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Dislocation bends in a film/substrate heterostructure

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Threading dislocations in thin-film/substrate heterostructures interact elastically with the free surface. In the case of a plastically relaxed heterostructure $Si_{0.68}Ge_{0.32}$/Si(001), and thanks to a new contrast simulation programme, it is shown that the short skew emerging legs of the threading dislocations are of screw character, which explains the easy production of 60° interfacial dislocations by multiple cross-slips of the emerging legs.

Keywords: Dislocations; Interfaces; Transmission electron microscopy (TEM); Simulation

Different techniques, including transmission electron microscopy (TEM) and transmission or reflection X-ray topography, are used to observe the formation of the first dislocations in heteroepitaxial systems formed by the deposition of a small amount of crystalline matter onto a single crystalline substrate (e.g. [1,2]). They are produced from the glide of threading dislocations (TDs) to accommodate as much as possible the lattice mismatch between the two crystals and therefore to decrease the total elastic energy stored in the system by the interfacial coherency between the film and the substrate.

For cubic to cubic heterostructures, according to the growth mode adopted by the system (layer by layer, or the Volmer–Weber or Stranski–Krastanov regime), the interfacial legs of these TDs can have Burgers vectors of types $1/2\langle 110\rangle$ and $1/6\langle 112\rangle$. With respect to a $\langle 110\rangle$ interfacial dislocation direction, these vectors are oriented either at 30° (Shockley partials, e.g. [3]), 60° (e.g. [2]) or 90° (e.g. [4]), mostly identified from high-resolution TEM observations. In the film, TDs can glide in planes different from the usual $\{111\}$ planes [5] or have line directions not contained in these planes, as shown by some high-resolution or stereo TEM observations [6]. They can also glide in the substrate of a flexible specimen [2,7].

For $Si_{0.68}Ge_{0.32}$/(001)Si films [8,9], threading dislocations have been shown to be generated from isolated surface dislocation sources under the form of successive dislocation half-loops gliding in the usual $\{111\}$ planes. However, for a $Si_{0.67}Ge_{0.33}$/(001)Si super-lattice [6], it was shown that the non-interfacial TD segments are not contained in the usual $\{111\}$ slip planes but can have directions almost parallel to the [001] zone axis.

The variety of these results and the need to identify very short dislocation legs near the free surface of a heterostructure observed in a plan-view specimen in TEM led the present authors to built a new investigation tool. More precisely, the identification of the TDs is desirable because the interfacial and emerging legs of a TD can have image contrasts very sensitive to the proximity of a free surface, which makes the application of the common invisibility criterion [10] rather controversial for both legs of the TD in a very thin-film. In an attempt to gain a better insight into their contrasts, the present authors have built a devoted programme that constructs computer-aided images. It is able to account for the measured geometry of a TD and tests all possible Burgers vector of the TD. It uses image matching from two-beam experimental TEM images, as proposed long ago [11,12].

Since the elastic field of a curved dislocation piercing the free surface seems intractable analytically [13], a simplified geometry is adopted hereafter: the TD is assumed to be undissociated and composed of two straight dislocations legs. This prerequisite is not restrictive for a

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semi-conductor system since dislocation segments are very commonly observed to lie along directions $\langle 1\,1\,0 \rangle$ (see e.g. [9,14–17]). In addition, its elastic field only relaxes at the upper surface of the thin foil. The interfacial leg is semi-infinite, while the short leg in the film pierces the upper surface on the skew at any direction. Numerical applications apply to dislocation bends in the $Si_{0.68}Ge_{0.32}/Si(0\,0\,1)$ system.

Figure 1 is a schematic drawing which represents a TD composed of a straight interfacial semi-infinite leg, TO, and a short leg oriented **OD**, piercing the free surface on the skew. The free surface normal, **N**, is oriented from inside to outside the material, supposed elastically homogeneous and isotropic (μ is the Young modulus, v the Poisson ratio). The Burgers vector associated to the dislocation bend TOD is denoted **b**. The elastic displacement field **u** of this dislocation is not available in the literature, but can be obtained from the superposition of some elastic equilibria relative to the semi-infinite material. The principle is to sum the elastic field of three appropriate dislocations with Burgers vectors equal to $\pm$**b**:

– A semi-infinite dislocation piercing the free surface at point D. Its orientation is along FOD and its Burgers vector is **b**. Its displacement field is explicitly given in Refs. [18,19].
– An angular dislocation TOG oriented by its interfacial leg **TO** with a leg GO parallel to **N**. Its Burgers vector is also **b**. Its angle at the apex O is equal to $\pi/2$.
– An angular dislocation FOG oriented by its leg **OG** parallel to $-$**N**. Its Burgers vector is $-$**b**. Its angle at the apex O, smaller than $\pi/2$, is determined by the crystallographic direction of the leg FO, i.e. that of the short emerging segment OD.

