Burgers Vector Content of an Interfacial Ledge

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A new way of investigating the elastic field around a ledge of a faceted interface is proposed for crystalline materials. The length and/or angular misfits along two adjacent facets are accommodated by slightly deforming the atomic structural units with an appropriate distribution of translation dislocations. The Burgers vector content of the ledge is not defined as usual from a circuit crossing the interface twice, a method which proves to be sometimes misleading. An example treats, at the atomic scale, an unusual ledge of the interface $TiAl/Ti_3Al$.

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In solid-state transformations, linear deformation singularities along crystalline interfaces play a crucial role. Much effort has been devoted to their characterization by conventional or high-resolution transmission electron microscopy (CTEM or HRTEM) (e.g., [1]), because of their importance in solid-state physics and materials science. For example, interface strain may dramatically influence the electronic properties of lattice-matched III-V semiconductor superlattices [2]; the density of interfacial ledges, or facets, may influence considerably the measured barrier height on *p*-type Si [3]; when interfacial ledges move, under a stress or temperature change, a phase transformation occurs [4]; gliding matrix dislocations generally leave ledges when cutting interfaces; etc.

Although some interfacial singularities can now be observed at the atomic scale thanks to a new generation of electron microscopes, it is not yet possible, in most cases, to describe their associated elastic deformation fields. This is a challenge for scientists and has motivated this Letter, in which an analytical solution is proposed for an interfacial ledge separating two parallel facets. The present difficulties in estimating the deformation field around a ledge, and consequently its related Burgers vector content (BVC), were faced first by Howe, Dahmen, and Gronsky [4], when treating ledges at Al/Al_2Ag interfaces observed in HRTEM: Does a translation dislocation as defined in [5] suffice to describe the elastic field of a ledge? In this case, how does one determine the Burgers vector from which the entire deformation field can be derived? Where should the theoretical dislocation core be placed when treating a ledge? How should one draw a circuit around the ledge using an HRTEM image, from which the BVC of the ledge can uniquely be obtained? In fact, the solution presented in [4] does not account for any length or angular interfacial misfit since the authors used a translation dislocation with a core arbitrarily chosen at a corner of a facet. Interestingly enough, these authors questioned the meaning of a circuit crossing the interface twice to distinguish between possible BVC's.

Our method to treat the problem is developed below. First, a short description of the classical interpretations of interfacial singularities and the associated terminology will be given.

For twin boundaries in cubic crystals, it has been shown, using CTEM, that many singularities have deformation fields similar to those of essentially isolated translation dislocations if they are sufficiently far from each other (e.g., [6]). The attached Burgers vectors were first identified as part of the displacement shift complete (DSC) lattice defined as the coarsest common lattice that contains both crystal lattices as subsets [7,8]. The DSC lattice usually serves as a reference lattice to draw Burgers circuits across the interface in the same manner that a crystal lattice is used for matrix dislocations [7,9]. Later, it was observed by CTEM that a deformation singularity can sometimes separate two structurally different interfacial domains [10]. Each domain has its own atomic structure, denoted as structural units (SU's) in [11], which repeat with a short period. Such a singularity was interpreted as a translation dislocation involving a DSC vector plus a rigid-body translation (e.g., [10,12]). More recently, new periodic singularities were observed in gold by HRTEM [13], which do not behave as DSC dislocations and still separate similar SU's. For an interface separating noncubic crystals, there are other difficulties. The most dramatic one is the fact that the DSC lattice cannot always be determined uniquely [8,14], which makes the determination of a Burgers vector by using a circuit passing twice across the interface problematic. Since a unique displacement field is observed, it is not acceptable to continue with the DSC concept only, despite its widespread use in the literature.

Our analysis of the displacement field around a ledge is built from elemental ideas: (i) The misregistry of two

lattices meeting along an interfacial facet has a linear dependence with coordinates along the facet and can therefore be accommodated by a continuous distribution of infinitesimal dislocations over the facet [15]; (ii) the geometrical need to reconstruct the same SU's along each facet implies, in general, the presence of a finite translation dislocation located at each of the two ends of the facet [16]; (iii) since a Burgers vector has meaning in an elastic continuum [5], a circuit drawn step by step on an HRTEM image, crossing the interface twice, is therefore *not necessary* to characterize the complete displacement field; (iv) the position of each atomic column can be derived from (i) and (ii) and then compared to its experimental position.

