

ON THE THEORY OF DISLOCATIONS IN A TWO-ROW MODEL OF A CRYSTAL

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Abstract

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PHYSICS

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ON THE THEORY OF DISLOCATIONS IN A TWO-ROW MODEL OF A CRYSTAL

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1. The behavior of dislocations largely determines the mechanical properties of metals ⁽¹⁾. Up to the present time, a continuum description of the elastic field and energy of an individual dislocation has been used, introduced by Taylor ⁽²⁾ as early as 1934 and based on the identification of dislocations in a crystal with elastic dislocations ^(1,3). Such a description is obviously inapplicable to the description of the dislocation core. A rigorous theory of dislocations must proceed from the concept of a crystal lattice.

For many problems it has proved useful to consider a two-row crystal. However, the well-known Frenkel-Kontorova dislocation model ^(4,5) contains an undesirable restriction—the assumption that the lower row of atoms is undeformable. In addition, in all works, with the exception of ⁽⁶⁾, difference equations are replaced by differential ones, which essentially means a transition to the continuum. An attempt at a consistent lattice treatment of a complete dislocation in a two-row crystal was undertaken by B. A. Grinberg and A. N. Orlov ⁽⁷⁾. But, as will be shown below, their model is incompatible with the conditions for lattice stability, and a dislocation cannot exist in it. In the present work a method is indicated for calculating various dislocations in a two-row crystal. For the first time, the configuration and energy of a partial dislocation in a two-row lattice are calculated. Previously, it had been considered by Frank and van der Merwe ⁽⁸⁾ in the Frenkel-Kontorova model with replacement of the difference equations by differential ones.

Fig. 1. Dislocation in a two-row crystal: a —partial, $b(e)$ —split, $v(d)$ —complete in a rectangular (hexagonal) lattice

2. Let us consider a lattice consisting of two rectilinear infinite atomic rows

separated from one another by a distance a_2 . From symmetry considerations it is obvious that such a lattice will have two allotropic modifications: rectangular and hexagonal (triangular). As a consequence, various dislocations may exist in a two-row lattice (Fig. 1): partial (a), split (b), complete (v) in a rectangular lattice, and split (e) and complete (d) in a hexagonal lattice. The segment of the lattice in split dislocations that connects the partial dislocations plays the role of a stacking defect. It is evident that a rectangular lattice cannot be stable for central forces when only nearest-neighbor interactions are taken into account. It is not difficult to see that if second-neighbor interactions are taken into account, then for po-

of the Morse potential ⁽⁹⁾

$$v(r) = D(\beta^2 e^{-2\alpha r} - 2\beta e^{-\alpha r}) \quad (1)$$

the lattice is stable for $\ln \beta < 1.94$ (D , β , α are constants). The authors ⁽⁷⁾ took into account only nearest interactions. In addition, they adopted the value $\ln \beta = 4$, for which the lattice is unstable even when the interaction of second neighbors is included.

Below we take into account the interaction of first and second neighbors in the rectangular lattice and of nearest neighbors in the hexagonal lattice.

The essence of the method reduces to selecting, for any arrangement of dislocations, a certain initial configuration of atoms consisting of segments of rectangular and triangular lattices. For a partial dislocation it is shown in Fig. 1a by the dashed line and is formed by two undeformed semi-infinite segments of rectangular and hexagonal lattices, connected by the common atom 00. Allowing the atoms to relax from the positions $x_{\mu\nu}^0$ corresponding to the initial configuration into the equilibrium positions $x_{\mu\nu}$, we obtain the dislocation configuration ($-\infty < \mu < \infty$ is the number of the atom in a row; $\nu = 0; 1$ is the row number). The displacements $\xi_{\mu\nu} = x_{\mu\nu} - x_{\mu\nu}^0$ may be regarded as small. Expanding the potential energy of the chain in $\xi_{\mu\nu}$, we obtain the following equations of the linear approximation for the "rectangular tail" of the dislocation ($\mu \geq 1$):

$$A(2\xi_{\mu\nu} - \xi_{\mu+1,\nu} - \xi_{\mu-1,\nu}) + B(\xi_{\mu\nu} - \xi_{\mu,1-\nu}) + C(2\xi_{\mu\nu} - \xi_{\mu+1,1-\nu} - \xi_{\mu-1,1-\nu}) = 0, \quad (2)$$

where $A = v''(a_1)$; $B = v'(a_2)/a_2$; $C = a_2^2 L^{-3} v'(L) + a_1^2 L^{-2} v''(L)$; $L = (a_1^2 + a_2^2)^{1/2}$, and a_1 is the interatomic distance in a row for the ideal rectangular lattice.

Introducing the variables

$$\alpha_\mu = \xi_{\mu 1} + \xi_{\mu 0}; \quad \beta_\mu = \xi_{\mu 1} - \xi_{\mu 0}, \quad (3)$$

we arrive at simple difference equations

$$\alpha_{\mu-1} + \alpha_{\mu+1} - 2\alpha_{\mu} = 0; \quad \beta_{\mu-1} + \beta_{\mu+1} - 2\gamma\beta_{\mu} = 0, \quad (4)$$

where $\gamma = (A + B + C)/(A - C)$.

