New features of dislocation structures arising from lattice discreteness.

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Abstract

New aspects of a relation between lattice and dislocation structures are examined within a physically transparent theoretical scheme. Predicted features originating from the lattice discreteness include: (i) multiple core dislocation structures and (ii) their dependence on the position of the dislocation axis. These effects, which in principle can be observed directly and may also manifest themselves in dislocation motion or/and transformation (cross-slip) characteristics, are very general and present in any crystal in which they may be more or less pronounced depending on the material.
It is widely accepted that such defects as dislocations significantly influence a number of properties in real materials. Thus, understanding the relationship between lattice and dislocation structures is one of the fundamental problems of materials physics. Despite recent developments of powerful atomistic simulation techniques, up to now our understanding of the relation between lattice and dislocation structures is based on results obtained within the framework of the Peierls-Nabarro (PN) model \[1,2\]. This model has provided both language for interpretation experimental/theoretical results and simple relations between dislocation properties and lattice discreteness characteristics (periodicity, symmetry, etc.) \[1–4\]. This remarkable breakthrough in understanding how dislocation properties are related with lattice characteristics became possible due to two features of this model: (i) its high tractability and (ii) its combined different length scale descriptions.

The combined "continuum/atomistic" descriptions in the PN model follow clearly from the structure of the energy functionals \[3,4\], \(E_{tot}\), of the dislocation displacement distribution \(\vec{u}(x)\) (here \(x\) is a distance from the dislocation axis in the slip plane)

\[
E_{tot}(\vec{u}(x)) = E_{el}(\vec{u}(x)) + E_{mis}(\vec{u}(x))
\]

(1)

with a linear elastic \(E_{el}\) and a non-linear atomistic misfit energy term \(E_{mis}\)

\[
E_{mis} = h \sum_n \Phi(\vec{u}(nh - l))
\]

(2)

where \(\Phi(\vec{u}(x))\) is a periodic energy profile which is often approximated by the so-called generalized stacking fault energy (GSF) or \(\gamma\)-surface \[3\]. Indeed, the \(E_{mis}\) term represents the most apparent and important lattice properties - discreteness/periodicity/symmetry - and allows one to investigate within the PN model the relation between lattice and dislocation properties. \(E_{mis}\) can be expanded in a Fourier series as

\[
E_{mis} = E_{mis}^0 + h \sum_{s=1}^{\infty} J_s \cos \frac{2\pi s l}{h}
\]

(3)

where \(E_{mis}^0 = \int_{-\infty}^{\infty} \Phi(\vec{u}(x))dx\) is independent of the position of the dislocation axis \(l\) and terms which are oscillatory with \(h\) being a repeat distance normal to the dislocation line and \(n\) an integer number that counts atomic rows in the same direction.
Now, a minimization of $E_{tot}(\vec{u}(x))$ allows one to find the equilibrium dislocation structure, $\vec{u}(x)$. In order to perform this minimization in analytic form, a critical approximation $E_{mis} = E_{mis}^0$ has been made \[1\]. This "continuum" approximation in representing the misfit energy - which is supposed to describe lattice discreteness - results in an obvious inconsistency which has been a subject of debate for years, mainly in the context of Peierls stress determinations \[3,7,8\]. Thus, an interesting and fundamental issue arises - if consistently represented in the atomistic interaction energy, how will lattice discreteness be manifested in the structure of dislocations?

Several recent attempts to overcome this inconsistency resulted in purely numerical procedures \[7,8\]. Thus, one of the most advantageous features of the PN model - high tractability and transparency - has been sacrificed. These authors also focused on the Peierls stress determination and demonstrated that indeed the discrete representation of the misfit energy brings theoretical estimates much closer to experimental results.

In this Letter, using a physically transparent solution of the PN model with a consistent discrete representation for the misfit energy, we examine how lattice discreteness may influence dislocation structure. This allows us to predict new generic features of the dislocation structure that are independent of the PN model assumptions, and driven by lattice discreteness such as multiple core structures and their dependence on the position of the dislocation axis.