The following assumptions are made: The ledge height is not more than a few interplanar spacings; two adjacent facets have identical misfits; there are well-defined (possibly different) SU's. The ledge *STEP*, Fig. 1(a), is supposed to be part of an elastically deformed continuum. Along the two facets *ST* and *EP*, which can have different widths, SU's repeat within some elastic distortions to accommodate the angular and/or length misfit(s) along the interface. Two planar unit cells of crystals + and −, denoted M^+ and M^-, match along each facet. This in effect determines the quasiperiodicity of the SU's arrangement along a deformed facet. First, by a thought experiment, atomic bonds are cut along a theoretical faceted interface, separating the matter into two undeformed half crystals. No long-range rotations are assumed to result, and a fixed point C_1 is chosen for both crystals, located in the center of the right facet. The center of the left facet now splits into C_2^+ and C_2^-, Fig. 1(b). Two free surfaces with ledges h^+ and h^- are generated, respectively denoted $S^+T^+E^+P^+$ and $S^-T^-E^-P^-$. In the following, by convention, the ledge is denoted "ledge h^+/h^-." From Fig. 1(b), the general result which is of interest is that, keeping the crystal fixed, a displacement vector **t** must be applied in general to the crystal + along S^+T^+ to superimpose C_2^+ and C_2^-. It is easy to prove [16] that **t** can always be expressed as a difference between a lattice vector of crystal + and a lattice vector of crystal −, whatever the crystals and their misfits are. At this stage, note that no use is made of the DSC formalism.

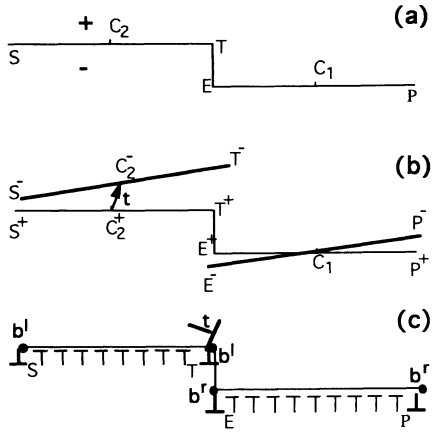

FIG. 1. Schematic representation of the cut-and-paste process leading to the surrounding displacement field around the interfacial ledge *STEP*, separating crystals + and −. The height *TE* of the ledge has been exaggerated relative to the widths of the facets: (a) deformed state; (b) after cut, the free surfaces $S^+T^+E^+P^+$ and $S^-T^-E^-P^-$ are generated; (c) elastic field in terms of a continuous distribution of translation dislocations.

To reconstruct the elastic displacement field along the ledge and the correct SU's is now straightforward. The two free surfaces are welded as schematically described in Fig. 1(b): A displacement is applied to map E^+P^+ onto E^-P^-. Along E^+P^+, it changes linearly from C_1 to account for the misfits of M^+ and M^-. S^+T^+ maps onto S^-T^- similarly, except for the addition of an extra constant shift $\mathbf{t}=C_2^+C_2^-$ [16]. In [17], where misfits are zero and a three-dimensional DSC lattice is assumed, **t** is a DSC vector. The resulting elastic field can be described readily, *in a continuum*, in terms of a continuous distribution of infinitesimal translation dislocations over the facets and finite translation dislocations in *S*, *T*, *E*, and *P*. Figure 1(c) is a schematic representation for dislocations oriented towards the reader and brought along *EP* from the right and along *ST* from the left. In this analysis the small contribution of the disordered part *TE* of the ledge core, the height of which is only a few interplanar spacings, has been neglected.

The elastic field in the close vicinity of the ledge can be characterized by its BVC: the sum of the Burgers vectors of the translation dislocations placed at *T* and *E*. From Figs. 1(b) and 1(c), it is either the vector $T^+T^- - E^+E^-$ or $\mathbf{t}+\mathbf{b}^l+\mathbf{b}^r$, where $\mathbf{b}^l$ and $\mathbf{b}^r$ are the finite Burgers vectors of the dislocations located at *T* and *E* only due to the misfits. These vectors can be determined from the undeformed state [Fig. 1(b)]. Let us first consider an initial state for which (i) the planar unit cells M^+ and M^- have a common node, and (ii) their orientation is such that a planar pure deformation *D* permits one to pass from M^+ to M^-. Then M^- is subjected to a three-dimensional rotation *R* to orient it according to Fig. 1(b). Note that the length misfits are only taken into account by *D*, while *R* takes account of the angular misfit. $A=RD$ is a linear operator transforming the planar unit cell M^+ into the planar unit cell M^-. If *I* is the identity operator, $\mathbf{b}^r=(A-I)C_1P^+$ and $\mathbf{b}^l=(A-I)C_2^+T^+$. Since, roughly, the main part of the elastic energy around the ledge changes with the square of the BVC, this vector is expected to be small. This offers a systematic way to determine the possible **t**'s. Because of the translation dislocation attached to **t**, it is expected that a series of ledges such as that described in Fig. 1(c) will be associated with long-range stresses. Interfaces close to mechanical equilibrium must hence be searched for $\mathbf{t}=0$ or an

