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A R T I C U L O

A thin two-phase foils deformed by an interfacial dislocation in anisotropic elasticity

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The purpose of this work is the numerical resolution, in the case of anisotropic elasticity, of the problem of a dislocation parallel and near to the two free surfaces of a thin bicrystal. This case is obtained while making the period of a network of misfit dislocations much greater than the thickness of the two foils. As a result, in the vicinity of the dislocation, the limiting bondary conditions will be close to that of Volterra translation dislocation. The elastic fields of displacement and stress are calculated for various orientations of the burgers vector. Before this calculation, we tested the precision of the results of the program by comparing the interfacial relative displacement obtained from this one to the results of the analytical expression describing this same displacement. The thin bicristal Al/Al_2Cu, that made the object of several investigations, is treated like example. The results obtained are compared to those obtained in isotropic elasticity.

Keywords: dislocation, misfit, interface, networks

Lámina delgada bifásica deformada por dislocación interfacial en elasticidad elástica

Este trabajo aborda la resolución numérica en anisotropía elástica, del problema de una dislocación paralela cercana a las superficies libres de un bi-cristal delgado. Este problema se genera cuando el periodo de la red de dislocaciones desplazadas es mucho mayor que el espesor de la bi-lámina. Como resultados, en la vecindad de la dislocación, las condiciones de contorno estarán cercanas a la dislocación de traslación de Volterra. Los campos elásticos de desplazamiento y las tensiones se calcularon para distintas orientaciones del vector de burgers. Como paso previo a los cálculos, se comprobó la precisión de los resultados del programa comparando le desplazamiento relativo interracial obtenido con los resultados de la expresión analítica que describen dicho desplazamiento. Se emplearon como ejemplo bi-cristales de Al/Al_2Cu, debido a su empleo en varias investigaciones. Los resultados fueron comparados con los obtenidos en elasticidad isótropa.

Palabras claves: dislocación,desacoplot, interface, red cristalina

1. INTRODUCTION

Efficient experimental methods have been developed in the past 50 years for studying matrix dislocations and dislocations located at crystalline interface by transmission electron microscopy.

When an interfacial dislocation is parallel and near of the two free surfaces of a thin bicristal, its field of displacements and stresses will necessarily depend on distance to these two free surfaces. The problem becomes more difficult when the bicristal is constituted of two plates of different nature (heterostructure) (1). R. Bonnet (2) proposed a method to solve this problem analytically and got the field of displacements and stresses in the case of isotropic elasticity.

The aim of our work consists in solving numerically this same problem but in the case of anisotropic elasticity. The thin bicristal Al/Al_2Cu, that made the object of several investigations (2-5), is treated like example..

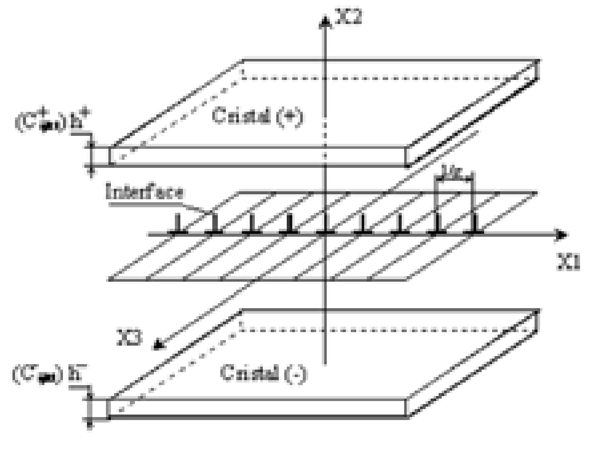

Fig. 1.- Schematic drawing of a thin two-thin foils +/-, with a network of unidirectional dislocations at the interface, 1/g is the period. The crystal stiffenesses are C^{+}_{ijkl} and C^{-}_{ijkl} with thickness h^{+} and h^{-} respectively.

2. GEOMETRY OF THE PROBLEM

Figure 1, present in detail the geometry of the problem for a network of misfit dislocations parallel to the axis Ox_3 of a cartesian frame $Ox_1x_2x_3$ with a period 1/g in the plan of an interface separating two different anisotropy media. For the limiting case corresponding to 1/g>>h + and h -, the problem reduces to a single straight interfacial defect interacting with the free surfaces.

3. FORMULATION OF THE PROBLEM

The displacement field, which results from the strain, is periodic and can be described quite generally by the function

$$u_k^{(n)} = \sum_{n \neq 0} U_k^{(n)}(x_2)\exp(2.i\pi.g.n.x_1) \qquad k=1,2,3 \tag{1}$$

where $U(x_2)$ is a complex function depending on x_2.
the linearity of the relative displacement, along a period (Λ = 1/g), can be written as:

$$u_k^+ - u_k^- = \left(\frac{b_k}{\Lambda}\right).x_1 - \frac{b_k}{2} \tag{2}$$

In order to fulfil Hooke's law and the local requirements the displacement in each medium must be such that

$$C_{ijkl}.U_{k,l} = 0 \tag{3}$$

In order to simplify the resolution of the problem, and also to perform the numerical calculation, the final expression of the displacements field can be written as :

