplest operator is the wave-vector operator k_j, $j = (x, y)$ (the momentum operator),

$$\begin{aligned}\frac{1}{\sigma^*}\int_{BZ} k_x\widetilde{u}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\mathrm{d}\mathbf{k} &= \frac{1}{\sigma^*}\int_{BZ}\widetilde{u}(\mathbf{k})\frac{1}{i}\frac{\partial}{\partial x}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\mathrm{d}\mathbf{k}\\ &= \frac{1}{\mathrm{i}}\frac{\partial}{\partial x}\frac{1}{\sigma^*}\int_{BZ}\widetilde{u}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\mathrm{d}\mathbf{k} = \frac{1}{\mathrm{i}}\frac{\partial u}{\partial x},\end{aligned}$$

so

$$k_x \longrightarrow \frac{1}{\mathrm{i}}\frac{\partial}{\partial x},$$

and similarly

$$k_y \longrightarrow \frac{1}{\mathrm{i}}\frac{\partial}{\partial y},$$

i.e.,

$$\mathbf{k} \longrightarrow \frac{1}{\mathrm{i}}\nabla. \tag{10}$$

For the square of the modulus (the kinetic energy operator)

$$k^2 = k_x^2 + k_y^2,$$

The operator is

$$k^2 \longrightarrow -\nabla^2.$$

Observing the following identity:

$$\begin{aligned}\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y\frac{1}{r^3}\mathbf{r}\cdot\nabla\,\mathrm{e}^{\mathrm{i}\mathbf{r}\cdot\mathbf{k}} &= \frac{1}{2\pi\,\mathrm{i}}\int_0^{\infty}\mathrm{d}r\int_0^{2\pi}\mathrm{d}\theta\frac{k\cos\theta}{r}\,\mathrm{e}^{\mathrm{i}rk\cos\theta}\\ &= \frac{k}{2\pi\,\mathrm{i}}\int_0^{\infty}\mathrm{d}x\int_0^{2\pi}\mathrm{d}\theta\frac{\cos\theta}{x}\,\mathrm{e}^{\mathrm{i}x\cos\theta} = k,\end{aligned} \tag{11}$$

one has

$$\frac{1}{\sigma^*}\int_{BZ} k\widetilde{u}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\,\mathrm{d}\mathbf{k} = \frac{1}{\sigma^*}\int_{BZ}\frac{-1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y\frac{\mathbf{r}_1\cdot\nabla_{\mathbf{1}}}{r_1^3}\widetilde{u}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}+\mathbf{r}_1)}\,\mathrm{d}\mathbf{k}. \tag{12}$$

Redefining the integral variable in the last expression, $\mathbf{r}_1 = \mathbf{r}^{'} - \mathbf{r}$,

$$\begin{aligned}&\frac{1}{\sigma^*}\int_{BZ}\frac{-1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})\cdot\nabla'}{|\mathbf{r}'-\mathbf{r}|^3}\widetilde{u}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}\mathrm{d}\mathbf{k}\\ &\quad= \frac{-1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})\cdot\nabla'}{|\mathbf{r}'-\mathbf{r}|^3}\frac{1}{\sigma^*}\int_{BZ}\widetilde{u}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}\mathrm{d}\mathbf{k}\\ &\quad= \frac{-1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})\cdot\nabla'}{|\mathbf{r}'-\mathbf{r}|^3}u(\mathbf{r}'),\end{aligned}$$

one sees that the modulus operator is a integral operator

$$k \longrightarrow \frac{-1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}x' \int_{-\infty}^{\infty} dy' \frac{(\mathbf{r}'-\mathbf{r})\cdot\nabla'}{|\mathbf{r}'-\mathbf{r}|^3}. \tag{13}$$

