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Dislocation equation from the lattice dynamics*

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Abstract

A dislocation equation satisfied by both horizontal displacement parallel to the glide plane and vertical displacement perpendicular to the glide plane has been derived generally from the lattice dynamics. In the slow-varying approximation that can be well applied to the dislocation, the equation has been changed into an integro-differential equation that possesses a universal form except the coefficients. If the higher-order derivatives of the displacement are canceled, the classic Peierls equation is recovered. The terms proportional to the higher-order derivatives represent the lattice effects that cannot be obtained in the continuum theory, and cannot be neglected in the core of the dislocation. The results are helpful to link the plasticity with the electronic structure of material because it is rigorously shown that the dislocation structure is mainly controlled by a few factors.

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1. Introduction

The relationship between the electronic structure and plasticity of material remains to be a challenge in the condensed matter theory. On the atomic level, the plasticity can be interpreted by virtue of the dislocation. The plastic deformation in metals and semiconductors is controlled by the mobility of dislocation and interactions of dislocations with each other and with other defects in the crystal [1]. The mobility and interactions are controlled by the core structure of the dislocation. Hence, the key is the core structure of the dislocation. In order to understand the relationship between electronic structure and plasticity, it is essential to understand first what control the structure of the dislocation and reveal the general relationships between the dislocation structure and the crystal characteristics from first principles.

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Since the dislocation mechanism of the material plasticity was introduced by Orowan, Polanyi and Taylor [2], great efforts have been made in understanding the structure of the dislocation. The most famous and successful theory is the Peierls–Nabarro (P–N) theory [3–5]. The P–N theory provides a conceptual framework for the dislocation structure and energetics. Appearance of dislocation will break the global order and make the crystal differ from a perfect crystal in topology. The different topology can be obtained by the different gluing. A well known example is the Mobius strip that can be obtained by gluing a band in a non-trivial way. In the P–N theory, the crystal is divided into two parts along the glide plane of the dislocation. Due to nonlinear interaction, dislocation defect is produced when the two parts are glued non-trivially. Unfortunately, although the gluing idea light the way for solving the problem involving the topology, the classical P–N theory has not thought useful as a predictive tool because prediction lack a quantitative agreement with experiments [1]. There are drawbacks that should be improved. In the P–N theory, the fundamental equation (Peierls equation) that determine the dislocation structure is a balance between the nonlinear force due to misfit gluing and the linear force due to deformation. Initially, the linear force was obtained through an assumption that the crystal can be approximated as an elastic continuum. The nonlinear force was approximated by the sinusoidal force law. Later, Christian and Vitek [6] suggested that the nonlinear interaction can be identified with the generalized stacking fault (GFS) energy. The GSF energy is an effective interplanar potential energy which can be obtained from first principles. The theoretical predictions have been improved remarkably since the GFS energy could be evaluated accurately [7–12]. However, the drawback of the continuum approximation remain to be relaxed. At the core of the dislocation, the displacement field varies so abruptly that Peierls equation is no longer valid in particular for the narrow dislocation. Therefore, the accuracy of prediction can be effected strongly by the continuum approximation. The discrete effects had been incorporated into the P–N theory by replacing the integrations by the discrete sums [7, 8]. However, in order to include the lattice effects adequately, one should relax the continuum approximation at the beginning and derive the modified equation from the first principles. Recently, author has made an effort to derive the Peierls equation from the lattice dynamics rather than the elastic mechanics. A modified equation has been derived for some simplified models [13, 14]. In this paper, it is shown that from the lattice dynamics an improved dislocation equation which includes the lattice effects can be derived generally. The equation is an integro-differential equation that possesses a universal form except the coefficients. If the higher-order derivatives of the displacement are canceled, the classic Peierls equation is recovered. The terms proportional to the higher-order derivatives represent the lattice effects that cannot be obtained in the continuum theory, and cannot be neglected in the core of the dislocation.

The context is organized as follows. In the following section, the problem of a half-infinite crystal with the external force imposed on the surface is solved formally. In section 3, the reduced dynamical matrix (RDM) in the wave-vector space has been discussed based on general features of the crystal. It is found that the behavior of the RMD can be qualitatively determined from the general features of the lattice. In section 4, based on the results obtained, the elements of the RDM in the k-space are expanded in the Fourier series, and the related operators in the real space are given in the slow-varying approximation. In section 5, the chiral symmetry has been introduced to understand the structure of the equation. The chiral symmetry may be also called parity symmetry because it is originated from equivalence of the left and right. In section 6, the dislocation equation is derived within the local interaction approximation between two half-infinite crystals. The last section is a brief discussion and summary.

2. Border equation of a two-dimensional half-infinite lattice

For a two-dimensional (2D) half-infinite lattice, if the external force is imposed only on the atoms located at the border, one can derive a balance equation that relates the displacement of the border atoms to the external force. The equation can be easily obtained by introducing the concept of compensating force. Let's image the half-infinite lattice as the upper half of an infinite lattice. In the harmonic approximation, internal force felt by the atom in the infinite lattice can be written as $-Du$, where D is the 2×2 dynamical matrix,

$$D = \begin{pmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{pmatrix},$$

and $u = (u_x, u_y)$ is the displacement field. Focusing on the atoms in the upper half, the internal force only from the atoms in the upper half can be obtained by extracting the contribution of the lower half from the total force $-Du$. The contribution from the atoms in the lower half will be referred to as compensating force and denoted by $-\Gamma u$. In the equilibrium, the external force $f = (f_x, f_y)$ is balanced by the internal force that is given by the difference of the total force and compensating force

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

This is the balance equation that is written in the matrix form for convenience. Obviously, the compensating force is closely related to the dynamics of the lattice. If the dynamical matrix D is given, the compensating matrix Γ can be separated from the D [13, 14].