To determine dislocation structure, we perform a minimization of the total energy functional, Eq. 1, with a discrete representation of the misfit energy, Eq. 2, using trial functions, $\vec{u}(x)$, defined from the Laurent expansion \[9,10\] of their derivatives $\rho_\beta(x)$

$$\rho_\beta(x) = \frac{du_\beta(x)}{dx} = Re \sum_{k=1}^{N} \sum_{n=1}^{p_k} \frac{A_{nk}^\beta}{(x - z_k^\beta)^n},$$

(4)

where $N$ is the maximal number, $p_k$ is the maximal order of the poles $z_k^\beta$ and $A_{nk}^\beta$ are expansion coefficients. It is important to note that, by definition, these trial functions provide a minimum of $E_{tot}$ for an arbitrary $\Phi(u)$ potential (not only sinusoidal, as trial functions used in \[3\] to parameterize total energy functional in the convenient form) in case
of the "continuum" approximation, \( E_{\text{mis}} = E_{\text{mis}}^0 \). This choice of trial functions not only provides good accuracy and stability of the minimization procedure [10] but also allows one to express \( E_{\text{tot}} \) through parameters describing the dislocation structure. Indeed, the poles \( z_k^\beta = x_k^\beta + i\omega_k^\beta \) have a clear meaning: \( x_k^\beta \) gives the position and \( \omega_k^\beta \) gives the width of the partials for the screw (\( \beta = 1 \)) and edge (\( \beta = 2 \)) components of the displacement in the partial cores. For example, for the ordinary dislocations dissociated into two Shockley partials, \( x_k^\beta = l \pm d^\beta/2 \), where \( d \) is the partials separation and \( l \) gives the position of the whole ordinary dislocation center. In the general case with these trial functions, \( E_{\text{tot}} \) can be presented as a numerical function of geometrical parameters, in particular, for an ordinary dislocation as a function of the set of parameters (\( \{g\} = \{d, \omega, l\} \)) describing the dislocation’s structure (\( d, \omega \)) and its position in the lattice (\( l \)).

As examples, we consider ordinary dislocations for fcc metal, Ir, and an ordered alloy, CuAu, with L1_0 structure. In these materials, this type of dislocation normally splits into two Shockley partials [2][10] and represents a very typical example of dislocation structures. To illustrate graphically minimization of \( E_{\text{tot}} \), let us introduce elastic (\( F_{\text{el}}(d) \)) and misfit (\( F_{\text{mis}}(d) \)) generalized forces which are defined as, \( F_{\text{el}}(d) = -\partial E_{\text{el}}(d)/\partial d \) (the sign is chosen for convenience) and \( F_{\text{mis}}(d) = \partial E_{\text{mis}}(d)/\partial d \) (here and further we drop the \( \beta \) index since \( d^1 \approx d^2 \)). In this definition, for a given \( d \) other geometrical parameters from the complete set \( \{g\} \) are taken to be such that they minimize \( E_{\text{tot}} \). Obviously, in this case the intersection of \( F_{\text{el}}(d) \) and \( F_{\text{mis}}(d) \) gives a partial separation \( d \) which corresponds to the minimum of Eq.[1], provided that the second derivatives are positive.

The generalized forces calculated according to this definition using ab-initio \( \gamma \)-surfaces (see [10] for details) in the case of the screw orientation of the unit dislocation for Ir and CuAu are presented in Fig.1 (a, c). For comparison, we also determine generalized forces for dislocations with simple model density distribution displacements composed of two delta functions, \( \rho(x) = b_1\delta(x + d/2) + b_2\delta(x - d/2) \) (see Fig. 1 (b, d)). In this case, we have a step function shaped dislocation for which \( E_{\text{tot}} \) has a very simple form,
\[
E_{\text{tot}} = H \cdot \ln\left(\frac{1}{d}\right) + \gamma_{\text{isf}} \cdot d \quad (5)
\]
and corresponding generalized forces \(F_{\text{el}}^{\text{step}} = H/d\) and \(F_{\text{mis}}^{\text{step}} = \gamma_{\text{isf}}\), where \(\gamma_{\text{isf}}\) is the intrinsic stacking fault energy and \(H\) is a so-called prelogarithmic factor (see for example [5]). Interestingly enough, for this model type of dislocation the well-known simple relation between the equilibrium partials separation and stacking fault energy, \(d = H/\gamma_{\text{isf}}\) [2], can be easily recovered from the functional dependence in Eq. (5). As can be seen in Fig. 1, in the limit of large separation distances \((d >> \omega)\), the PN model generalized forces defined within the "continuum" approximation approach those for the step function shaped dislocation.

