Thin Solid Films 599 (2016) 7–13

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

Free surface relaxation of a semicoherent interface in an isotropic thin plate

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ARTICLE INFO

Article history:
Received 6 March 2015
Received in revised form 12 October 2015
Accepted 8 December 2015
Available online 18 December 2015

Keywords:
Thin film
Dislocation
Elastic field
Free surface

ABSTRACT

A method leading to an explicit evaluation of the elastic field of a planar semicoherent interface placed in a thin isotropic plate is proposed. It is assumed that the interface contains a single family of straight, periodically distributed, misfit dislocations. The known properties of continuous distributions of dislocations and periodic elastic fields in an unbounded medium are used to solve the problem. Surface stresses are cancelled from the addition of appropriate fields applying to an infinite medium. Numerical applications illustrate, for a near Σ9{122} semicoherent grain boundary in silicon, the dependence of the deformation field on the plate thickness and on the orientation parameters of the interface.

1. Introduction

Since the beginning of transmission electron microscopy (TEM), the displacement fields attached to many crystalline defects have been introduced in imaging calculations [1,2]. A few of them include peculiar effects due to the elastic interaction of the defect with both free surfaces of thin plate-like crystals. Results are known for an isolated dislocation perpendicular to surfaces with a strong screw component, e.g., [3–6]. To date, for crystalline interfaces, which often induce elastic fields due to their own intrinsic structures, free surface relaxations remain completely ignored in imaging calculations. In high resolution TEM (HRTEM), the observed sample should have a thickness 2h less than 10 nm to reach a resolution better than 0.1 nm [5]. Therefore, there is an increasing need to refine the description of the elastic field (displacement $\mathbf{u}$, stresses σ_{jk}) attached to a crystalline interface inside a thin plate, i.e. a need to evaluate more precisely the "image" field that takes into account for the particular effect of the free surfaces. The parameters to include in such a description should include: the intrinsic structure of the interface, the thickness of the thin plate, the interface orientation in the plate, the dislocation directions and their spacings.

The novel aspect of the present work is to give a way to quantify these interface relaxation effects in the frame of the three-dimensional isotropic elasticity theory, for the case of a planar and semicoherent interface containing a single family of parallel misfit dislocations inclined in a thin crystal plate. By the term "semicoherent interface", we follow the usual definition [7–13]. Let us note that the problem was solved in [7] for a semicoherent interface parallel to the two free surfaces.

Techniques such as HRTEM and annular dark-field (ADF) imaging in scanning transmission electron microscopy (STEM) are commonly used to observe such semicoherent interfaces. They show at near-atomic, or even at atomic scale, that the misfit between the two adjacent crystal lattices is accommodated by more or less periodic deformations of both crystal lattices. Any attempt to quantify or evaluate the strain field is therefore useful, as already proposed from two-dimensional approaches [12–17].

To simplify the calculation, the elastic properties of the two adjacent crystals are assumed isotropic and identical. The basic idea is to combine three different solutions applying to the same unbounded bicrystal, so as to cancel the stresses applying on two planes separated by the distance 2h and cutting at any angle the semicoherent interface.

To illustrate the solution developed in the present work, some numerical applications are presented for a near-Σ9{122} grain boundary in a silicon bicrystal. The data are inspired from a recent work [17] performed on this interface. The reported observations show that a single family of intrinsic dislocations is part of the interface structure, the role of which is to accommodate a small angular misfit as a simple small-angle tilt boundary does [10,11] with respect to the exact Σ9 twin orientation.

Before presenting the calculation method, it is useful to define some geometrical symbols attached to the dislocation pattern.

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http://dx.doi.org/10.1016/j.tsf.2015.12.035
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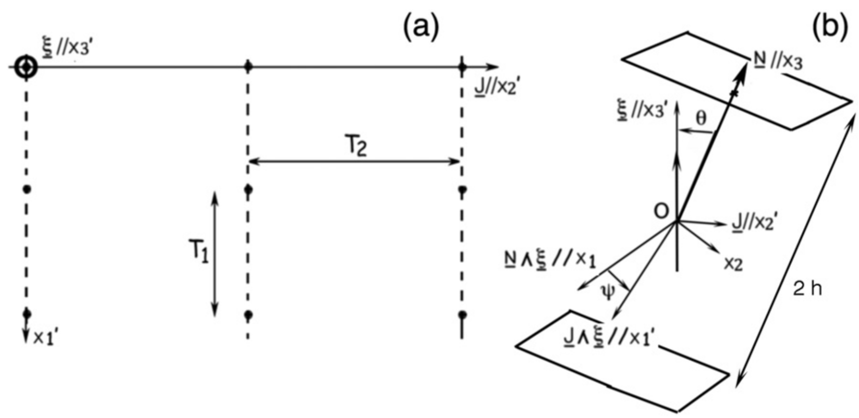

Fig. 1. (a, b) Geometry and symbols attached to the dislocation pattern. (a) The elastic medium is unbounded. The set of planar semicoherent interfaces, marked in dotted lines, is periodic with T_2. Along each interface, misfit dislocation lines are viewed edge-on, marked by black points, and are periodic with T_1. (b) A slice is cut in the unbounded medium represented in (a). The two free surfaces are inclined with respect to the dislocations and the semicoherent interfaces.