In terms of Green's function G

$$DG = 1,$$

the solution of equation (1) can be written as

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

If the force f does not vanish only for the atoms on the border and the displacements of the border atoms are interested, equation (2) gives the relation between the imposed force and the displacements of the atoms on the border. In order to show this explicitly, let's introduce

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

and rewrite equation (2) explicitly as

$$u_i(n, l) = \sum_{n'l'} \sum_j \Lambda_{ij}^{-1}(n, n', l - l') f_j(n', l'),$$

where $n, n' = 0, 1, 2, \ldots$, is the order number of the atom chains parallel to the border and integers $l, l' = 0, \pm 1, \pm 2, \ldots$, are used to label the atoms on the chain. The translation symmetry along the border direction has been used in the expression. Since displacements of the atoms on the border $n = 0$ are considered only and $f_j(n', l') = 0$ if $n' \neq 0$, so equation (2) reduces as unidimensional

$$u_i(0, l) = \sum_{l'} \sum_j \Lambda_{ij}^{-1}(0, 0, l - l') f_j(0, l').$$

In brief,

$$u_i(l) = \sum_{l'} \sum_j \Lambda_{ij}^{-1}(l - l') f_j(l'),$$

or

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

Equation (4) is a balance equation of the border acted by the external force. It will be named as the border equation and the matrix $\Lambda_{ij}(l-l')$ will be named as the reduced dynamical matrix (RDM).

In the wave-vector space (k-space), the border equation becomes

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

with

$$u(l) = \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{u}(k)\,\mathrm{e}^{-\mathrm{i}lka}\,\mathrm{d}k,$$

$$\Lambda(l) = \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}(k)\,\mathrm{e}^{-\mathrm{i}lka}\,\mathrm{d}k,$$

where a is the period of the border.

If the external force is imposed along the direction parallel to the border, that is

$$\widetilde{f}_y = 0,$$

then the vertical component $\widetilde{u}^y$ can be simply expressed by the parallel component $\widetilde{u}^x$,

$$\widetilde{u}_y = -\frac{\widetilde{\Lambda}^*_{xy}}{\widetilde{\Lambda}_{yy}}\widetilde{u}_x, \tag{6}$$

and the parallel component $\widetilde{u}^x$ satisfies the following equation:

$$\left(\widetilde{\Lambda}_{xx} - \frac{|\widetilde{\Lambda}_{xy}|^2}{\widetilde{\Lambda}_{yy}}\right)\widetilde{u}_x = \widetilde{f}_x. \tag{7}$$

3. General properties of the RDM in the *k*-space

Because the RDM $\widetilde{\Lambda}(k)$ is a Hermitian matrix

$$\widetilde{\Lambda}^+(k) = \widetilde{\Lambda}(k), \tag{8}$$

the diagonal elements are real

$$\widetilde{\Lambda}^*_{xx}(k) = \widetilde{\Lambda}_{xx}(k), \qquad \widetilde{\Lambda}^*_{yy}(k) = \widetilde{\Lambda}_{yy}(k),$$

and the off-diagonal elements are conjugated

$$\widetilde{\Lambda}^*_{xy}(k) = \widetilde{\Lambda}_{yx}(k).$$

From the fact that $\Lambda(l)$ is a real matrix, it is easy to obtain

$$\widetilde{\Lambda}^*(k) = \widetilde{\Lambda}(-k). \tag{9}$$

From equations (8) and (9) it is clear that in the k-space the diagonal elements are real even functions,

$$\widetilde{\Lambda}_{xx}(-k) = \widetilde{\Lambda}_{xx}(k) = \widetilde{\Lambda}^*_{xx}(k), \qquad \widetilde{\Lambda}_{yy}(-k) = \widetilde{\Lambda}_{yy}(k) = \widetilde{\Lambda}^*_{yy}(k).$$

As for the off-diagonal elements, the real part is an even function and the imaginary part is an odd function,

$$\widetilde{\Lambda}^*_{xy}(k) = \widetilde{\Lambda}_{xy}(-k).$$

Let's decompose the matrix $\widetilde{\Lambda}(k)$ into the real part and the imaginary part

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

Then, the real part $\widetilde{\Lambda}^r(k)$ is even,

$$\widetilde{\Lambda}^r(-k) = \widetilde{\Lambda}^r(k),$$

and the imaginary part $\widetilde{\Lambda}^i(k)$ is odd,

$$\widetilde{\Lambda}^i(-k) = -\widetilde{\Lambda}^i(k).$$

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

$$\sum_{l'} \Lambda(l - l')u(l') = \sum_{l} \Lambda(l)u = 0.$$

Because u is an arbitrary vector, one obtains

$$\sum_{l} \Lambda(l) = 0$$

or

$$\widetilde{\Lambda}(0) = 0. \tag{10}$$

Therefore, the matrix $\widetilde{\Lambda}$ vanishes at the center of the Brillouin zone. At the ends of the Brillouin zone $k = \pm\pi/a$, it can be proved that the imaginary part vanishes

$$\widetilde{\Lambda}^i|_{k=\pm\frac{\pi}{a}} = 0,$$

and the derivative of the real part $\widetilde{\Lambda}^r$ vanishes

$$\left.\frac{\mathrm{d}\widetilde{\Lambda}^r}{\mathrm{d}k}\right|_{k=\pm\frac{\pi}{a}} = 0.$$

The proof is simple. From the periodicity

$$\widetilde{\Lambda}\left(k + \frac{2\pi}{a}\right) = \widetilde{\Lambda}(k),$$

one has

$$\widetilde{\Lambda}\left(k + \frac{\pi}{a}\right) = \widetilde{\Lambda}\left(k - \frac{\pi}{a}\right).$$