average t close to zero. An additional property can be derived for the BVC if the following question is answered: What happens to the BVC when the two facets have varying widths, i.e., when the extremities S,T,E,P move? For simplicity, C_1 is still maintained as a fixed point for the two crystals and the section TE is assumed to move parallel to itself. Moving the extremities of the facets does not change the straight lines S^-T^- and E^-P^-, which are parallel and attached to the theoretical free surface of crystal $-$. As a result, the BVC remains unchanged.

For practical purposes, the BVC of a ledge is deduced as follows. First, the length and angular misfits are measured in areas far from the interface to avoid lattice distortions. Atomic structural units are then analyzed for both facets so that the positions of their atomic columns can be reproduced by computer. Second, the lengths of the two facets ST and EP are measured. The vector $\mathbf{b}^l$ (or $\mathbf{b}^r$) is then derived, since its components are proportional to the length and/or angular misfits of the left (right) facet. Third, a set of small vectors $\mathbf{t}$ is obtained by computer, and added to $\mathbf{b}^l$ and $\mathbf{b}^r$ to form the smallest possible BVC's. Finally, for each BVC obtained, the displacement field around the ledge is computed using the scheme in Fig. 1(c), and compared to that of the HRTEM image in the vicinity of the ledge. Since the elastic field is uniquely determined from the given boundary conditions, a unique BVC will result. An illustration will now be presented, for which there is no angular misfit.

Recent work in HRTEM of $(1\bar{1}1)$TiAl/$(0001)$$Ti_3Al$ interfaces has revealed the presence of deformation singularities, which have elastic deformation fields similar to that of Shockley dislocations of the TiAl phase and are associated with ledges $h^+=2$ and $h^-=2$, or ledge 2/2 [18]. Other singularities are nevertheless present, like the unusual example of the ledge 4/4, in Fig. 2. The positions of the facets are indicated by the white bars. Examination of this micrograph shows that there are no obvious extra atomic planes visible. This can be readily verified by drawing a circuit around the ledge, using jumps on lattice sites. As a result, it can be inferred that the ledge is not linked to a significant deformation field. This is false as shown below.

TiAl has a tetragonal atomic structure $L1_0$ with lattice parameters $c=a=0.40713$ nm [18]; Ti_3Al is hexagonal (DO_{19}) with $a=0.5775$ nm and $c=0.4638$ nm [19]. The SU's are formed by close-packed stacking of atoms along the two facets. There is no angular misfit between the dense planes $(1\bar{1}1)$ and (0001), which have practically the same spacing. The electron beam is parallel to $[10\bar{1}]$TiAl$\parallel\langle 11\bar{2}0\rangle Ti_3Al$, this latter vector being the largest one (misfit 0.001). As a result, t is practically zero, while $\mathbf{b}^l=\mathbf{b}^r$ are close to $\frac{1}{12}[121]$, giving a BVC close to $\frac{1}{6}[121]$. Using the anisotropic elastic constants for TiAl in [19] gives the theoretical atomic column positions

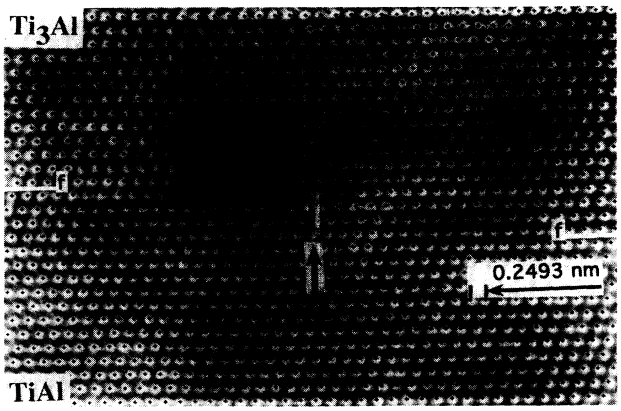

FIG. 2. HRTEM image of a ledge 4/4 at the interface $(1\bar{1}1)$TiAl/$(0001)Ti_3Al$. The electron beam is along $[10\bar{1}]$TiAl. The white bars labeled f indicate the positions of the facets. The arrow indicates the position of the theoretical ledge. The predicted atomic positions (small black crosses) conform reasonably well with the experimental positions (white dots). The Burgers vector content (BVC) of the ledge is $\frac{1}{6}[121]$TiAl.