2. The dislocation pattern

2.1. Symbols and conventions

The dislocation pattern of interest is the same in the entire work, but according to the case it is either placed in an unbounded medium, Fig. 1(a), or in a plate, Fig. 1(b). Fig. 1(a) depicts a periodic set (period T_2) of identical and parallel semicoherent interfaces, represented in dotted lines, along which lie a single family of periodic misfit dislocation lines (period T_1) viewed edge-on. All misfit dislocations have the same Burgers vector **b** and are oriented by the vector **ξ**. In Fig. 1(b), the same dislocation pattern is limited by two free surfaces with a normal **N** inclined of θ with respect to **ξ**. A Cartesian frame $Ox_1x_2x_3$ is fixed with respect to the plate with (Ox_3//**N**) and Ox_1//**N**Λ**ξ**, the origin O being located at the median plane of the plate. Another Cartesian frame $Ox_1'x_2'x_3'$ is attached to the interfaces (common normal **J**//Ox_2') and to the dislocations. It is such that Ox_1' is obtained from Ox_1 via a rotation of axis **ξ** and angle ψ. One of the misfit dislocations has its line along Ox_3'. The interfaces are therefore oriented by the two angles θ and ψ. Therefore, **J** is inclined with respect to **N** of the angle.

$$\phi = \arccos[\sin[\theta]\cos[\psi]] \tag{1}$$

In general, HRTEM observations are performed for zero or small angle θ, while the angle ψ can be large and reach π/2. For this peculiar case the interfaces are parallel to **N** and ξ.

2.2. The concept of extended core dislocation (ECD)

In references [18,19], the concept of ECD leads the way to evaluate the elastic field of an isolated classical dislocation in a thin plate. In these references, an ECD is constructed from a theoretical straight,

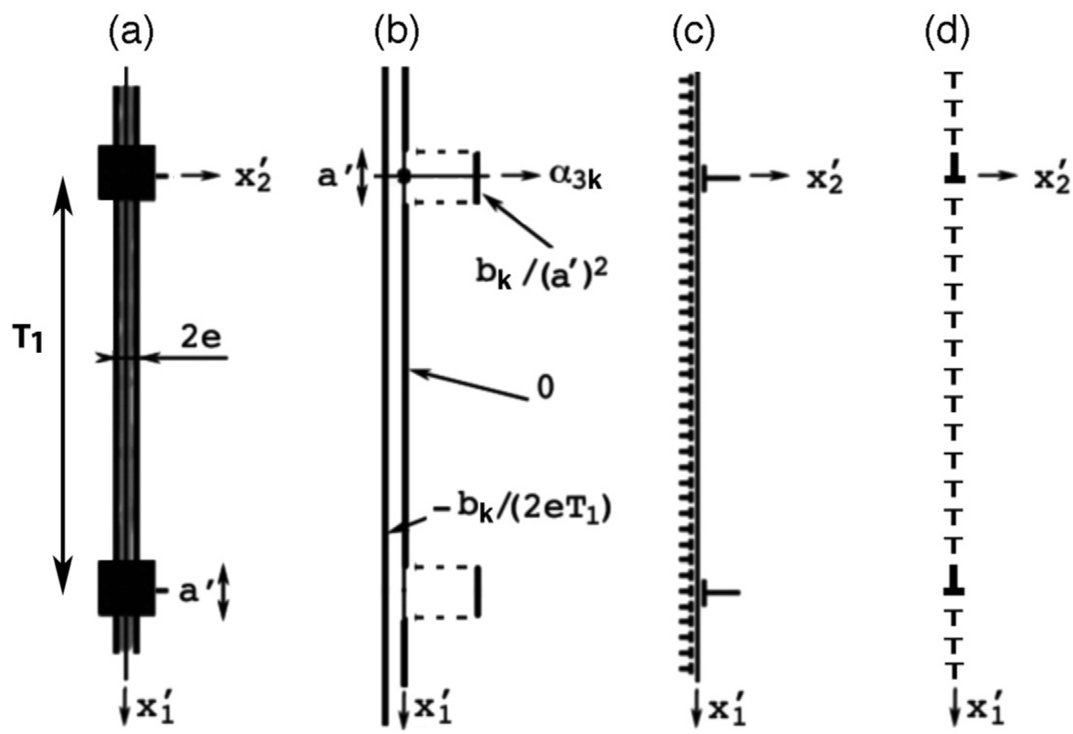

Fig. 2. Description of the deformation sources along the semicoherent interface placed at $x_2' = 0$ in an unbounded medium. (a) Two kinds of extended core dislocations (ECDs) are used: one has a core with a square cross-section (side a′) and the other has a core with an elongated rectangular cross-section (surface $2eT_1$). (b) Changes of the tensor components α_{3k} (k = 1–3) along the axis Ox_1'. (c, d) Description of the elastic fields according to refs. [9–11] for the two edge cases **b**(b_1,0,0) and **b**(0,b_2,0).