Because $\widetilde{\Lambda}^r$ is a periodic even function, one has

$$\widetilde{\Lambda}^r\left(k + \frac{\pi}{a}\right) = \widetilde{\Lambda}^r\left(-k + \frac{\pi}{a}\right). \tag{11}$$

Taking differential to the both sides of equation (11), then let $k = 0$, one obtains

$$\left.\frac{\mathrm{d}\widetilde{\Lambda}^r}{\mathrm{d}k}\right|_{k=\frac{\pi}{a}} = -\left.\frac{\mathrm{d}\widetilde{\Lambda}^r}{\mathrm{d}k}\right|_{k=\frac{\pi}{a}} = 0.$$

Because $\widetilde{\Lambda}^i$ is a periodic odd function, one has

$$\widetilde{\Lambda}^i\left(k + \frac{\pi}{a}\right) = -\widetilde{\Lambda}^i\left(-k + \frac{\pi}{a}\right). \tag{12}$$

Taking $k = 0$, one obtains

$$\widetilde{\Lambda}^i\left(\frac{\pi}{a}\right) = -\widetilde{\Lambda}^i\left(\frac{\pi}{a}\right) = 0.$$

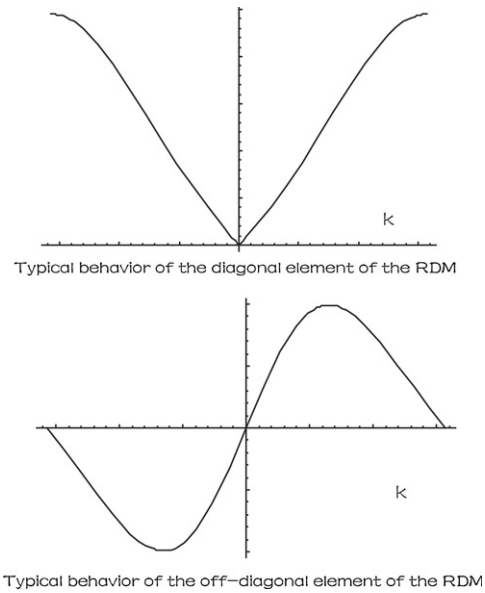

Figure 1. The typical behaviors of the elements of the RDM in the k-space. All the elements vanish at the origin, $k = 0$. The diagonal elements have singularity at the origin while the off-diagonal is smooth in the Brillouin zone.

In figure 1, the matrix elements as a function of the wave vector k have been plotted qualitatively. The behaviors of the real elements look like the phonon dispersion relation. Its derivative is not continuous at the origin. The imaginary elements are smooth functions.

If the matrix $\widetilde{\Lambda}$ is expanded in the power series at the origin $k = 0$, its real part will be

$$\widetilde{\Lambda}^r = |k| \left[\frac{\mathrm{d}\widetilde{\Lambda}^r}{\mathrm{d}k}(0) + \frac{1}{3!}\frac{\mathrm{d}^2\widetilde{\Lambda}^r}{\mathrm{d}k^3}(0)k^2 + \cdots \right] + \frac{1}{2!}\frac{\mathrm{d}^2\widetilde{\Lambda}^r}{\mathrm{d}k^2}(0)k^2 + \frac{1}{4!}\frac{\mathrm{d}^4\widetilde{\Lambda}^r}{\mathrm{d}k^4}(0)k^4 + \cdots,$$

and its imaginary part will be

$$\widetilde{\Lambda}^i = \frac{\mathrm{d}\widetilde{\Lambda}^i}{\mathrm{d}k}(0)k + \frac{1}{3!}\frac{\mathrm{d}^3\widetilde{\Lambda}^i}{\mathrm{d}k^3}(0)k^3 + \cdots.$$

Apparently, $\widetilde{\Lambda}^r$ is consisted of singular part and regular part

$$\widetilde{\Lambda}^r = \widetilde{\Lambda}^{rs} + \widetilde{\Lambda}^{rr},$$

with

$$\widetilde{\Lambda}^{rs} = |k| \left[\frac{\mathrm{d}\widetilde{\Lambda}^r}{\mathrm{d}k}(0) + \frac{1}{3!}\frac{\mathrm{d}^3\widetilde{\Lambda}^r}{\mathrm{d}k^3}(0)k^2 + \cdots \right],$$

$$\widetilde{\Lambda}^{rr} = \frac{1}{2!}\frac{\mathrm{d}^2\widetilde{\Lambda}^r}{\mathrm{d}k^2}(0)k^2 + \frac{1}{4!}\frac{\mathrm{d}^4\widetilde{\Lambda}^r}{\mathrm{d}k^4}(0)k^4 + \cdots.$$

The singularity of $\widetilde{\Lambda}^r$ at the origin is a representative of the long-range interaction. The Hermitian property of the RDM in the k-space implies

$$\Lambda^T(l) = \Lambda(-l), \tag{13}$$

in the real space.

4. The Fourier series and slow-varying approximation

Following the method given in ref [14], the Fourier series and slow-varying approximation of the RDM are discussed in this section. For the imaginary part, the Fourier series is simple

$$\widetilde{\Lambda}^i = \sum_n b_n^i \sin(nka), \qquad b_n^i = \frac{a}{\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}^i \sin(nka)\,\mathrm{d}k,$$

where the property of the odd function has been used. For the regular part of the real part, the Fourier series is also simple

$$\begin{aligned}
\widetilde{\Lambda}^{rr} &= \sum_n b_n^{rr}\cos(nka),\\
b_0^{rr} &= \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}^{rr}\,\mathrm{d}k,\\
b_n^{rr} &= \frac{a}{\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}^{rr}\cos(nka)\,\mathrm{d}k, \qquad n\neq 0,
\end{aligned}$$

where the property of the even function has been used.