We now focus on how the oscillatory part of the misfit energy, usually neglected in the PN model analysis, affects dislocation structure. Remarkably enough, there are not only oscillations with \(l\) which can be expected from the Fourier expansion of the misfit energy, Eq. (3), but also oscillations with partials separation \(d\) for fixed \(l\). As can be seen in Fig. 1, for Ir, despite the rather small amplitude of these oscillations, the effect of the misfit energy discrete representation is quite visible since the intersection of the generalized forces happens to be in the area where \(d\) dependence of the \(F_{\text{el}}\) is rather weak and so solutions are affected most by the \(F_{\text{mis}}\) oscillations. Finally, for CuAu the effect is dramatic since the amplitude of the oscillations is very large. It is significant that the discrete representation of the misfit energy not only changes quantitatively parameters of the dislocation structure (as in the case of Ir) but may also result in qualitatively new effects (as in the case of CuAu). As is evident from Fig. 1, one such general effect, which is independent of the PN model approximations, is the appearance of multiple stable dislocation core configurations. Indeed, conclusions we draw in this study about the possibility of multiple core configurations are based on generic features of the \(F_{\text{el}}(d)\) and \(F_{\text{mis}}(d)\) dependencies (see Fig. 1) which follow from the general physics of the linear (elastic part) and non-linear (misfit part) lattice response [11].

Moreover, within the proposed scheme it is possible to derive [12] the following convenient and physically transparent form for the energy functional, Eq. (4).

\[
E_{\text{tot}} = E_{\text{tot}}^0(d, \omega) + A(d, \omega) \cos \frac{2\pi l}{h} \cos \frac{\pi d}{h} \quad (6)
\]
Here the $l$ independent first term $E_{\text{tot}}^0 = E_{\text{el}} + E_{\text{mis}}^0$ is the energy in the “continuum” approximation and the second term has an explicit oscillatory dependence both on $l$ and $d$.

This form reveals that the appearance of the above features associated with lattice discreteness are dependent on the relative contribution of the energies represented by the $E_{\text{tot}}^0$ and the oscillatory terms. In turn, the character of $E_{\text{tot}}^0(d)$ dependence and corresponding generalized forces is driven by the competition of the partials attraction described by $E_{\text{mis}}^0$ (term which is dependent upon the $\gamma$-surface energetic characteristics and for large $d$, it can be well approximated by Eq. 5) and the elastic repulsion ($E_{\text{el}}$ which is dependent on the elastic constants and in the limit $d \gg \omega$, has a simple dependence, see Fig.1). The influence of the oscillatory term is predetermined by its amplitude $A(d, \omega)$ which according to our analysis is strongly dependent on characteristics of the $\gamma$-surface [13].

It is important that Eq. 6 describes dislocation energetics for a wide range of $d$ and $\omega$ [14] and correspondingly a complex interdependence of all geometrical parameters ($d$, $\omega$ and $l$). Features of dislocation structure originating in this interdependence of geometrical parameters and their impact on dislocation energetics can be seen from the calculated $d$ and $l$ dependencies of the $E_{\text{tot}}$ in Fig.4. Indeed, proof that there are can be more than one stable dislocation core configuration (CuAu) can be seen in Fig.2(a). Next, the dependence of the partials separation on the position of the dislocation axis in the lattice is clearly seen in Fig.2(b). A comparison of the $d(l)$ dependencies determined within the “continuum” approximation and with a discrete representation for $E_{\text{mis}}$ makes it evident that lattice discreteness is the origin of the variation in equilibrium dislocation structure depending on the position of the dislocation axis (core “relaxation”). This variation may result in changes in the number of stable core configurations and abrupt transitions between them (as for CuAu, see Fig.2(a,b)).

These predicted features may have a profound impact on dislocation energetics. As can be seen in Fig.2(c), the dependence of the dislocation structure on the position of the dislocation axis may not only lower significantly the Peierls barrier (as also have been found in [7,8]) but may even modify the shape of the Peierls potential. It is remarkable that core
“relaxation” along with the existence of the multiple core configurations (the case of CuAu) adds a new feature to the Peierls potential - an additional minimum - which according to the model analysis may result in characteristic changes of the temperature dependence of the yield stress [13]. As can be seen clearly in Fig.4, the unusual shape of the Peierls potential in CuAu originates in the abrupt transitions between two stable core configurations, “1” and “2”.

We find that in addition to the known dislocation structure features, lattice discreteness is the origin of (i) multiple core configurations and (ii) their dependence on the position of the dislocation axis. Combination of these effects may result in rather complex variations of the dislocation structure over the crystal including changes in the number of stable core configurations and transitions between them. As a result, one may have to consider a distribution of the core configurations in a crystal under ambient conditions rather than one characteristic core structure which determines dislocation motion or cross-slip properties.

