Generalized stacking fault energetics and dislocation properties: compact vs. spread unit dislocation structures in TiAl and CuAu.

Oleg N. Mryasov¹, Yu. N. Gornostyrev¹,² and A.J. Freeman¹

¹ Department of Physics and Astronomy, Northwestern University Evanston, IL 60208-3112.
² Institute of Metal Physics, Ekaterinburg, Russia.

We present a general scheme for analyzing the structure and mobility of dislocations based on solutions of the Peierls-Nabarro model with a two component displacement field and restoring forces determined from the ab-initio generalized stacking fault energetics (ie., the so-called γ-surface). The approach is used to investigate dislocations in L1₀ TiAl and CuAu; predicted differences in the unit dislocation properties are explicitly related with features of the γ-surface geometry. A unified description of compact, spread and split dislocation cores is provided with an important characteristic "dissociation path" revealed by this highly tractable scheme.

61.72.Lk, 61.72.Bb, 61.72.Nn, 61.82.Bg, 62.20.Fe

I. INTRODUCTION

In the development of modern materials with advanced high-temperature structural properties, there is a growing awareness of the importance of a fundamental understanding of the role of specific lattice defects. One such defect, dislocations, is always present in most real materials and influences a variety of properties, including mechanical, electric, optical and magnetic. High-temperature intermetallics is one of the most vivid examples where particular dislocations control deformation, fracture and other properties that are most important in terms of their technological applications.

Dislocations are a unique example of the extended defect for which a single length scale description (atomistic or continuum) is not quite appropriate - a feature that is one of the main sources of difficulties in their theoretical description. There are hundreds of atoms in a dislocation core (requiring an atomistic treatment) and thousands of atoms involved in the formation of the elastic dislocations fields (where a continuum description is more appropriate) so that neither entirely atomistic nor continuum descriptions are suitable to the problem but rather need to be combined.

Classical atomistic simulations, however, proved to be very useful and provided important insights into their fundamental properties in metals. To make use of atomistic simulations for modeling dislocations in particular material reliable model of interatomic interaction has to be developed. This, however, poses major principal problem for the use of classical atomistic simulations. Unfortunately, in most of interesting cases (including intermetallics like L1₀ TiAl) interatomic interactions are very complex and so their satisfactory description cannot be guaranteed with existing central force models. This significantly limits abilities of classical atomistic simulations for predictive analysis dislocations properties particularly in intermetallic alloys with their complex character of interatomic interactions. To date, the few quantum molecular dynamic simulations of dislocations have been restricted to s,p systems (Si, SiC), employing periodic boundary conditions with a few hundred atoms in the supercell. This approach remains unexceptionally expensive and has principal difficulties to be applied for intermetallics containing 3d-elements.

The complexity of the problem has stimulated renewed interest in the simple but tractable Peierls-Nabarro (PN) dislocation model, which incorporates atomistic effects in an approximate way into a continuum framework. In this model, the effects of lattice discreteness are confined to a slip plane with a local relation for non-linear atomistic restoring forces which can be determined from an effective rigid shift interplanar potential known as a generalized stacking fault (GSF) energy. The PN model proved to be very useful and has strongly influenced conceptually the theory of dislocations, fracture and related mechanical properties. Naturally appeared in PN model, the energy of the relative displacements of two halves of the crystal (ie., the so-called generalized stacking fault (GSF) energy, or γ-surface) was introduced and studied as an important general characteristic of the mechanical response in solids.