It should be careful when the singular part $\widetilde{\Lambda}^{rs}$ is expanded in the Fourier series. Because of the singularity, $\widetilde{\Lambda}^{rs}$ cannot be expanded simply like $\widetilde{\Lambda}^i$ and $\widetilde{\Lambda}^{rr}$. In order to expand $\widetilde{\Lambda}^{rs}$ in a correct way, instead of the whole Brillouin zone, one should take the half Brillouin zone $(0, \pi/a)$ as the domain in which $\widetilde{\Lambda}^{rs}$ is smooth. This can always be done because $\widetilde{\Lambda}^{rs}$ is an even function. The $\widetilde{\Lambda}^{rs}$ as a function defined in the half Brillouin zone satisfies the following boundary conditions:

$$\widetilde{\Lambda}^{rs}|_{k=0} = 0, \qquad \left.\frac{\mathrm{d}\widetilde{\Lambda}^{rs}}{\mathrm{d}k}\right|_{k=\frac{\pi}{a}} = 0.$$

Therefore, it can be expanded as

$$\begin{aligned}
\widetilde{\Lambda}^{rs} &= \sum_n b_n^{rs}\sin\left(n+\frac{1}{2}\right)ka,\\
b_n^{rs} &= \frac{2a}{\pi}\int_0^{\frac{\pi}{a}} \widetilde{\Lambda}^{(rs)}\sin\left(n+\frac{1}{2}\right)ka\,\mathrm{d}k.
\end{aligned} \tag{14}$$

Substituting $\widetilde{\Lambda}$ expressed in the Fourier series into the equation

$$\Lambda(l) = \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}(k)\,\mathrm{e}^{-\mathrm{i}lka}\,\mathrm{d}k,$$

one can express $\Lambda(l)$ in terms of Fourier coefficients,

$$\begin{aligned}
\Lambda^{rr}(l) &= \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}^{rr}(k)\,\mathrm{e}^{-\mathrm{i}lka}\,\mathrm{d}k\\
&= \frac{1}{2}\sum_n(\delta_{n+l}+\delta_{n-l})b_n^{rr},\\
\Lambda^{i}(l) &= \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}^{i}(k)\,\mathrm{e}^{-\mathrm{i}lka}\,\mathrm{d}k\\
&= \frac{\mathrm{i}}{2}\sum_n(\delta_{n+l}-\delta_{n-l})b_n^{i},
\end{aligned}$$

$$\Lambda^{rs}(l) = \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \widetilde{\Lambda}^{rs}(k)\,\mathrm{e}^{-\mathrm{i}lka}\,\mathrm{d}k$$
$$= \frac{a}{2\pi}\sum_n \frac{2n+1}{\left(\frac{2n+1}{2}\right)^2 - l^2} b_n^{rs}.$$

Now it is time to discuss the border equation in the slow-varying approximation. First,

$$\sum_{\ell'}\Lambda^{rs}(\ell-\ell')u(\ell') = \frac{1}{2\pi}\sum_{\ell'}\sum_{n=1}^{\infty}\frac{(2n+1)b_n^{rs}}{\left(\frac{2n+1}{2}\right)^2-(\ell-\ell')^2}u(\ell')$$
$$= \frac{-1}{2\pi}\sum_{n=1}^{\infty} b_n^{rs}\sum_{\ell'}\left[\frac{u(\ell')}{\ell-\ell'-\frac{2n+1}{2}} - \frac{u(\ell')}{\ell-\ell'+\frac{2n+1}{2}}\right]$$
$$= \frac{-1}{2\pi}\sum_{n=1}^{\infty} b_n^{rs}\sum_{\sigma}\frac{u\left(\sigma+\frac{2n+1}{2}\right)-u\left(\sigma-\frac{2n+1}{2}\right)}{\sigma-\ell},$$

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

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

In addition, from equation (14), it is easy to get an identity

$$\sum_{n=1}^{\infty}\left(\frac{2n+1}{2}\right)^{2j+1} b_n^{rs} = (-1)^j\frac{\mathrm{d}^{2j+1}\tilde{\Lambda}^{rs}(k)}{\mathrm{d}k^{2j+1}}\bigg|_{k=0^+}.$$

By virtue of the identity, one can arrive at

$$\sum_{\ell'}\Lambda^{rs}(\ell-\ell')u(\ell') = \frac{-1}{\pi}\sum_{\sigma}\frac{1}{\sigma-\ell}\sum_{j=0}^{\infty}\frac{(-1)^j}{(2j+1)!}\frac{\mathrm{d}^{2j+1}\tilde{\Lambda}^{rs}(k)}{\mathrm{d}k^{2j+1}}\bigg|_{k=0^+}\frac{\mathrm{d}^{2j+1}u(\sigma)}{\mathrm{d}\sigma^{2j+1}}$$
$$= \frac{-1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\frac{1}{1!}\frac{\mathrm{d}\tilde{\Lambda}^{rs}}{\mathrm{d}k}\bigg|_{k=0^+}\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{1}{3!}\frac{\mathrm{d}^3\tilde{\Lambda}^{rs}}{\mathrm{d}k^3}\bigg|_{k=0^+}\frac{\mathrm{d}^3u}{\mathrm{d}x^3}+\cdots\right]\bigg|_{x=x'},$$
$$= \frac{-1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\frac{1}{1!}\frac{\mathrm{d}\tilde{\Lambda}^{r}}{\mathrm{d}k}\bigg|_{k=0^+}\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{1}{3!}\frac{\mathrm{d}^3\tilde{\Lambda}^{r}}{\mathrm{d}k^3}\bigg|_{k=0^+}\frac{\mathrm{d}^3u}{\mathrm{d}x^3}+\cdots\right]\bigg|_{x=x'}, \tag{15}$$