$$\begin{aligned} U_k = \sum_{n=0}^{\infty}\left(\frac{1}{\pi.n}\right)\sum_{\alpha=1}^{3}[\{\cos[n.\omega(x_1+r_\alpha.x_2)]\} \\ \times \mathrm{Re}[(-i.X_\alpha^{(n)}.\lambda_{k\alpha}).\exp(-n.\omega.s_\alpha.x_2)+(-i.Y_\alpha^{(n)}.\bar{\lambda}_{k\alpha}).\exp(n.\omega.s_\alpha.x_2)]] \\ +\{\sin[n.\omega(x_1+r_\alpha.x_2)]\} \times \mathrm{Re}[(X_\alpha^{(n)}.\lambda_{k\alpha}).\exp(-n.\omega.s_\alpha.x_2)+(Y_\alpha^{(n)}.\bar{\lambda}_{k\alpha}).\exp(n.\omega.s_\alpha.x_2)]] \end{aligned} \tag{4}$$

where $\omega = 2.\pi.g$,

the stress field is readily found from equation 3 using Hooke's law

$$\begin{aligned} \sigma_{ij} = 2.g\sum_{n=0}^{\infty}\sum_{\alpha=1}^{3}[\{\cos[n.\omega(x_1+r_\alpha x_2)]\}+ \\ \times \mathrm{Re}[X_\alpha^{(n)}L_{\alpha ij}.\exp(-n.\omega s_\alpha.x_2)+Y_\alpha^{(n)}\bar{L}_{\alpha ij}.\exp(n.\omega s_\alpha.x_2)]+\{\sin[n.\omega(x_1+r_\alpha x_2)]\}+ \\ \times \mathrm{Re}[i.X_\alpha^{(n)}L_{\alpha ij}.\exp(-n.\omega s_\alpha.x_2)+i.Y_\alpha^{(n)}\bar{L}_{\alpha ij}.\exp(n.\omega s_\alpha.x_2)] \\ \text{avec} \quad L_{\alpha ij} = \lambda_{k\alpha}[C_{ijk1}+p_\alpha C_{ijk2}] \qquad i,j=1,2,3 \qquad ,l=1,2 \end{aligned} \tag{5}$$

When the period tends to infinity, the limiting boundary conditions in the vicinity of any intrinsic dislocations tend to those of a translation dislocation placed along a hetero-interface: continuity of the stresses σ_{2k} and Heaviside step function for the discontinuity of each component of the interfacial relative displacement ($u_K^+ - u_K^-$).
Expressing in detail these boundary condition leads to a system of 12 linear complex equations with 12 complex unknowns $(X_\alpha^+, Y_\alpha^+, X_\alpha^-, Y_\alpha^- \quad \alpha = 1,3)$.

4. APPLICATION

To examine the precision of the calculations carried out by the program, we plotted the curves of relative displacements according to x_1 ($\Delta U_k = F(x_1)$) which correspond on the one hand to the theoretical expression (equation 2) and on the other hand with the result given by the program in the case of a thin bicrystal Al/Al_2Cu, (figure 2).

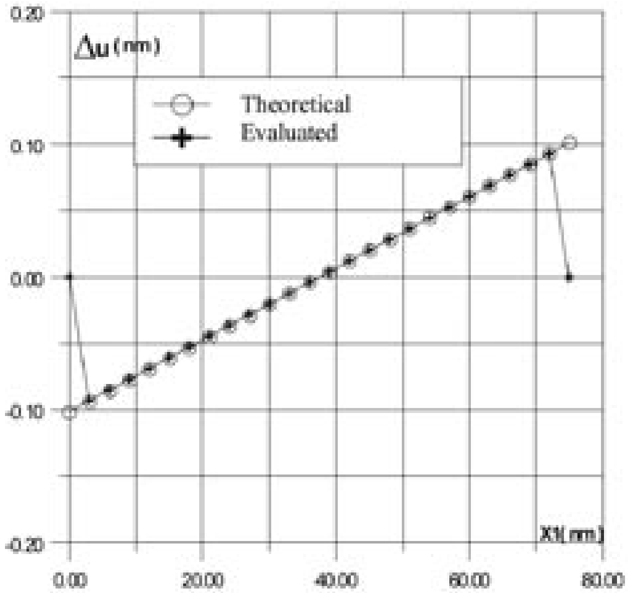

Fig. 2.- Representation of the interfacial relative displacement

This figure shows well that the curves are perfectly superposable in the field of validity of the theoretical expression which is between the first dislocation placed at x_1 = 0 and the second dislocation placed at x_1 = 75 nm corresponding to one period. It should be noted that the comparison between the two curves must be done far from the core of the misfit dislocations.

However while moving away from some b of each dislocation, we obtain more precise results. Therefore for x_1= 5b, the relative error defined by:

$$\Delta R = \left|(\Delta U_{program} - \Delta U_{theoretical} / \Delta U_{theoretical}\right|$$

is 3.3 %. This perfect superposition of the curves along one period is due to the theoretical method used, the selected number of harmonics (n = 100) and the double precision of calculations.