Despite its well-known approximations, the PN model is very attractive since it offers a tractable description with parameters (γ-surface) accessible by highly accurate quantum mechanical calculations. As was recently demonstrated, the applicability of the Peierls model framework can be extended in a semi-discrete version even for such an extreme case as narrow dislocation cores in Si. In this work, the classic Peierls model dislocation energy functional is minimized using a discrete scheme which allows avoiding assumptions of the dislocation core planarity and the Nabarro approximation for calculating Peierls stresses. Unfortunately, the proposed semi-discrete scheme is purely numerical; however, in the theory of such complex lattice defects as dislocations it is highly desirable to keep the high tractability of the theoretical approach as much as possible.
To date, the PN model analysis with first-principles parametrization for GSF energetics was restricted, however, to considering dislocations with a single component displacement field (one dimensional (1D) PN model) in Si, and in B2 intermetallic compounds. The abilities of the PN model to deal with dislocation cores in intermetallics has not yet been studied systematically, except for our earlier overall encouraging experience with the 1D-PN model for dislocations in B2 NiAl and FeAl. However, the two component displacement field (two-dimensional (2D) PN model) with the possibility of dislocation dissociation is quite typical situation in general and, in particular, is necessary to be considered in the case of unit dislocations for L1_0 TiAl and CuAu, materials with similar fcc-like structure but very different mechanical behaviour.

In contrast with the 1D PN model, exact solutions of the 2D-PN model are unknown even for the simplest sinusoidal restoring force law. Recently, Schoeck presented a direct variational method for analyzing, on the energy functional level, the 2D-PN model using ansatz solutions with geometric parameters. This method has been used to calculate dislocation core structures corresponding to model GSF surfaces. Here we present an alternative scheme for solving 2D-PN model equations within a wide class of analytic functions which makes this scheme unified (i.e., free of parameters and assumptions on dislocation dissociation) suitable for analyzing realistic/complex γ-surface and physically transparent. We apply this scheme to analyze unit dislocation structure and mobility in L1_0 TiAl and CuAu alloys with GSF energetics determined from ab-initio calculations.

In this work, we demonstrate how advantages of the PN model’s high tractability can be fully revealed due to the use of a general and physically transparent scheme for analyzing solutions in the generalized case of a two component displacement field (2D) and with a first-principles determination of the γ-surface energetics. We focus on an analysis of the unit dislocation structure in L1_0 TiAl and CuAu using the proposed scheme since this type of dislocation is important for understanding these materials with very different mechanical behaviour. We demonstrate that this proposed approach explains qualitative differences in dislocation structure and mobility in a very natural way and establishes an explicit relation between γ-surface geometry and dislocation properties within the 2D PN model. This allows one to relate GSF energetics determined from ab-initio electronic structure calculations with dislocation structure using a unified and highly transparent procedure.

II. APPROACH AND METHOD

The structure of dislocations within the 2D PN model is described from a balance between elastic and atomistic restoring forces which is expressed in a system of integrodifferential equations:

\[
\frac{K_{a\beta}}{2\pi} \int_{-\infty}^{\infty} \frac{d\xi}{\xi - x} \frac{du_\beta(\xi)}{d\xi} = F_a(\vec{u})
\]  

(1)

Here \(\beta\) is the index for components of the displacement \(\vec{u}\), with \(\beta=1\) for screw and \(\beta=2\) for edge, and \(K_{a\beta} = \mu D_{a\beta}\). \(D_{\beta}\) is a parameter equal to 1 for \(\beta = 1\) and \(1/(1-\nu)\) for \(\beta=2\). There are at least two difficulties to applying the PN model for realistic situations: (i) the restoring force law is unknown in general and (ii) an analysis of Eq. (1) seems to be difficult for an arbitrary restoring force law. We follow the GSF concept and define the restoring force in the local approximation as \(F_\beta(\vec{u}) = -dE(\vec{u})/du_\beta\), where GSF energies \(E(\vec{u})\) are calculated for experimental lattice structure parameters employing the local density full-potential linear muffin-tin orbital (FLMTO) band structure technique with the Ceperly-Alder form for the exchange-correlation potential.