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

$$-\mathrm{i}\sum_{\ell'}\Lambda^{i}(\ell-\ell')u(\ell') = \frac{1}{2}\sum_{n=1}^{\infty} b_n^i[u(\ell+n)-u(\ell-n)]$$
$$= \frac{1}{1!}\frac{\mathrm{d}\tilde{\Lambda}^i}{\mathrm{d}k}\bigg|_{k=0}\frac{\mathrm{d}u}{\mathrm{d}x} - \frac{1}{3!}\frac{\mathrm{d}^3\tilde{\Lambda}^i}{\mathrm{d}k^3}\bigg|_{k=0}\frac{\mathrm{d}^3u}{\mathrm{d}x^3}+\cdots, \tag{16}$$

$$\sum_{\ell'}\Lambda^{rr}(\ell-\ell')u(\ell') = \frac{1}{2}\sum_{n=1}^{\infty} b_n^{rr}[u(\ell+n)+u(\ell-n)-2u(\ell)]$$
$$= -\frac{1}{2!}\frac{\mathrm{d}^2\tilde{\Lambda}^{rr}}{\mathrm{d}k^2}\bigg|_{k=0}\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \frac{1}{4!}\frac{\mathrm{d}^4\tilde{\Lambda}^{rr}}{\mathrm{d}k^4}\bigg|_{k=0}\frac{\mathrm{d}^4u}{\mathrm{d}x^4}+\cdots$$
$$= -\frac{1}{2!}\frac{\mathrm{d}^2\tilde{\Lambda}^{r}}{\mathrm{d}k^2}\bigg|_{k=0}\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \frac{1}{4!}\frac{\mathrm{d}^4\tilde{\Lambda}^{r}}{\mathrm{d}k^4}\bigg|_{k=0}\frac{\mathrm{d}^4u}{\mathrm{d}x^4}+\cdots. \tag{17}$$

If each series in terms of the derivatives is truncated suitably, the discrete border equation will be changed into an integro-differential equation. A practically useful equation will be given in the following section.

5. Chiral symmetry

For the case interested practically, the half-crystal generally possesses a mirror symmetry with regard to the mirror plane perpendicular to the border. Existence of the mirror symmetry indicates that the left and right are equivalent. One has the freedom to choose a right-hand coordinate system or a left-hand coordinate system. The border equation would take the same form for the both coordinate systems. So, it is convenient to call such a symmetry as the chiral symmetry.

Under the transformation from the right-hand to the left-hand coordinate system, i.e. the chiral transformation, the coordinate of an atom on the border changes a sign,

$$l \longrightarrow -l,$$

the displacement component parallel to the border changes a sign,

$$u_x \longrightarrow -u_x,$$

the displacement perpendicular to the border keeps invariant,

$$u_y \longrightarrow u_y,$$

and the force vector changes in the same way as the displacement vector. Introducing the transformation matrix

$$M = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

the change of a vector like the displacement can be written as

$$u \longrightarrow Mu = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} u_x \\ u_y \end{pmatrix} = \begin{pmatrix} -u_x \\ u_y \end{pmatrix}.$$

Now, it is ready to obtain the transformation relationship between the RDM given in the right-hand and left-hand coordinate systems. In order to avoid the confusion, the variables given in the right-hand (left-hand) coordinates system will be denoted with the subscript $R(L)$, for example, l_R (l_L), u_R (u_L), f_R (f_L). First, let's write the border equation in the right-hand coordinates system,

$$\sum_{l'_R} \Lambda_R(l_R - l'_R) u_R(l'_R) = f_R(l_R). \tag{18}$$

As shown above, the displacement and force in different coordinate system are related through the chiral transformation

$$l_R = -l_L, \qquad u_R(l_R) = Mu_L(l_L), \qquad f_R(l_R) = Mf_L(l_L).$$

Substituting into equation (18), one obtains

$$\sum_{l'_L} \Lambda_R(-l_L + l'_L) Mu_L(l'_L) = Mf_L(l_L).$$

Multiplying M^{-1} to both sides of this equation,

$$\sum_{l'_L} M^{-1} \Lambda_R(-l_L + l'_L) Mu_L(l'_L) = f_L(l_L),$$

it is easy to identify that

$$\Lambda_L(l) = M^{-1}\Lambda_R(-l)M. \tag{19}$$

This is the transformation relationship of the RDM under the chiral transformation. The border equation should take the same form if there exists the chiral symmetry

$$\Lambda_L(l) = \Lambda_R(l) = M^{-1}\Lambda_R(-l)M, \tag{20}$$

or explicitly

$$\begin{pmatrix} \Lambda_{xx}(l) & \Lambda_{xy}(l) \\ \Lambda_{yx}(l) & \Lambda_{yy}(l) \end{pmatrix} = \begin{pmatrix} \Lambda_{xx}(-l) & -\Lambda_{xy}(-l) \\ -\Lambda_{yx}(-l) & \Lambda_{yy}(-l) \end{pmatrix},$$

the subscript has been dropped in the last equation. Therefore, one can conclude that the diagonal elements of the RDM matrix are even functions, the off-diagonal elements are odd functions if the RDM is invariant under the chiral transformation. In the k-space, the conclusion is the same,

$$\begin{aligned} \widetilde{\Lambda}_{xx}(-k) &= \widetilde{\Lambda}_{xx}(k), & \widetilde{\Lambda}_{yy}(-k) &= \widetilde{\Lambda}_{yy}(k), \\ \widetilde{\Lambda}_{xy}(-k) &= -\widetilde{\Lambda}_{xy}(k), & \widetilde{\Lambda}_{yx}(-k) &= -\widetilde{\Lambda}_{yx}(k). \end{aligned}$$

