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Isotropic Stress Distribution in Cu/(001) Fe Two Sheets

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***Abstract*—**The nanotechnology based on epitaxial systems includes single or arranged misfit dislocations. In general, whatever is the type of dislocation or the geometry of the array formed by the dislocations; it is important for experimental studies to know exactly the stress distribution for which there is no analytical expression [1, 2]. This work, using a numerical analysis, deals with relaxation of epitaxial layers having at their interface a periodic network of edge misfit dislocations. The stress distribution is estimated by using isotropic elasticity. The results show that the thickness of the two sheets is a crucial parameter in the stress distributions and then in the profile of the two sheets.

A comparative study between the case of single dislocation and the case of parallel network shows that the layers relaxed better when the interface is covered by a parallel arrangement of misfit. Consequently, a single dislocation at the interface produces an important stress field which can be reduced by inserting a parallel network of dislocations with suitable periodicity.

***Keywords*—**Parallel array of misfit, interface, isotropic elasticity, single crystalline substrates, coherent interface

I. INTRODUCTION

RECENTLY several technologies are focused on the use of nano-materials but the question is how to produce substrates with adequate relaxed surface topology [3,6].

In many cases, studies concerning structural properties have been stopped by the problem of the interface. In fact, structural studies must be preceded by the determination of elastic properties at the interface which is not always possible in experiments. On the other hand, the METHR images are important to know what kind of array could be inserted at the interface [7, 10]. Much of the motivation behind the research in this area remains what it always has been. Advances in computing continue to “up the pressure” for improved constitutive descriptions of interfacial mechanisms.The growth processes are sophisticated, but they are now routinely performed by any or several techniques in many laboratories. In any case, in these methods atoms are deposited one at a time in such a way as to establish the crystalline structure of the growing film, using the crystalline structure of the substrate as a template. Under appropriate conditions, the interface is coherent or epitaxial, at least, in the early stages of growth. A principal difficulty with a strained-layer structure is that the stress associated with the strain gives rise to a driving force for structural defects in the strained-layer lattice. However, hetero-epitaxial interfaces and semi coherent phase boundaries form a class of interfaces defined by the meeting of two crystals with the same orientation, but different lattice parameters.In the simplest case, it is possible to accommodate the strain with an array of edge dislocations, with Burgers vectors lying in the plan of the interface. In the present instance, this array of dislocations produces a stress field for which there is no analytical expression. Consequently, it is important to find a route allowing the calculations with precision of the stress distribution at surfaces and in thin film directly. A first estimation of the stress distribution caused by the dislocations in periodic array can be obtained by basing the calculation on the mean elastic strain in the two crystals.

In this work, the model of two single crystalline sheets has been exploited successfully in numerical analysis using mathematica language to quantify the stress field when parallel array of misfit dislocations lays the plane interface.

The results show that the thickness of the two sheets is a crucial parameter in the stress distribution. In fact, the two sheets are completely relaxed when the total thickness H is about 30 nm. Also, in the present work, an isolated dislocation is taken into consideration in order to preview mechanical behavior of the two sheets. The use of isolated dislocation suggests that the normal stresses gradually increase as the spacing between dislocation arrays become higher.

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II. PATTERN

Suppose a uniform film of some single crystal and lattice parameter a_1 is grown on the surface of second material of the same orientation but lattice parameter a_2. With reference to the configuration illustrate in figure 1, suppose the film and substrate are both modeled as isotropic elastic materials, each with a shear modulus μ and Poisson ratio ν. Let us consider a parallel arrangement of edge misfit dislocations lying in the plane interface between two sheets with specific thicknesses h_1 and h_2. The total thickness of the epitaxial system is $H = h_1 + h_2$. If the dislocations are inserted periodically with a suitable period Ω. The spacing between dislocations for a given thickness follows from the relation:

$$\Omega = \frac{a_1 a_2}{(a_1 - a_2)\sqrt{2}} \tag{1}$$

Let us define a Cartesian frame $Ox_1x_2x_3$ such as the center O is fixed on the core of the dislocation, x_1 is perpendicular to the line of dislocations and x_3 is parallel to it. We note that this coordinate system corresponds to that conventionally used in dislocation mechanics. The components of Burgers vectors b normal to the free surface are: **b** (b_1, 0, 0). The sign of b_1 is essentially fixed by the sign of the mismatch strain but there is some flexibility in selection of components of Burgers vector and, then, b_1 has a positive orientation.