In fact, special points on the γ-surface known as planar stacking fault energies (APB, ISF, CISF etc.) have been calculated by various ab-initio methods for a number of metals, alloys and compounds (see references in [2]). Thus, calculations of the entire γ-surface do not pose principal difficulties but may be rather challenging from a numerical standpoint if one would like to achieve, as much as possible, equably high accuracy for all γ-surface sampling points. Most of the numerical aspects one may face in ab-initio calculations of the GSF energetics have been summarized by Paxton. Probably, the first example of the entire γ-surface determined using ab-initio techniques is a pseudopotential plane wave (PPW) calculation for Si by Kaxiras and Duesberg. The PPW approach, however, is somewhat less natural to use if rather localized d and f electrons are present in a system. Thus, in this work we make use of the all-electron FLMTO technique which allows one to treat equally well both localized and delocalized electronic states with reasonable accuracy and high numerical efficiency.

One should emphasize here that only in the local approximation is so simple a relation provided with GSF energies and hence restoring forces are so easily accessible by ab-initio techniques. As demonstrated by Miller and Phillips using MD simulations, the local approximation merely affects dislocation structure but may be important for calculating Peierls stresses. Any corrections beyond the local approximation involve a much more complex procedure and to the best of our knowledge have not yet been realized using ab-initio calculations.

An analysis of the solutions of Eq. (1) is rather complex from a mathematical point of view. An elegant idea proposed by Lejeck for finding solutions of the 1D PN model equations in a wide class of analytic functions seems to be general and suitable for cases of complex/realistic restoring force laws. Details of such an analysis for the 1D PN model with generalized restoring forces determined for NiAl from ab-initio calculations are discussed.
in our earlier work. Our results for this realistic example demonstrate that the scheme for solving the PN model type equations based on Lejeck’s idea can be very convenient and provides the accuracy and numerical stability desired. In the 2D PN model case, however, additional complications related with the coupling of equations (cf. Eq. (6)) have to be overcome. In this work, we present a scheme for solving the 2D PN model equations with an arbitrary restoring force law which is based on Lejeck’s idea as generalized for the 2D case.

Solutions of Eq. (6) are found by constructing an analytic complex function \( G_\beta(x) = \rho_\beta(x) + i \cdot \frac{1}{\mu D_\beta} F_\beta(x) \) where \( \rho_\beta(x) = du_\beta(x)/dx \) is the dislocation density, and \( F_\beta(\bar{u}(x)) \) the restoring force and are given as expansions

\[
\rho_\beta(x) = \text{Re} \sum_{k=1}^{N} \sum_{n=1}^{p_k} \frac{A_{nk}^{\beta}}{(x - z_k^n)^n}, \tag{2}
\]

\[
\frac{2}{\mu D_\beta} F_\beta(x) = -Im \sum_{k=1}^{N} \sum_{n=1}^{p_k} \frac{A_{nk}^{\beta}}{(x - z_k^n)^n}. \tag{3}
\]

Here \( N \) is the number of poles with maximal order \( p_k \) at points in the complex plane, \( z_k^n = x_k^n + i\zeta_k^n, (k = 1,...,N) \). This representation is not only mathematically justified (the structure of the PN model equations is analogous to the Hilbert transform) but is also physically transparent. Indeed, the number of poles in the expansion for \( \rho_\beta(x) \) determines the number of cores (partial or fractional dislocations) with a width \( \zeta_k^n \) and positions of the centers, \( x_k^n \). The solutions, \( u_\beta(x) \), can be found by integrating \( \rho_\beta(x) \) with appropriate boundary conditions. Then, for an fcc lattice and a screw orientation of the unit dislocation in the \{111\} plane, the functions \( u_\beta(x) \) and \( F_\beta(\bar{u}(x)) \) for \( p_k = 2 \) and \( N = 2 \) can be written in the convenient parametric form

\[
\frac{2\pi u_1}{b} = \frac{1}{2} \left[ \theta_1^2 + \theta_2^2 - \frac{\alpha_1 - 1}{\alpha_1} (\sin \theta_1^2 + \sin \theta_2^2) \right] \tag{4}
\]

\[
\frac{\pi u_2}{b_e} = \frac{1}{2} \left[ \theta_1^2 - \theta_2^2 - \frac{\alpha_2 - 1}{\alpha_2} (\sin \theta_1^2 - \sin \theta_2^2) \right] \tag{5}
\]