The first two equations are satisfied automatically as shown previously. The last two equations are new relations resulted from the chiral symmetry. The new relations imply that the off-diagonal elements are pure imaginary

$$\widetilde{\Lambda}^r_{xy} = \widetilde{\Lambda}^r_{yx} = 0.$$

In the slow-varying approximation, keeping the derivatives up to the third order, the border equations (4) with the chiral symmetry read

$$\begin{aligned} &-\frac{1}{2}\tilde{\Lambda}^{(2)}_{xx}(0)\frac{\mathrm{d}^2u^x}{\mathrm{d}x^2} + \mathrm{i}\tilde{\Lambda}^{(1)}_{xy}(0)\frac{\mathrm{d}u^y}{\mathrm{d}x} \\ &\qquad - \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\tilde{\Lambda}^{(1)}_{xx}(0)\frac{\mathrm{d}u^x}{\mathrm{d}x} - \frac{1}{6}\tilde{\Lambda}^{(3)}_{xx}(0)\frac{\mathrm{d}^3u^x}{\mathrm{d}x^3}\right]\Bigg|_{x=x'} = f^x, \end{aligned} \tag{21}$$

$$\begin{aligned} &-\frac{1}{2}\tilde{\Lambda}^{(2)}_{yy}(0)\frac{\mathrm{d}^2u^y}{\mathrm{d}x^2} - \mathrm{i}\tilde{\Lambda}^{(1)}_{xy}(0)\frac{\mathrm{d}u^x}{\mathrm{d}x} \\ &\qquad - \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\tilde{\Lambda}^{(1)}_{yy}(0)\frac{\mathrm{d}u^y}{\mathrm{d}x} - \frac{1}{6}\tilde{\Lambda}^{(3)}_{yy}(0)\frac{\mathrm{d}^3u^y}{\mathrm{d}x^3}\right]\Bigg|_{x=x'} = f^y. \end{aligned} \tag{22}$$

6. Dislocation equation

The crystal with a dislocation can be viewed as two half-infinite crystals glued together along the glide plane in a non-trivial way. If the half-infinite crystal above or below the glide plane is concerned only, it can be viewed as a perfect crystal distorted weakly. So, the half-infinite crystal itself can be described in the frame of the harmonic approximation. The large distortion occurs in the transition region where two half-infinite crystals are connected. Because of the large distortion, the nonlinear interaction between the two half-infinite crystals must be taken into account. The total force imposed on the border atom located at position l is consisted of two parts: one is from the internal interaction of the half crystal that can be expressed as

$$-\sum_{l'}\Lambda^a(l-l')u^a(l')$$

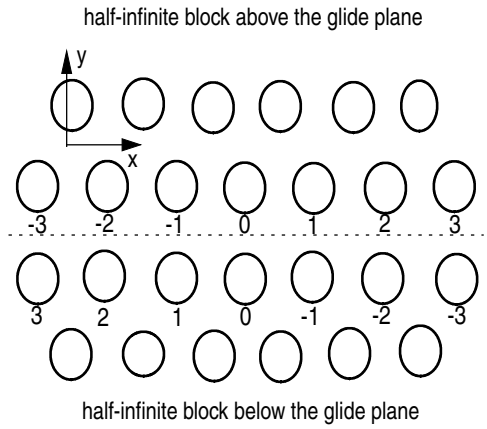

Figure 2. The intrinsic coordinates for deriving the dislocation, in which the two atoms are paired, are labeled by l and $-l$. The crystal has been cut along the glide plane (the dot line).

for the atom l on the border above the glide plane, and

$$-\sum_{l'} \Lambda^b(l-l')u^b(l')$$

for the atom l on the border below the glide plane; another is the 'external force' that is from the other half crystal. In the equilibrium, the balance equations are

$$\sum_{l'} \Lambda^a(l-l')u^a(l') = f^a(l), \qquad \sum_{l'} \Lambda^b(l-l')u^b(l') = f^b(l),$$

where $f^a(l)$ ($f^b(l)$) is the force acting on the atom l of the half crystal above (below) the glide plane and imposed by the half crystal below (above) the glide plane. Obviously, if the half crystal above (below) the glide plane rotates π, it will change into the half crystal below (above) the glide plane. Therefore, if the intrinsic coordinates systems shown in figure 2 are used for different half crystals, it must be

$$\Lambda^a = \Lambda^b.$$

In figure 2, the origins of the coordinates system are chosen so that the atom l in the upper crystal is aligned vertically with the atom l' in the lower crystal. The two atoms aligned vertically will be referred to as an atom pair. For an atom pair, the balance equations can be written as

$$\sum_{l'} \Lambda(l-l')u^a(l') = f^a(l), \tag{23}$$

$$\sum_{l'} \Lambda(-l+l')u^b(-l') = f^b(-l). \tag{24}$$

Now, introducing the mass center and relative displacement for the two atoms paired,

$$u^c(l) = \tfrac{1}{2}[u^a(l) + u^b(-l)], \qquad u^r(l) = \tfrac{1}{2}[u^a(l) - u^b(-l)],$$

from equation (23) plus equations (24) and (23) minus equation (24), one can obtain

$$\sum_{l'}[\Lambda^e(l-l')u^c(l')+\Lambda^o(l-l')u^r(l')]=\frac{1}{2}[f^a(l)+f^b(-l)], \tag{25}$$

$$\sum_{l'}[\Lambda^e(l-l')u^r(l')+\Lambda^o(l-l')u^c(l')]=\frac{1}{2}[f^a(l)-f^b(-l)], \tag{26}$$

where Λ^e is the even part of the dynamical matrix

$$\Lambda^e(l)=\tfrac{1}{2}[\Lambda(l)+\Lambda(-l)],$$

and Λ^o is the odd part of the dynamical matrix

$$\Lambda^o(l)=\tfrac{1}{2}[\Lambda(l)-\Lambda(-l)].$$

In the k-space, equations (25) and (26) become

$$\widetilde{\Lambda}^e\widetilde{u}^c+\widetilde{\Lambda}^o\widetilde{u}^r=\tfrac{1}{2}(\widetilde{f}^a+\widetilde{f}^b|_{k=-k}), \tag{27}$$

$$\widetilde{\Lambda}^e\widetilde{u}^r+\widetilde{\Lambda}^o\widetilde{u}^c=\tfrac{1}{2}(\widetilde{f}^a-\widetilde{f}^b|_{k=-k}). \tag{28}$$