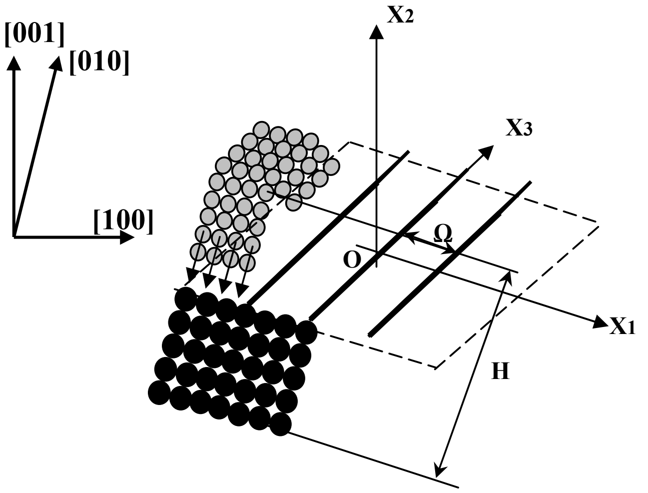


Fig. 1: Description of the array pattern's dislocations.

Since the deformation of the upper surface is a wavy one, the solution for a periodic array of identical edge dislocations can be found using a Fourier series. The displacement field of a periodic dislocation array is given by the sum of contributions from the individual dislocations:

$$u_k = \sum_{n=-\infty}^{\infty} U_{ki}^{n} \exp(in\omega x_1) = \sum_{n=1}^{\infty} 2U_k^n [\cos(n\omega x_1) - i \sin(n\omega x_1)] \quad (2)$$

Where: $\omega = \dfrac{\Omega}{2\pi}$.

Elastic stresses are derived from Hooke's law:

$$\sigma_{ij} = \lambda \delta_{ij} u_{kk} + \mu (u_{i,j} + u_{j,i}) \quad i, j = 1, 2, 3 \text{ and } k = 1, 2, 3 \quad (3)$$

Where: λ and μ are the Lamé coefficients for isotropic solid and δ_{ij} is the Kronecker's symbol.

The components of normal stresses used for the calculations are as follows:

$$\sigma_{22} = \frac{2u\nu}{1-2\nu}[(1-\nu)u_{2,2} + \nu u_{1,1}]$$

$$\sigma_{11} = \frac{2u\nu}{1-2\nu}[(1-\nu)u_{1,1} + \nu u_{2,2}] \quad (4)$$

$$\sigma_{21} = \mu(u_{2,1} + u_{1,2})$$

$$\sigma_{23} = \mu(u_{2,3} + u_{3,2})$$

For the pattern defined, limiting boundaries conditions are set to simplify the development of the expressions (2) and to determine the final expressions of the elastic fields. The limiting boundaries are:

i) The continuity of the relative displacement Δu.

$$\Delta u = u_2 - u_1 = \sum_{n=1}^{\infty} \frac{-b_k}{\pi n} \sin(n\omega x_1) \quad (5)$$

b_k is the Burgers vector with k =1, 2, 3.

ii) The continuity of the normal stresses through the interface which can be expressed by:

$$\sigma_{2k}^{(1)}\Big|_{x_2=0} = \sigma_{2k}^{(2)} \qquad k = 1, 2, 3 \quad (6)$$

iii) The nullity of the normal stresses at the free surfaces:

$$\sigma_{2k}^{(1)}\Big|_{x_2=h_1} = 0 \text{ and } \sigma_{2k}^{(2)}\Big|_{x_2=h_2} = 0 \quad k = 1, 2, 3 \quad (7)$$

When boundary conditions are applied, the expressions (2, 7) become heavy to manipulate. The main problem is to determine the analytical expressions of Fourier's coefficients. Then, we use the mathematica language to write a program which allows us to obtain easily the analytical expressions and to calculate finally the elastic fields. In this type of program, the first step is to verify the Fourier series convergence. For this, we choose a Cu/ (001) Fe system because it presents a very specific physical properties. Mathematica language gives a good convergence of the Fourier series such as the harmonic number noted n can reach 2000 with a very economic time of calculations. In this application, the harmonic number n is taken equal to 500 because it gives satisfying results.