\[
\frac{4\pi \omega_1^1}{\mu D_1 b} F_1 = -\frac{1}{2\alpha_1} \left[ \sin \theta_1^2 + \sin \theta_2^2 + \frac{2(\alpha_1 - 1)}{\alpha_1} \times \right. \left. (\sin^2(\theta_1^2/2)\sin \theta_1^2 + \sin^2(\theta_2^2/2)\sin \theta_2^2) \right] \tag{6}
\]

\[
\frac{2\pi \omega_2^0}{\mu D_2 b_e} F_2 = -\frac{1}{2\alpha_2} \left[ \sin \theta_1^2 - \sin \theta_2^2 + \frac{2(\alpha_2 - 1)}{\alpha_2} \times \right. \left. (\sin^2(\theta_1^2/2)\sin \theta_1^2 - \sin^2(\theta_2^2/2)\sin \theta_2^2) \right] \tag{7}
\]

Here \( \theta_k^\beta = 2\arccot((x - x_k^\beta)/\zeta_k^\beta), \zeta_k^\beta = \alpha_\beta \omega_0^\beta \), where \( \omega_0^\beta \) is the width of the dislocation core which appears in the solution of the original PN model for a sinusoidal restoring force law, \( b \) is the total Burgers vector and \( b_e \) is the edge component of the partial dislocation Burgers vector. Thus, the complete set of dislocation structure parameters, \( \alpha_\beta \) and \( x_k^\beta \) (including possible splitting) can be determined from the general restoring force law \( F_\beta(\bar{u}) \).

However, there is a complication related with an essential feature of the 2D PN model. Now, the 2D PN model equations (Eq. (6)) are coupled only through the restoring force which is a function of the unknown a priori “dissociation path” determined in the two component displacement space and given by the dependence \( u_2 = f(u_1) \) of the edge \( u_2 \) on the screw \( u_1 \) component. Thus, function \( f(u_1) \) has to be found along with solutions of Eq. (6). Hence, we propose an iterative procedure which starts with calculations of the restoring forces, \( F_\beta(u_1, u_2) \), and the corresponding dislocation structure parameters for a linear “dissociation path” \( u_2 = K \cdot u_1 \). Then, as convergence is achieved, both the actual “dissociation path” and the solutions \( \bar{u}(x) \) can be determined.

### III. RESULTS AND DISCUSSION

The results of such an analysis for a unit dislocation structure in L10 TiAl and CuAu are presented in Fig. 1. As can be seen, a unit dislocation in TiAl is compact - in contrast with CuAu. The unit dislocation structure predicted here for TiAl (compact core) is consistent with available experimental data and atomistic simulation results for an embedded atom potential that gives a value of the CSF energy that is similar to our ab-initio calculations but our analysis is performed within a highly tractable scheme which allows one to relate qualitative differences in dislocation properties to the ab-initio \( \gamma \)-surface geometry.

_Disslocation dissociation and \( \gamma \)-surface geometry._ Focus now on the details of the \( \gamma \)-surface geometry which determine the difference in the structure of TiAl and CuAu unit dislocations. These \( \gamma \)-surfaces, calculated for the \{111\} plane with the FLMT method using six layer supercells and homogeneous periodic boundary conditions without relaxation, are presented in Fig. 2 as contour plots along with actual “dissociation” paths. Note that the dislocation axis is taken along \langle 110 \rangle so that displacements along \langle 112 \rangle correspond to an edge and those along \langle 110 \rangle have a pure screw component. We label several special points on the \( \gamma \)-surface section along \langle 112 \rangle for the screw component \( u_1 = 0.5 \): (i) the complex stacking fault (CSF), labeled C, (ii) the inflection point, labeled I, and (iii) the point \( C' = (0.5, f(0.5)) \), where \( f(0.5) \) is the calculated maximal edge component. There is a noticeable difference in the relative location of I and C for TiAl and CuAu which results in striking differences in the properties of the unit dislocations.

