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## تأثير المتباين على حقل الضبط لبلورة ثنائية تحت تاثير شبكة من الخلوع الحدودية

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### المخلص:

الهدف من هذا العمل هو نمذجة السلوك المتوقع عند العديد من القياسات وإعادة إنتاج بعض المشاهدات التجريبية وذلك بواسطة المحاكاة العددية التي تقوم على نظرية المرونة المتباينة. هذه الأخيرة تسمح لنا بالتعبير عن كل العلاقات الضرورية لوصف حقل التشوه، و ذلك بنشر متتاليات فورييه، مما يؤدي إلى جملة من المعادلات الجبرية الخطية التي حلت عدديا للحصول على معاملات فورييه المركبة والتي ثم استخدمت لحساب الحقول المرنة للانتقال والجهود. في هذا العمل ركزنا على تطوير برنامج رياضي لحساب حقل الضبط المرن المتباين، وكتطبيق على ذلك قمنا بنمذجة بلورة ثنائية من رقائق النحاس والحديد .Cu/(001)Fe



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# Influence of anisotropy on the constraints field of a bicrystal (layer/substrate) under the effect of a network of interfacial dislocations

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## KEYWORDS

Anisotropic elasticity;  
Misfit;  
Interface;  
Dislocation network

**Abstract** The purpose of this work is to model the monoscale predictive behavior and to reproduce certain experimental observations by using numerical simulation based on the theory of anisotropic elasticity. The latter allows us to express all the necessary expressions describing the strain field. The Fourier series expansion of the strain field leads to a system of linear algebraic equations which are solved numerically to obtain the complex Fourier coefficients which are used to calculate the elastic fields of displacements and stresses. In this work we focused our effort towards the development of a mathematical code that calculates the anisotropic elastic constraints field. As an application, we have treated the case of a bicrystal Cu/(001) Fe.

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## 1. Introduction

Any defect informs us about the potential presence of buried dislocations. These dislocations can be interfacial. They are grouped into different networks whose associated dislocation is measurable by microscopic observations (Jesser and Matthews, 1967); while theoretically obtaining the calculation of elastic fields by Eshelby et al. (1953).

The structural understanding of networks of dislocations by diffraction experiments or microscopy can be supplemented by calculations of elasticity. Studies carried out on thin films

deposited on monocrystalline substrates reveal the existence of networks of interfacial well organized dislocations, and whose density, stability and character depend on the differences between parametric and angular crystals along the interface as well as the temperature factor. It is when the networks of interfacial dislocations become more regular that the interfaces become more stable (WP Wu et al., 2011).

These same elastic fields (constraints) are calculated using another approach which is the finite elements method (FEM) by Peralta et al. (1993) whose results were in accordance with the predicted values for a predictive model.

From a mechanical point of view, one of most exciting issues, both in its fundamental and applied aspects, is the comprehension of the deformation mechanisms of these nanomaterials by Fabien (2003). The miniaturization of products in the semiconductor industry poses in fact mechanical constraint problems which engender problems of failure and reliability. We take into account these constraint fields when designing has become a critical element in the development of new bilayer, trilayer (Brioua et al., 2005) or multilayer

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(Wang et al., 2007) products. Based on a double Fourier series formulation of Bonnet (1981), we present in this work solutions in anisotropic elasticity for an intrinsic unidirectional dislocation network situated at the interface of a thin bicrystal. We encounter in our calculations a sixth degree polynomial equation that is solved numerically. The determination of Fourier coefficients (Bonnet, 2003) leading to the calculation of required elastic fields consists of the numerical resolution of a linear system having 24 matrix of equations in 24 complex unknowns.

And for a good exploitation of these fields we must take into account the effect of elastic anisotropy, which significantly affects the material behavior, this analysis is presented by Peralta et al. (2001) for the treated case Cu/sapphire.

## 2. Presentation of the problem and boundary conditions

Fig. 1 shows the geometry of the problem for two spaces (+) and (-) of thickness  $h^+$  and  $h^-$ , anisotropy characterized by the elastic constants  $C_{ijkl}$  and separated by a plan interface comprising an intrinsic unidirectional dislocation network with a network period  $1/g$ .

Modeling our case means giving explicit solution to the elastic field of a unidirectional dislocation network. For that we must take into consideration conditions at the limits situated at the interface of this bicrystal in anisotropic elasticity using an approach based on a double Fourier series analysis.