Figure 1 shows that the two superimposed legs along FO (respectively GO) do not contribute to the elastic field since their line orientations and their Burgers vectors are opposed. As a result, this addition leads to the elastic field of the dislocation bend TOD. The problem reduces consequently to the evaluation of the two angular dislocations TOG and FOG, which have a leg parallel to **N**.

As shown below, each of them can be explicitly written from a solution proposed by Comninou and Dundurs [20]. These authors actually discovered a way to find the displacement field $\mathbf{u}^N$ of an angular dislocation for the peculiar case of a leg parallel to **N** and an apex angle less than or equal to $\pi/2$. Briefly, the logic is as follows. First, they consider an infinite material and a plane P with a normal **N**. They insert a first angular dislocation with a Burgers vector **b** and its mirror image with respect to plane P. The first angular dislocation should have a leg perpendicular to P but not crossing it. Then, they apply Yoffe's expressions [21] to obtain the resultant elastic field. However, since non-zero normal stresses remain along the mirror plane P, extra terms are added to find the field $\mathbf{u}^N$. These terms are found from the use of appropriate harmonic functions specific to each component of the Burgers vector **b**.

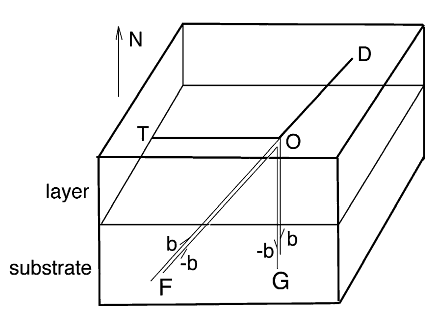

Figure 1. Representation of a dislocation bend TOD in a layer/substrate system. The thin half arrows indicate the line orientations of dislocations FOD, TOG and FOG. The dislocation legs along FO and OG are superimposed.

Therefore, for the dislocation bend TOD in Figure 1, the total **u** field is obtained by adding:

– Once, the elastic field of a semi-infinite dislocation [18,19].
– Four times, that of an angular dislocation in an infinite material [21].
– Twice, the extra terms calculated in Ref. [20].

Since the expressions in Refs. [18–21] are fairly long to write, they could contain typographical errors. For safety, we have tested them numerically and found some errors not yet outlined in the literature (to the authors' knowledge). Adapted corrections are available to interested readers.

The computation of a simulated image of a TD is performed in the assumption of a bright-field two-beam condition. The principle of the technique is well known since the pioneer works of Hirsch et al. [10] and Head et al. [11,12] on the straight dislocations: the Howie–Whelan equations [22] are numerically integrated over the foil thickness crossed by the electron beam and the intensity is recorded in close nodes included in the perimeter of the simulated image. A grey scale then transforms the intensity into an image, the resolution of which depends on the spacing between two consecutive nodes.

The main difficulties in this sort of question are (i) to obtain the displacement field **u** attached to the defect with the best possible approximation; and (ii) to be able to calculate explicitly the β' function to insert into the Howie–Whelan equations. This latter point was the most tedious part of the present work since this function depends on the nine derivatives of the three-dimensional **u** field and on the tilting angles of the thin foil via the diffracting vector **g**. The β' function is calculated in the same frame $OX_1X_2X_3$ as in Ref. [23], except that the origin O is chosen here as the apex of the TD: the axis OX_2 is directed towards the screen, while the axis OX_3 is chosen along the projection onto the screen of the crystallographic direction of the dislocation leg **OD**. The axis OX_2 is chosen opposite to the crystallographic orientation of the beam, denoted **BM**. In a simulated image, OX_3 is directed from bottom to top. A simulated image includes the projections the two dislocation legs and is limited by a parallelogram with sides parallel to the two dislocation legs.

To obtain a good resolution, each simulated image is constructed as the sum of 80×80 adjacent small parallelograms. Inside each small parallelogram the grey intensity is assumed to be constant, as computed at the centre of the parallelogram via the Runge–Kutta–Merson procedure [24]. This method has already been