As follows from our analysis, predicted features of dislocation structure originating in lattice discreteness are always present in crystals, but as we demonstrate with Ir and CuAu as examples, they appear more or less pronounced depending on characteristics of the given material. These fundamental characteristics can be identified within the proposed theoretical analysis primarily due to its tractability and physical transparency [13]. While these features, namely multiple core configurations, can be directly verified, in principle, in high resolution electron microscopy experiments, they may also reveal themselves indirectly in low temperature internal friction experiments [17] and in mechanical properties which depend on elementary processes that are sensitive to the dislocation structure. Among such processes, we would emphasize cross-slip, where dislocation core structure and its changes under local stress may play an important role.

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[11] For drawn here conclusions about features of dislocation structures originating in lattice discreteness only the character of the $F_{el}(d)$ and $F_{mis}(d)$ is important. The oscillatory $F_{mis}(d)$ dependence originates in lattice discreteness/periodicity. Characteristic $F_{el}(d)$ dependence originates from the long wave length limit behavior of the linear lattice response Green function.

[12] This form can be derived if (i) summation in Eq. [3] is limited to the $s=1$ oscillatory term (a well justified approximation, since this series is very rapidly converging ($J_2/J_1 \ll 1$)); (ii) a dislocation density distribution function represented as a sum of the partial dislocation densities, $\rho(x) = \rho^1(x+d) + \rho^2(x-d)$; and (iii) parity properties - positive for $\rho(x)$ and negative for the $\partial \Phi(u(x))/\partial u$ functions are taken into account.
The estimate (based on the saddle point method) allows to find that $A(d, \omega) \sim \exp(-\frac{2\pi \omega}{h})b_k H_k$, where $H_k$ are the main values of the $\gamma$-surface curvature tensor at the unstable stacking fault point (H). We also find that $\omega$ is the inverse proportional to the $H$, thus $A(d, \omega)$ is strongly dependent on the geometrical ($H$) and energetic ($\gamma_{\text{isf}}$) characteristics of the $\gamma$-surface. Details of the analysis of the relation between dislocation structure and $\gamma$-surface geometry/energetics will be published elsewhere.

In the limit $d \gg \omega$, $A(d, \omega) \approx A$ and derived in this paper expression Eq.6 can be transformed to the one which similar to suggested by Schoeck [13].

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FIGURES

FIG. 1. Dependence of the generalized elastic and misfit forces (in $J/m^2$) on partials separation $d$ (in lattice constant units) for Ir and CuAu calculated within the PN model (left panel (a), (c)) and for simple model step function shaped ordinary dislocation (right panels (b), (d)). The misfit forces corresponding to the consistent discrete representation of the misfit energy in the PN model are presented by solid lines and those calculated within the ”continuum” approximation by dotted-dashed lines.

FIG. 2. Dislocation energy (in $J/m$) as (a) a function of the partials separation $d$, (b) a corresponding dependence of $d$ on $l$ (for more than one stable core configuration, solutions which are close in energy are numbered “1” and “2”) and (c) a corresponding dependence of the total energy on the position of the ordinary dislocation center given by $l$ in units of a repeat distance in the direction normal to the dislocation line ($h$), calculated for Ir (left panels) and CuAu (right panels); the ones determined within the ”continuum” approximation (see text) are presented by the dotted-dashed lines.
Fig. 1(a, b) O.N. Mryasov, Yu. N. Gornostyrev and A.J. Freeman

(a) Elastic Force
(b) Misfit Force

Ir

Generalized forces (J/m^2)

Elastic Force
Misfit Force
Fig. 1(c,d) O.N. Mryasov, Yu. N. Gornostyrev and A.J. Freeman
Fig. 2(a) O.N. Mryasov, Yu. N. Gornostyrev and A.J. Freeman

(a) 

Ir

CuAu

total energy (J/m)

partial separation d/a

l = 0.166

l = 0.66

l = 0.75

l = 0

l = 0.75

l = 0
Fig. 2(b) O.N. Mryasov, Yu. N. Gornostyrev and A.J. Freeman

![Graphs showing partials separation (d/a) for Ir and CuAu](image-url)
Fig. 2(c) O.N. Mryasov, Yu. N. Gornostyrev and A.J. Freeman

\[ E(l) - E(0) \ (\text{mJ/m}) \]

\[ l/h \]

- \( E(l) - E(0) \) for Ir and CuAu materials.

\[ 0.0 \ 0.2 \ 0.4 \ 0.6 \ 0.8 \ 1.0 \]

\[ 0.00 \ 0.01 \]

\[ 0.0 \ 0.01 \]

\[ 0.0 \ 0.01 \]

\[ 0.0 \ 0.01 \]

\[ 0.0 \ 0.01 \]