III. Cu/ (001) Fe System

Using two sheets formed by Cu/ (001) Fe epitaxial system, we calculate the stress distributions with the data given in the table 2. The elastic constants are taken in the Nye referential. The relation (8) gives the values of these constants in function of the Lamé coefficients.

$$C_{11} = \lambda + 2\mu,\ C_{12} = \lambda \text{ and } C_{44} = \mu \quad (8)$$

$$\lambda = \frac{2\mu\nu}{1-2\nu} 2\mu \quad (9)$$

To have an idea about if dissociation can be predicted, we calculate the misfit of this system according the relation (10) and reported on the table 2 :

$$\varepsilon = \frac{a_1 - a_2}{a_1} \quad (10)$$

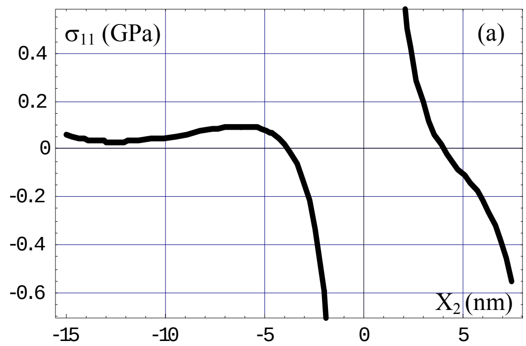
IV. Results And Discussion

The stress distribution on the two surfaces is identical due to the periodicity of the elastic field. When we consider the same thickness of the two sheets, the normal stresses σ_{11} and σ_{22} are equal in magnitude but opposite in sign. Up to this point in the discussion of the symmetry of normal stresses, it has been tacitly assumed that the normal stresses σ_{22} are equal to zero at the free surfaces of the two sheets. For thinner film h_1= 7.5 nm, the stress σ_{11} are commonly found to be greater than that in the substrate. There are two main reasons for this outcome, both of which are listed by the limiting boundaries. Thus,

TABLE II
DATA FOR THE C_U/ (001) F_E TWO SHEETS

Symbol	Parameter	Value
a_1	Lattice parameter of Cu	0.361 nm
a_2	Lattice parameter of Fe	0.355 nm
C^1ij	Elastic constants of Cu	C_{11}=168.4,C_{12}= 121.4 and C_{44}=75.4 GPa
C^2ij	Elastic constants of Fe	C_{11}=232,C_{12}= 136 and C_{44}=117 GPa
Ω	Period	15.1032 nm
h_1	Thickness of Cu	7.5 nm
h_2	Thickness of Fe	15 nm
b	Burgers Vector	0.25344 nm
ε	Misfit	1.66 %

Fig. 2 illustrates the large discontinuity through the interface even if x_1 is taken far from the core of dislocation (Fig.2 (c)) or close to it (Fig.2 (b)). The stress σ_{11} is about 0.22 GPa at the free upper surface and can reach 0.5 Gpa when the calculations are made far from the core of dislocations while it is about 0.4GPa in the lower free surface whatever is the value of x_1. In effect, the stress σ_{11} is low when the thickness is at least as large as a period. For the case of normal stresses σ_{22}, the formulation used provides an easy way to understand the surface profile at different distances from the core of dislocations. As shown in Fig. 3, when the dislocation is situated on X_1 = b the value of stress σ_{22} is 3 GPa (Fig. 3 (a)).



σ_{11} (GPa) (b)

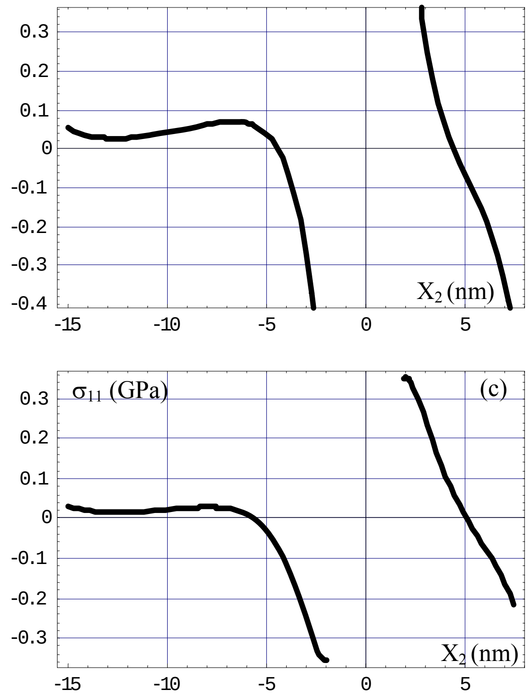
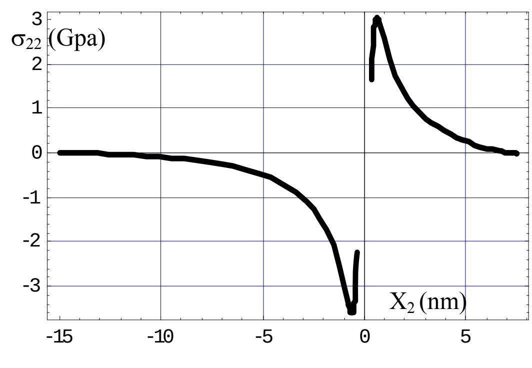