In the local approximation, the interaction Hamiltonian between the two half crystals is a sum of effective pair interaction

$$H_{\text{int}}=\sum_l \phi[u^a(l)-u^b(-l)].$$

As a consequence, the total force felt by an atom pair vanishes

$$f^a(l)+f^b(-l)=0 \qquad \text{or} \qquad \widetilde{f}^a+\widetilde{f}^b|_{k=-k}=0,$$

and equation (27) can be solved

$$\widetilde{u}^c=-(\widetilde{\Lambda}^e)^{-1}\widetilde{\Lambda}^o\widetilde{u}^r. \tag{29}$$

Substituting equation (29) into equation (28), one has an equation for the relative displacement

$$\widetilde{\Omega}\widetilde{u}^r=\widetilde{f}^a, \tag{30}$$

with

$$\widetilde{\Omega}=\widetilde{\Lambda}^e-\widetilde{\Lambda}^o(\widetilde{\Lambda}^e)^{-1}\widetilde{\Lambda}^o. \tag{31}$$

From the discussion in section 3, it is known that $\widetilde{\Lambda}^e$ is the real part of $\widetilde{\Lambda}$, which is a symmetry matrix

$$\widetilde{\Lambda}^e=\begin{pmatrix}\widetilde{\Lambda}_{xx} & \widetilde{\Lambda}^r_{xy}\\ \widetilde{\Lambda}^r_{xy} & \widetilde{\Lambda}_{yy}\end{pmatrix}, \tag{32}$$

and $\widetilde{\Lambda}^o$ is the imaginary part of $\widetilde{\Lambda}$, which is an antisymmetry matrix

$$\widetilde{\Lambda}^o=\begin{pmatrix}0 & \mathrm{i}\widetilde{\Lambda}^i_{xy}\\ -\mathrm{i}\widetilde{\Lambda}^i_{xy} & 0\end{pmatrix}. \tag{33}$$

Therefore, the matrix $\widetilde{\Omega}$ can be obtained explicitly

$$\widetilde{\Omega}=\left[1-\frac{\left|\widetilde{\Lambda}^i_{xy}\right|^2}{\widetilde{\Lambda}_{xx}\widetilde{\Lambda}_{yy}-\left(\widetilde{\Lambda}^r_{xy}\right)^2}\right]\widetilde{\Lambda}^r. \tag{34}$$

In general, the equations satisfied by the relative displacement are coupled. However, if the RDM is invariant under the chiral transformation, the matrix $\widetilde{\Omega}$ is a diagonal matrix

$$\widetilde{\Omega} = \begin{pmatrix} \widetilde{\Lambda}_{xx} - \frac{|\widetilde{\Lambda}_{xy}|^2}{\widetilde{\Lambda}_{yy}} & 0 \\ 0 & \widetilde{\Lambda}_{yy} - \frac{|\widetilde{\Lambda}_{xy}|^2}{\widetilde{\Lambda}_{xx}} \end{pmatrix}, \tag{35}$$

and so the equations are decoupled.

As do usually, it is reasonable to assume that if the interval between the upper and lower border is kept at its equilibrium value, the vertical of the force will be negligible

$$f_y^a \longrightarrow 0 \qquad \text{as} \quad u_y^r \to 0.$$

Choosing $u_y^r = 0$ for the dislocation solution, one finally obtains a simplified dislocation equation

$$\widetilde{\Omega}_{xx}\widetilde{u}_x^r = \widetilde{f}_x^a, \qquad \widetilde{\Omega}_{xx} = \widetilde{\Lambda}_{xx} - \frac{|\widetilde{\Lambda}_{xy}|^2}{\widetilde{\Lambda}_{yy}}. \tag{36}$$

In the real space, equation (36) reads

$$-\frac{1}{2}\widetilde{\Omega}_{xx}^{(2)}(0)\frac{\mathrm{d}^2 u_x^r}{\mathrm{d}x^2} - \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\widetilde{\Omega}_{xx}^{(1)}(0)\frac{\mathrm{d}u_x^r}{\mathrm{d}x} - \frac{1}{6}\widetilde{\Omega}_{xx}^{(3)}(0)\frac{\mathrm{d}^3 u_x^r}{\mathrm{d}x^3}\right]\Bigg|_{x=x'} = f_x^a, \tag{37}$$

with

$$\widetilde{\Omega}_{xx}^{(j)}(0) = \left.\frac{\mathrm{d}^j \widetilde{\Omega}_{xx}}{\mathrm{d}k^j}\right|_{k=0^+}, \qquad j = 1, 2, \ldots,$$
$$\widetilde{\Omega}_{xx} = \widetilde{\Lambda}_{xx} - \frac{|\widetilde{\Lambda}_{xy}|^2}{\widetilde{\Lambda}_{yy}},$$

in the slow-varying approximation. This is the dislocation equation that will be closed when the force law is given.