For the field of displacement, the not deformed free surfaces and the interface are represented by the horizontal lines located respectively at -5 nm, 0 nm and 2.5 nm.

After introduction of an edge dislocation at the origin of the frame Ox_1x_2, the results, presented in figure 3 are obtained.

These results correspond to the case of a thin bicristal Al/Al_2Cu. This model was the subject of several studies in the approximation of an isotropic elasticity in particular those of R. Bonnet (2-5). The positive crystal was choosen Al with a thickness of h^+ = 2.5 nm. In the same way the negative crystal was choosen Al_2Cu with the thickness of h^- = 5 nm.

For the calculation, the period has been taken as ten times the foil thikness, i.e. 75 nm. This value (75 Nm) is usually met in M.E.T.H.R.

The elastic constants are given by (5) and are (in GPa):

- For Al_2Cu $C_{11} = 159$, $C_{12} = 63$, $C_{44} = 29$
- For Al $C_{11} = 108.2$, $C_{12} = 61.3$, $C_{44} = 28.5$

Figure 3.a corresponds to $b = a_{Al}/2$ [110] while the figure 3.b corresponds to $b = a_{Al}/2$ [101] with $a_{Al} = 0.405$ nm. Let us note that to better suggest the foil deformation, the displacements u_K were taken in each point as three times its real value.

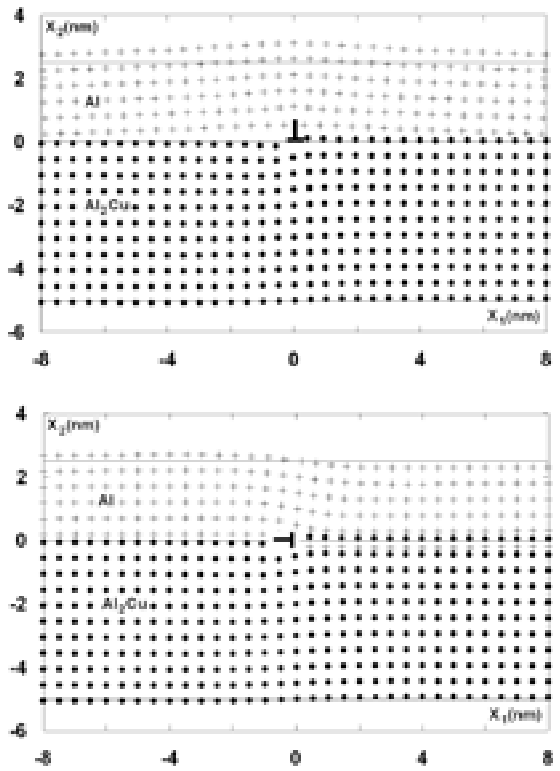

Fig. 3.- Schematic drawing describing the displacement fields of thin two layers Al/AL_2Cu deformed by interfacial edge dislocations.
(a) b // Ox_1, (b) b // Ox_2

The results obtained in this case are appreciably superposable with the results of Bonnet (4) obtained in isotropic elasticity.

In these two figures 3 (a & b) and like the isotropic case (3), along each heterointerface, the deformed lattice of points and crosses are discontinuous having modulus equal to $a_{Al}/2$, as expected. These figures illustrate also and clearly the fact that Al_2Cu is a harder phase, see e.g. figure 3.b the larger deformation of the upper free surface associated with Al.

In figure 4 (a & b), equistress curves $\sigma_{11} = \pm 150$ and ± 300 MPa are presented for the same thin bicristal Al_2Cu , theses curves, which there is no analytical formula, show that the presence of a second crystal modifies considerably the distribution of the stress field around a dislocation. These equistress reveal also an effect of surface, which was not mentioned in the case of isotropic elasticity.

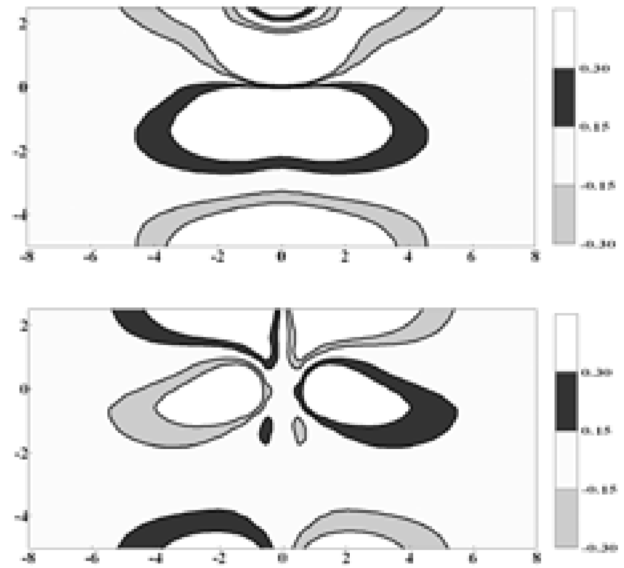

Fig. 3.- Equi-stresses curves $\sigma_{11} = \pm 150$ et ± 300 MPa of thin two layers Al/AL_2Cu deformed by interfacial edge dislocations.
(a) b // Ox_1, (b) b // Ox_2

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