In analogy, using the identity

$$\begin{aligned}\frac{1}{2\pi \mathrm{i}}\int_{-\infty}^{\infty}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y\frac{\mathbf{r}}{r^3}\,\mathrm{e}^{\mathrm{i}\mathbf{r}\cdot\mathbf{k}} &= -\frac{\nabla_{\mathbf{k}}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y\frac{1}{r^3}\,\mathrm{e}^{\mathrm{i}\mathbf{r}\cdot\mathbf{k}}\\ &= -\frac{\nabla_{\mathbf{k}}}{2\pi}\int_0^{\infty}\mathrm{d}r\int_0^{2\pi}\mathrm{d}\theta\frac{1}{r^2}\,\mathrm{e}^{\mathrm{i}rk\cos\theta} = \nabla_{\mathbf{k}}k\frac{-1}{2\pi}\int_0^{\infty}\mathrm{d}x\int_0^{2\pi}\mathrm{d}\theta\frac{1}{x^2}\,\mathrm{e}^{\mathrm{i}x\cos\theta} = \frac{\mathbf{k}}{k},\end{aligned} \tag{14}$$

the unit wave-vector operator $\mathbf{k}/k$ can be obtained,

$$\frac{\mathbf{k}}{k} \longrightarrow \frac{1}{2\pi \mathrm{i}}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}. \tag{15}$$

From the operator expressions given above, it is straightforward to obtain an equation in the real space in the long-wavelength approximation that reads

$$\begin{aligned}-a_2\nabla^2\mathbf{u} - b_0\nabla\nabla\cdot\mathbf{u} - c_0\nabla u_z - \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{1}{|\mathbf{r}'-\mathbf{r}|^3}[a_1(\mathbf{r}'-\mathbf{r})\cdot\nabla'\mathbf{u}\\ + b_{-1}(\mathbf{r}'-\mathbf{r})\nabla'\cdot\mathbf{u}] = \mathbf{f},\end{aligned} \tag{16}$$

$$-\widetilde{\Lambda}_{zz}^{(2)}\nabla^2 u_z + c_0\nabla\cdot\mathbf{u} - \frac{\widetilde{\Lambda}_{zz}^{(1)}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})\cdot\nabla' u_z}{|\mathbf{r}'-\mathbf{r}|^3} = f_z, \tag{17}$$

where $\mathbf{u}(\mathbf{r})$ and u_z are respectively the horizontal and vertical components of the relative displacement of the misfit planes that are glued together in an nontrivial way to produce a dislocation, $\mathbf{f}$ and f_z are respectively the horizontal and vertical components of the interaction force [8].

For the dislocation, the misfit is mainly focused on the shear (horizontal) component. Two misfit planes slip relatively while the space between the misfit planes is nearly unchanged. Therefore, the vertical component f_z is small and can be neglected. Besides, because the coefficient $\widetilde{\Lambda}_{zz}^{(2)}$ represents the force induced by inhomogeneous vertical deformation of the plane, it is also small and can be neglected. Now, equation (17) can be written as

$$\nabla\cdot\mathbf{u} = \frac{\widetilde{\Lambda}_{zz}^{(1)}}{2\pi c_0}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})\cdot\nabla' u_z}{|\mathbf{r}'-\mathbf{r}|^3}, \tag{18}$$

or simply

$$\mathrm{i}\mathbf{k}\cdot\mathbf{u} = -\frac{\widetilde{\Lambda}_{zz}^{(1)}}{c_0}ku_z,$$

where $\mathbf{k}$ and k are operators given above. It is clear that the vertical component can be expressed as

$$u_z = -\frac{c_0}{2\pi\Lambda_{zz}^{(1)}}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})\cdot\mathbf{u}(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|^3}, \tag{19}$$

and

$$\nabla u_z = -\frac{c_0}{2\pi\Lambda_{zz}^{(1)}}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{(\mathbf{r}'-\mathbf{r})\nabla'\cdot\mathbf{u}(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|^3}. \tag{20}$$