From (3) and (4) we obtain the solution of equations (2) in the form

$$\xi_{\mu\nu} = \frac{1}{2}\xi_{01} [1 - (-1)^{\nu} q^{-\mu}], \quad q = \gamma + (\gamma^2 - 1)^{1/2}. \quad (5)$$

Here the term corresponding to uniform stretching of the lattice along the chain has been discarded and it has been assumed that $\xi_{00} = 0$ (thereby excluding the displacement of the lattice as a whole). The displacement of the end atom of the rectangular tail ξ_{01} plays the role of the boundary condition in solving (2). The energy of the “tail” is expressed quadratically through ξ_{01} :

$$U_n = \text{const} + \frac{1}{2}v_{11}\xi_{01}^2, \quad (6)$$

where $v_{11} = \frac{1}{2} [B + (2A + B)^{1/2}(2C + B)^{1/2}]$.

The consideration of the “hexagonal tail” of the dislocation ($\mu < 0$) is carried out somewhat more complicatedly and ultimately leads to an equation of type (4) and a solution of type (5), where the role of the boundary condition is played by the displacement $\xi_{-1,1}$ (Fig. 1a). The tail energy is equal to

$$U_{\Gamma} = \text{const} + \frac{1}{2}v_{22}\xi_{-1,1}^2, \quad (7)$$

where v_{22} is expressed through the constants of the atomic-interaction potential.

The total energy of a two-row lattice in the presence of a partial dislocation, to within a constant, is expressed through ξ_{01} and $\xi_{-1,1}$:

$$U = v \left(\frac{1}{2}a_{\Gamma} + \xi_{01} + |\xi_{-1,1}| \right) + \frac{1}{2}v_{11}\xi_{01}^2 + \frac{1}{2}v_{22}\xi_{-1,1}^2, \quad (8)$$

(a_{Γ} is the interatomic distance in a row for the ideal hexagonal lattice).

The first term expresses the interaction of atoms 01 and $-1, 1$. In the linear approximation ξ_{01} and $\xi_{-1,1}$ are trivially determined from the minimum of (8). For the Morse potential we obtain

$$\xi_{01}/r_m = 0.121; \quad |\xi_{-1,1}|/r_m = 0.100$$

($r_m = \alpha^{-1} \ln \beta$ is the position of the minimum of the potential energy (1)). The energy of a partial dislocation produced by a shift in the rectangular lattice is, in the linear approximation,

Fig. 2. Configuration of a partial dislocation (with allowance for nonlinearity in the core). a —upper row of atoms; b —lower row of atoms

Figure 2: Fig. 2. Configuration of a partial dislocation (with allowance for nonlinearity in the core). a —upper row of atoms; b —lower row of atoms

$$U = 1.21D$$

(D is the energy of one interatomic bond).

The linear approximation, naturally, cannot give exact quantitative results. A direct calculation shows that the quadratic expressions (6) and (7) differ from the true ones by no more than 2%. The principal error in the linear approximation is due to the first term in (8). It therefore seems reasonable to take nonlinearity into account only in this term. Then the minimization of (8) reduces to the solution of a single nonlinear equation

$$v' \left(\frac{a_r}{2} + \frac{v_{11} + v_{22}}{v_{22}} \xi_{01} \right) + v_{11} \xi_{01} = 0,$$

which, for a given interaction law $v(r)$, is readily solved graphically. For the Morse potential we obtain:

$$\xi_{01}/r_m = 0.222, \quad |\xi_{-1,1}|/r_m = 0.184, \quad U = 0.87D.$$

Comparison with the data given above gives an idea of the error of the linear approximation.

It follows from (5) and the analogous expression for the “hexagonal tail” that the displacements of atoms at infinity tend to a certain limiting value (Fig. 2)

$$\xi_{\mu\nu} \rightarrow \frac{1}{2} \xi_{01}, \quad \mu \rightarrow +\infty;$$

$$\xi_{\mu\nu} \rightarrow \frac{1}{2} \xi_{-1,1}, \quad \mu \rightarrow -\infty.$$

Fig. 2. Configuration of a partial dislocation (with allowance for nonlinearity in the core). a —upper row of atoms; b —lower row of atoms

This is understandable from physical considerations. At the location of the dislocation, the interatomic distances in the lower row are increased in comparison with the equilibrium parameter a_1 . It is easy to see that at infinity a two-row lattice can be ideal (undeformed) only if all atoms at infinity are displaced by one and the same constant amount. In the Frenkel-Kontorova model the lower

row of atoms is not deformed, and there is no limiting displacement of atoms at infinity.

Apparently, this effect will be significant in calculating the Peierls-Nabarro force.

It should also be noted that the displacements of atoms decrease very rapidly with distance from the dislocation core (Fig. 2). For example, the displacement of the 5th atom in the upper row on the right differs from the limiting displacement by only 2.5%. The shear deformation of the lattice to the right of the dislocation is 6.2% in the 2nd cell, 0.7% in the 5th, and 0.02% in the 10th.

It is not difficult to verify that, if only nearest-neighbor interactions are taken into account, equations (2) have only solutions corresponding to a homogeneous de-

formation, i.e., the dislocation does not exist. The exception is the quite unrealistic case in which the lattice is stretched perpendicular to the rows.

This method is applicable for calculating the characteristics of other dislocations represented in Fig. 1, or of their combinations. The use of the Morse potential is not obligatory.

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