As long as the relative displacement is known, the mass center displacement can be obtained through equation (29). It is easy to obtain that

$$\widetilde{u}_x^c = 0,$$

i.e., the mass center is fixed in the horizontal direction, and

$$\widetilde{\Lambda}_{yy}\widetilde{u}_y^c = \widetilde{\Lambda}_{xy}\widetilde{u}_x^r, \tag{38}$$

i.e., a vertical displacement induced by the relative displacement in the horizontal direction takes place. In the real space, equation (38) reads

$$-\frac{1}{2}\widetilde{\Lambda}_{yy}^{(2)}(0)\frac{\mathrm{d}^2 u_y^c}{\mathrm{d}x^2} - \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\widetilde{\Lambda}_{yy}^{(1)}(0)\frac{\mathrm{d}u_y^c}{\mathrm{d}x} - \frac{1}{6}\widetilde{\Lambda}_{yy}^{(3)}(0)\frac{\mathrm{d}^3 u_y^c}{\mathrm{d}x^3}\right]\Bigg|_{x=x'} = \mathrm{i}\widetilde{\Lambda}_{xy}^{(1)}(0)\frac{\mathrm{d}u_x^r}{\mathrm{d}x}. \tag{39}$$

This is a linear integro-differential equation.

Because the mass center is fixed in the horizontal direction and the relative displacement vanishes in the vertical direction, equations (37) and (39) can be written in terms of the

displacements of the atoms on one border

$$-\frac{1}{2}\widetilde{\Omega}^{(2)}_{xx}(0)\frac{\mathrm{d}^2u^a_x}{\mathrm{d}x^2}-\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\widetilde{\Omega}^{(1)}_{xx}(0)\frac{\mathrm{d}u^a_x}{\mathrm{d}x}-\frac{1}{6}\widetilde{\Omega}^{(3)}_{xx}(0)\frac{\mathrm{d}^3u^a_x}{\mathrm{d}x^3}\right]\Bigg|_{x=x'}=f^a_x, \tag{40}$$

$$-\frac{1}{2}\widetilde{\Lambda}^{(2)}_{yy}(0)\frac{\mathrm{d}^2u^a_y}{\mathrm{d}x^2}-\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\left[\widetilde{\Lambda}^{(1)}_{yy}(0)\frac{\mathrm{d}u^a_y}{\mathrm{d}x}-\frac{1}{6}\widetilde{\Lambda}^{(3)}_{yy}(0)\frac{\mathrm{d}^3u^a_y}{\mathrm{d}x^3}\right]\Bigg|_{x=x'}=\mathrm{i}\widetilde{\Lambda}^{(1)}_{xy}(0)\frac{\mathrm{d}u^a_x}{\mathrm{d}x}. \tag{41}$$

The displacements of the atoms on the other border are given by

$$u^b_x=-u^a_x,\qquad u^b_y=u^a_y.$$

7. Discussion and summary

The dislocation equation has been derived generally and rigorously from the lattice dynamics. The vertical displacement as well as the horizontal displacement can be calculated in the same time. In contrast, the vertical displacement cannot be calculated at all in the classical P–N theory. It is known that the glide plane will bend in large scale due to appearance of the dislocation. The bend may be measured through x-ray diffraction. So the theoretical prediction may be checked by experiment.

The concept of chiral symmetry newly introduced is very important in understanding the structure of the dislocation. Apparently, in the most cases there always exist the chiral symmetry. Of course, the chiral symmetry may be broken sometimes. But it is reasonable to believe that the violation is small and can be neglected in the first approximation.

The dislocation equation in the slow-varying approximation is a modification of the Peierls equation. It includes corrections from the discrete effects of the lattice. Similar results had been given in [14], where the dislocation equation was presented for a simplified model of the cubic lattice. However, there are differences. First, the calculation formulae of the coefficients in the equation are not exactly the same. The previous expressions are approximation of those obtained here. Second, the equation of the vertical component is improved.

The dislocation equation has a universal form that does not depend on the type of the lattice. The difference of the lattice is reflected by the different coefficients appeared in the equation. Therefore, in addition to the GFS energy, the dislocation structure is controlled by a few coefficient factors related with small deformation of the crystal. Now, what one need to do is to determine the coefficients. In principle, these coefficients can be calculated when the dynamical matrix of the crystal is given. In particular, because the coefficients only relate to the behavior near the zero point of the RDM in the k-space, it can be calculated perturbatively. Besides, as a solution of the problem of the half-infinite lattice, the coefficients can be also evaluated by the first principle calculation.

The dislocation equation derived from the lattice dynamics is more transparent in physics than that derived from the elastic continuum theory. In the classical P–N theory, one may be confused with the question such as how to carry out the summation correctly. It is well known that there are arguments about how to evaluate the dislocation energy and the Peierls stress. In the lattice theory, everything is clear and definite because it is discrete from the beginning.

The dislocation equation obtained can be straightforwardly applied to the dislocation in a two-dimensional lattice like the bubble raft. It can also be applied to the dislocation in a three-dimensional lattice if the straight dislocation can be identified with a ‘point defect’ in a two-dimensional lattice. If the dislocation in a three-dimensional lattice has both edge and

screw components, one need to extend the classical P–N model (1D model) to be so-called the 2D model [5, 8, 11, 12]. Actually, in order to theoretically investigate the dislocation in a three-dimensional lattice, one needs to deal with the two-dimensional glide plane. It is necessary to find a general dislocation equation satisfied by the displacement field on the glide plane. The general dislocation equation can address the curved dislocation as well as the straight dislocation. The method used here is suitable to be generalized to derive such a dislocation equation.

In summary, the dislocation equation has been derived generally and rigorously from the lattice dynamics. It is more transparent in physics. It includes correction from the lattice effects that cannot be obtained in the continuum theory, and cannot be neglected in the core of the dislocation. It enables one to calculate the vertical displacement as well as the horizontal displacement. It indicates that the dislocation structure is dominated by a few factors even the lattice effects are taken into account. If the factors can be related with the electronic structure, it would be possible to predict and design the plasticity of material microscopically.

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