Substituting equation (20) into equation (16), one finally obtains

$$-a_2\nabla^2\mathbf{u} - b_0\nabla(\nabla\cdot\mathbf{u}) - \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x'\int_{-\infty}^{\infty}\mathrm{d}y'\frac{1}{|\mathbf{r}'-\mathbf{r}|^3}[a_1(\mathbf{r}'-\mathbf{r})\cdot\nabla'\mathbf{u} + b_1'(\mathbf{r}'-\mathbf{r})\nabla'\cdot\mathbf{u}] = \mathbf{f} \quad (21)$$

with

$$b_1' = b_1 - \frac{c_0^2}{\Lambda_{zz}^{(1)}}.$$

This is the equation satisfied by the horizontal-displacement field defined on the misfit plane. The different types of the dislocations can be described by this equation in a unified way. It is a unified dislocation equation. The relation between the interaction force **f** and the displacement **u** can be obtained through the γ surface calculated from first principles [5, 6]. The dislocation equation can be equivalently stated in the form of a variational principle. The variational functional is

$$J = \frac{1}{2}\int\mathrm{d}\mathbf{r}\left(a_2\sum_{ij}\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j} + b_0\sum_{ij}\frac{\partial u_i}{\partial x_i}\frac{\partial u_j}{\partial x_j}\right) + \frac{1}{4\pi}\int\mathrm{d}\mathbf{r}\int\mathrm{d}\mathbf{r}'\frac{1}{|\mathbf{r}'-\mathbf{r}|} \times\left(a_1\sum_{ij}\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j'} + b_{-1}'\sum_{ij}\frac{\partial u_i}{\partial x_i}\frac{\partial u_j}{\partial x_j'}\right) + \int\mathrm{d}\mathbf{r}\,\gamma(\mathbf{u}), \quad (22)$$

where $x_i = (x, y)$ has been used for convenience, $\gamma(\mathbf{u})$ is the so-called γ surface from which the nonlinear force can be obtained

$$\mathbf{f} = -\frac{\partial\gamma}{\partial\mathbf{u}}. \quad (23)$$

5. The coefficients in the equation

The coefficients a_2, b_0, a_1 and b_{-1}' appearing in the dislocation equation (21) can be interpreted physically. While the dislocation equation takes a universal form, these coefficients depend on the specific solid under consideration. For a straight dislocation line, it is easy to show that the dislocation equation becomes

$$-(a_2+b_0)\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2} - \frac{a_1+b_{-1}'}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\frac{\mathrm{d}u^x}{\mathrm{d}x}\bigg|_{x=x'} = f_x \quad (24)$$

$$-a_2\frac{\mathrm{d}^2u^y}{\mathrm{d}x^2} - \frac{a_1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\frac{\mathrm{d}u^y}{\mathrm{d}x}\bigg|_{x=x'} = f_y, \quad (25)$$

where the y-axis has been chosen to be parallel to the dislocation line. If the second-order differential terms are neglected, equations (24) and (25) are just the so-called $2D$ model proposed before. If an edge dislocation is considered, the first equations (24) recover the classical Peierls equation. By comparing, it is easy to express the coefficients a_1 and b_{-1}' in terms of the energy factors of dislocations

$$a_1 = K_s\sigma, \qquad b_{-1}' = (K_e - K_s)\sigma, \quad (26)$$

where K_e (K_s) is the energy factor of the edge (screw) dislocation [1], σ is the area of the primitive cell of the misfit plane. For an isotropic solid, the energy factors is given simply by

$$K_s = \mu, \qquad K_e = \frac{\mu}{1-\nu}, \quad (27)$$

where μ is the shear modulus and ν is the Poisson's ratio.

The second-order differential terms in the dislocation equation result from the surface effect. When a half crystal is viewed as a set of parallel planes, the plane at the top (surface) is not equivalent to the other planes. In the continuum approximation, the distinction does not manifest and so the surface effect is missed. When the modification due to the discreteness of the lattice is considered, such a surface effect represented by the second-order differential terms appears. The surface effect is a high-order correction which is important for the core structure of the dislocation. Actually, in the Frenkel and Kontorva (F–K) model [9], only the interaction of the atoms on the surface (the misfit plane) was considered while the interaction between the atom on the surface and the atom at the interior is neglected.