If the components of the restoring forces, Eq. (3), along the \( u_2 = f(u_1) \) path change sign then there is
more than one pole in the expansion, Eq. (2), and so solutions of Eq. (1) correspond to the partial/fractional (split/spread) dislocations. In particular, this condition is fulfilled if the corresponding $\gamma$-surface section has a minimum at $(u_1=0.5, u_2=f(0.5))$, where the maximal edge component $f(0.5)$ was found to be substantially smaller than the trial already after the first step of the iterative procedure. This "reduction" is a result of the overlap of the opposite sign partials displacement fields. As a consequence of such a "reduction", $C'$ may be located either before the I point (CuAu) or beyond (TiAl); this, in turn, determines whether there is a minimum on the $\gamma$-surface section and, correspondingly, whether the dislocation is split/spread or compact.

![Density of displacements $\rho(x)$ in the unit dislocation: a) the screw component in TiAl and for b) the screw and c) edge components in CuAu as a function of the distance ($x$) from the dislocation center (given in lattice constant units).](image)

The iterative procedure allows us to also find the actual "dissociation path", curve $u_2 = f(u_1)$, which is shown in Fig. 3 as a thick solid line. In the case of a spread unit dislocation (CuAu), the actual path is quite different from the usually assumed path. However, for a compact dislocation (TiAl) the difference of the actual "dissociation path" (solid line) from the assumed path (dashed line) is really dramatic (see Fig. 3). The possibility of such a transition from the split/spread to compact solution (with a corresponding transformation of the "dissociation path") has also been recently indicated by Schoeck in a 2D PN model analysis with model type $\gamma$-surfaces using the direct variational approach.

The equilibrium separation distance between partials of dissociated dislocations is traditionally determined from the balance between elastic (within linear elasticity theory) and stacking fault surface tension forces resulting in the widely used simple expression. The PN equations (Eq. (1)) do not contain, in an explicit form, the stacking fault energy ($\gamma_f$) which is related in a very simple manner with the equilibrium separation distance ($d$) between partials of dissociated dislocations. However, it is possible to demonstrate that this simple relation can be recovered within our more general PN model approach as the limiting case of large separation distances.

![Contour plots of the $\gamma$-surface (in J/m$^2$) for L1$_0$ a) TiAl and b) CuAu. The position of the CSF is denoted by C, the point corresponding to the calculated amplitude of the edge component by $C'$ and the inflection point of the corresponding section by I. The actual "dissociation path" (or dependence of the longitudinal on lateral to the Burgers vector components of the displacement) is presented by the thick solid lines and is compared with the usually assumed path (straight dashed line).](image)

Indeed, the energy $\gamma_f$ of the fault with vector $\vec{f}=(0.5, u_2)$ is uniquely determined within the local approximation through the two component restoring force vector $\vec{F}(\vec{u})$ defined for an arbitrary path $u_1 = f(u_2)$ as...
\[ \gamma_f = \frac{a_f}{\pi d} \left[ b_x^2 \left( 1 + \left( \frac{4K}{\pi d} \right) \right) \frac{b_y^2}{1 - \nu} \left( 1 - \frac{8\zeta}{\pi d} \right) \right] \]

where the separation distance in the limit considered is taken as \( d = 2x_1 = 2x_2 \) with \( \alpha = \alpha_1 = \alpha_2 \), \( b_x = b/2 \) is the screw component and \( b_\rho \) is the edge component of the Burgers vector and \( \alpha_{1,2}, \zeta_{1,2} \) are parameters in Eqs. (8) and (9). Then it is easy to see that the zeroth order terms of the \( \gamma_f \) power expansion in \( \zeta/d \) (for large separation distances \( 2x_1 = 2x_2 = \delta + \zeta \ll d \)) reproduce exactly the well-known relation between \( d \) and \( \gamma_f \). This simple estimate, however, becomes obviously inaccurate for dislocations with small separation distances, as in the case of CuAu and TiAl considered here. This result is non-trivial since it allows one to relate rigorously the PN model and often used simple elasticity descriptions. We also find that the higher order (in \( \zeta/d \)) contributions in Eq. (8) have negative sign, thus the simple relation \( \gamma \sim 1/d \) corresponds to an upper estimate which becomes increasingly inaccurate for dislocations with small separation distances, \( d \). We should emphasize, however, that in accordance with our 2D PN analysis the CSF energy alone is not a sufficient characteristic to describe important details of the dislocation structure. Hence, additional parameters of the entire \( \gamma \)-surface (see Eq. 8) have to be taken into account for a correct analysis - which is especially important in the case of small dislocation spreading (as found in our analysis for \( \gamma \)-surfaces calculated for TiAl and CuAu).