(small black crosses in Fig. 2) which can be compared to the experimental atomic projections shown in the HRTEM image Fig. 2 (white dots according to [18]).

Figures 3(a) and 3(b) depict, for the same ledge (but viewed from the opposite direction), why no extra plane can be detected by a circuit crossing the interface twice. Figure 3(a) describes schematically the stress-free state of the crystals. Broken lines RS and UV point out the mismatch between the lattices at the upper and lower parts of the ledge, due to the length misfit. By jumps using atomic column positions, as currently done, any circuit around the ledge cannot reveal the presence of an extra plane [Fig. 3(b)]. Such a circuit is thus misleading.

Of course, concerning the detailed atomic structure of a ledge core, no details can be given from elasticity only. On the other hand, we note that finite translation dislocations located at the ends of the facets may climb or dissociate towards one or both crystals, or along the facets.

In summary, a new method has been presented to describe the elastic field around an interfacial ledge when well-defined SU's repeat along the facets. For the first time, it has been shown how this field depends on the SU's (via vector t), on the heights h^+ and h^- of the ledge which can be different [16], and on the misfits of the crystal lattices along the facets (via the transformation A). In addition, the BVC of the ledge has been defined, which characterizes the strength of the surrounding elastic field without using any circuit crossing the interface twice. These theoretical results have been validated by an atomic scale study of a ledge 4/4. Beyond the analysis of HRTEM images they have important implications for the fundamental question of appropriate bound-

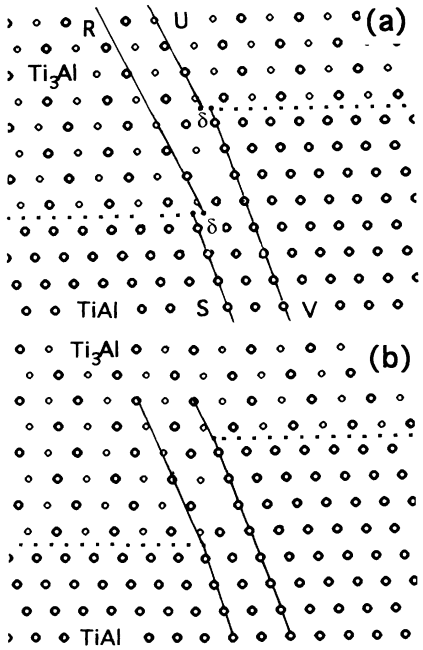

FIG. 3. Schematic representations of the displacement field associated with a ledge 4/4. (a) Stress-free state obtained after cutting the atomic bonds along the facets (in dotted lines). Discontinuities $\delta = \frac{1}{12}$ [121]TiAl at the upper and lower ends of the ledge, shown by the broken lines *RS* and *UV*. (b) Deformed state.

ary conditions to be applied at solid/solid interfaces.

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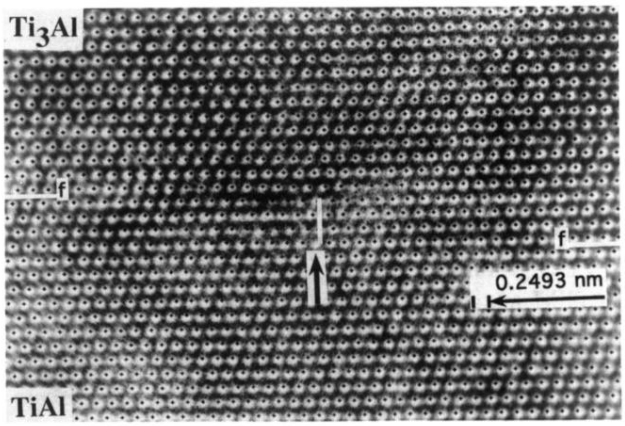

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