Fig. 2 illustration of σ_{11} stresses in the Cu/(001) Fe system (a) x_1 = b, (b) x_1 = 5b and (c) x_1 = 10b

This value becomes very weak (0.4 GPa) when x_1 = 5, 10 b (Fig 3. (b) and c)). Thus each position of the dislocations array gives a relative profile peak to valley of the free surfaces. Also, the stress σ_{22} changes versus the total thickness H of the sheets. Consequently, for relaxed film, the change in the surface profile with increasing film thickness should be a strong indicator of whether the morphology. The height undulations increase with increasing film thickness. Another way to confirm if the insertion of an array of dislocations on the interface could be a factor of relaxation of the two surfaces is to consider an isolated dislocation by imposing a large value of the spacing between the array dislocations.



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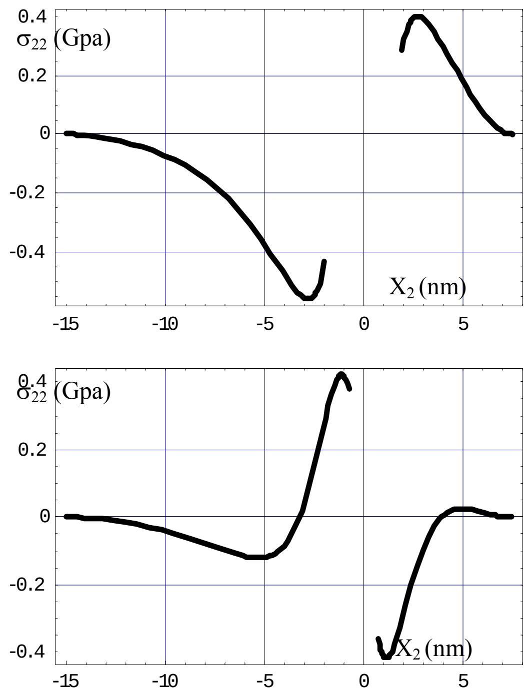

Fig. 3 illustration of σ_{22} stresses in the Cu/(001) Fe system
(a) $x_1 = b$, (b) $x_1 = 5b$ and (c) $x_1 = 10b$

In this context, the spacing between two dislocations has been taken equal to 10Ω. Fig. 4 describes the σ_{22} stress distribution in the case of single dislocation. It reveals that the normal stresses gradually increase as the spacing between dislocation arrays become higher. Consequently, a single interfacial dislocation produces an important stress field which can be reduced by inserting parallel array of misfit dislocations with convenient periodicity.

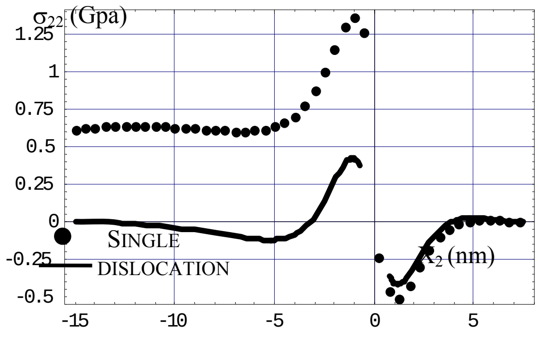

Fig. 4 Comparative curve between the case of single dislocation and the case of parallel array in the Cu/(001) Fe system.

V. Conclusion

In this paper, we have presented solutions for the elastic stress field for periodic array of dislocations pure edge character placed near free surfaces of elastically isotropic materials. These solutions include the effect of the free surfaces. We note that the stress field following from the derived displacement fields for periodic dislocations could be obtained in a different way from summation of Fourier series expressions. Using this technique, we write a mathematica language in the aim to determine the stress distribution in a two sheet materials. Through an application to the Cu/(001/ Fe system, we conclude that the relaxation of the two sheets can be obtained when the thickness is at least as large as a spacing between dislocations. Also, when a single dislocation is laying the interface, the stress field is high and it can be reduced by inserted parallel array.

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