**The Peierls stress.** - Consider now how such a characteristic of the dislocation mobility as the Peierls stress, \( \sigma_p \), can be determined within the proposed PN model analysis scheme. According to the approximations introduced by Nabarro (which often work reasonably well), \( \sigma_p \) is defined as

\[ \Phi_p(l) = \Phi_p(0) + \frac{h}{2} \sum_{s=1}^{n} J(s) \left[ \cos(2\pi s l/h) + \cos(2\pi s (l - \delta)/h) \right] \]

Here \( h \) is the lattice period in a direction perpendicular to the dislocation line, \( \delta \) and \( \sigma_p/\mu \) (here \( \mu \) is the shear modulus) for CuAu (0.0005) is significantly smaller than for TiAl (0.024). This difference is attributed to the spreading of the unit dislocation in CuAu, since \( \sigma_p/\mu \) for the unspread core solution is about the same as for TiAl. This result is quite remarkable since it clearly demonstrates the importance of the entire \( \gamma \)-surface geometrical parameters as an integrated characteristic of the interatomic interactions of solids (including chemical bonding contributions) in the context of the analysis of dislocation properties.

We emphasize here the importance of such characteristics that are naturally revealed in our 2D PN model analysis as a "dissociation path" for the analysis of the fracture behaviour. As is well-known in the scope of Rice-Thomson (R-T) criteria, crack propagation is described by the competition of the crack opening (characterized by the surface energy \( \gamma_s \)) and dislocation emission (characterized by unstable stacking fault energy \( \gamma_{us} \)) processes. An analysis of this competing process arrives at the criterion of brittle crack propagation, \( \gamma_s/\gamma_{us} > 2.9 \), which despite its simplicity captures the general tendencies in materials fracture behaviour. Dislocation emission from the crack tip within the R-T criterion is characterized by the energy barrier, \( \gamma_{us} \). This energy barrier is usually estimated assuming a straight line "dissociation" path. As we demonstrated above, the actual "dissociation" path may deviate significantly from an assumed straight line. In cases of spread dislocations (CuAu), corresponding changes in \( \gamma_{us} \) estimates are likely to be small but may be quite significant in cases of compact dislocation cores (TiAl). In fact, if features of the actual "dissociation" path are taken into account to determine \( \gamma_{us} \) for TiAl, the R-T criterion \( \gamma_s/\gamma_{us} = 1.7 \) predicts brittle crack propagation - opposite to the result which one obtains assuming a straight "dissociation" path \( \gamma_s/\gamma_{us} = 4.5 \).
IV. CONCLUSIONS

We proposed a general and physically transparent scheme for analyzing the 2D PN model with a general restoring force law. We provided realistic examples (TiAl, CuAu) and demonstrated that dislocation properties can be predicted and explained on the basis of first-principle calculations of the γ-surfaces. In particular, the actual "dissociation path" was determined and proved to be an essential feature of the 2D PN model and an important characteristic for understanding dislocation dissociation processes and related mechanical properties (tendencies in fracture behaviour). We showed that differences in dislocation properties (compact vs. spread) for realistic (complex) situations as in TiAl and CuAu can be explained from the first-principle calculations of the γ-surface geometry. This demonstrates the advantages of the proposed approach which establishes, within the 2D PN model, explicit relations between γ-surface geometry parameters (which can be accurately determined using ab-initio techniques) and dislocation structure and mobility (processes that approach mesoscopic scales).

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