In the long-wavelength approximation, the force attributed to the interaction among the atoms on a misfit plane with the rotational symmetry can be written as

$$\mathbf{f}_{\text{plane}} = \rho_s \sigma c_{st}^2 \nabla^2 \mathbf{u} + \rho_s \sigma \left(c_{sl}^2 - c_{st}^2\right) \nabla(\nabla \cdot \mathbf{u}), \tag{28}$$

where ρ_s is the mass in a unit area of the misfit plane, c_{st} (c_{sl}) is the acoustic wave velocity of a transverse (longitudinal) phonon of a misfit plane which has been uncoupled from the other planes and is considered as an isolated two-dimensional lattice. Obviously, the differential terms should be proportional to $\mathbf{f}_{\text{plane}}$ given by equation (28). Furthermore, from the solvable model, it is found that the ratio factor equals approximately $3/4$. Thus one can recognize

$$a_2 = \tfrac{3}{4} \rho_s \sigma c_{st}^2, \tag{29}$$

$$b_0 = \tfrac{3}{4} \rho_s \sigma \left(c_{sl}^2 - c_{st}^2\right). \tag{30}$$

Unfortunately, the velocity of an acoustic wave of an uncoupled plane cannot be measured directly. One needs to relate it with the velocity of the bulk acoustic wave. It is observed that for the bulk wave propagating along the direction parallel to the misfit plane, the transverse wave with polarization perpendicular to the plane is dominated by the coupling between the planes. In comparison, the longitudinal wave depends on both the inter-plane interaction and on-plane interaction. This indicates that the wave velocity of the uncoupled plane can be obtained from the bulk counterpart extracting the coupling contribution which is represented by the transverse wave mentioned above. Indeed, it is found that the following expressions are valid, in particular for the short-range interactions that are generally used for solids

$$c_{sl}^2 = c_l^2 - c_{tv}^2 \tan^2\theta \cos^2\phi, \tag{31}$$

$$c_{st}^2 = c_{th}^2 - c_{tv}^2 \tan^2\theta \sin^2\phi, \tag{32}$$

where c_l is the velocity of the longitudinal wave propagating along the misfit plane in the bulk crystal, c_{th} (c_{tv}) is the velocity of the transverse wave propagating along the misfit plane in the bulk crystal and polarized horizontally (vertically), θ and ϕ are the orientation angles of the relative-position vector of a pair of neighbor atoms in the intrinsic frame given by the three polarizations. The neighbor atoms should be chosen in such a way that their interaction dominates the transverse wave polarized vertically. For the misfit plane (100) in the SC lattice, $\tan\theta = 1$ and $\phi = 0$. For the (111) plane in the FCC lattice, $\tan\theta = 1/\sqrt{2}$ and $\phi = \pi/6$. In the isotropic approximation, the bulk-wave velocities are

$$c_{th}^2 = c_{tv}^2 = \frac{\mu}{\rho}, \qquad c_l^2 = \frac{2\mu(1-\nu)}{\rho(1-2\nu)},$$

where ρ is the bulk density of the mass. It is worthwhile to point out that the coefficients involved in the modification caused by the discreteness effects depend on the geometric structure as well as on the elastic constants.

6. Summary

A unified equation is presented for dislocations derived on the basis of lattice statics and symmetry principles. The equation satisfied by the displacement field defined on the two-dimensional misfit plane can be applied to curved dislocations as well as straight dislocations. It can also be applied to deal with the dislocation nets resulting from the mismatch. The equations obtained for half-infinite crystals are also useful for some relevant problems involving the surface, such as cracks and the deformation induced by the probe of an atomic-force microscope.

The dislocation equation is obtained on the assumption that the misfit plane has rotational symmetry, but not requiring that the bulk crystal is isotropic. For most cases of interest, the rotational symmetry of the plane holds up. If the rotational symmetry is broken, the equation can be straightforwardly generalized to include anisotropic effects at the price of introducing more coefficients.

The dislocation equation goes beyond the continuum theory because modifications due to discrete effects are included. Formally, the terms related to the discrete effects are the same as that appearing in the F–K equation. So the equation can be viewed as a unification of the Peierls equation and the F–K equation. Since the discreteness correction depends on the specific geometric structure, the core structure will be different for isotropic crystals with different structures. Provided that the nonlinear interaction between the misfit planes is given, the dislocation can be obtained as the solution of the equation. A detailed discussion for a specific dislocation will be presented elsewhere.

Acknowledgment

The work is supported by the National Natural Science Foundation of China (grant no 10774196)

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