### 2.1. Boundary conditions imposed in the displacement field

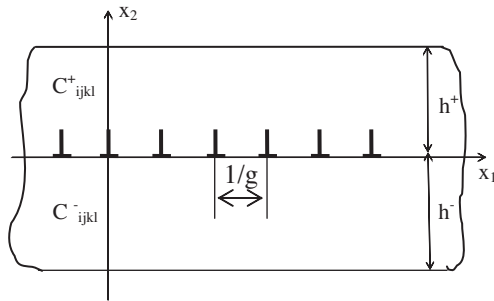
Fig. 2 shows the linearity of the displacement on the interface and the schematic representation of the displacement associated with a network of intrinsic dislocations described for each component  $u_k$ , which can be expressed by the following expression:

The linearity of the displacement on the interface can be expressed by:

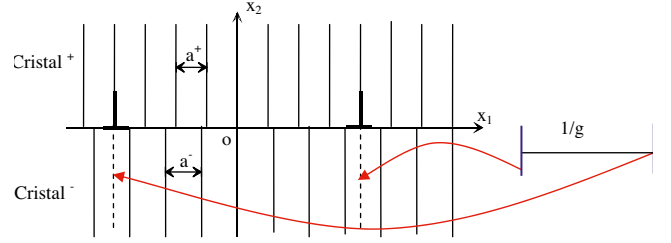
$$[u_k^+ - u_k^-]_{x_2=0} = -\frac{b_k}{\pi} \sum_{n=1}^{\infty} (1/n) \cdot \sin(n \cdot \omega \cdot x_1) \quad (1)$$

### 2.2. Boundary conditions imposed in the stress field

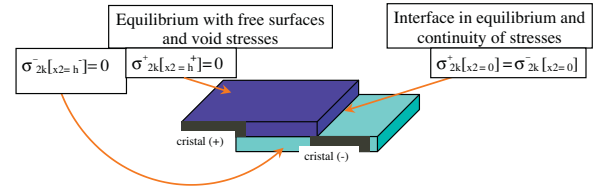
Fig. 3 shows the boundary condition:



**Figure 1** Schematic drawing of a two layer material +/−, with a network of unidirectional dislocations at the interface;  $1/g$  is the period. The crystal stiffnesses are  $C_{ijkl}^+$  and  $C_{ijkl}^-$ , with thickness  $h^+$  and  $h^-$ , respectively.



**Figure 2** Schematic representation of the interfacial plane misfit after cut along the interface. As a result, the relative displacement to apply along the interface from the free stress state should be a saw tooth curve.



**Figure 3** Boundary conditions in stresses.

## 3. Mathematical formulation and solution in anisotropic elasticity

Considering two spaces (+) and (-), Fig. 1, assumed to obey Hooke's law, both spaces (+) and (-) are separated by a plane interface with a network of intrinsic dislocations.

As the strain is assumed to be periodic along the axis  $Ox_1$ , it can be expanded in Fourier series at every point of the two spaces outside the areas of discontinuity:

$$\varepsilon_{ij}(x_1, x_2) = \sum_G \varepsilon_{ij}^{(G)}(x_2) \cdot \exp(2 \cdot i \cdot \pi \cdot n \cdot x_1 / L) \quad (2)$$

For  $|x_2|$  tending to infinity, all the coefficients tend towards zero (preservation of structural units). Using the Einstein summation convention on dumb indices, integration of Eq. (2) gives the following displacement field:

$$u_k = U_k^0 + V_{k1}^0 \cdot x_1 + V_{k2}^0 \cdot x_2 + \sum_{n0} U_k^{(n)}(x_2) \cdot \exp(2 \cdot i \cdot \pi \cdot g \cdot n \cdot x_1) \quad (3)$$

$$k = 1, 2, 3$$

With  $1/g = \Lambda$  ( $\Lambda$  is the period)

In the case of intrinsic dislocations  $V_{k1}^0$  and  $V_{k2}^0$  must be equal to zero to avoid the stresses at long distance. So the expression of the displacement field is written as follows:

$$u_k = \sum_{n0} U_k^{(n)}(x_2) \cdot \exp(2 \cdot i \cdot \pi \cdot g \cdot n \cdot x_1) \quad k = 1, 2, 3 \quad (4)$$

This displacement field  $u_k$  must satisfy the generalized Hooke's law, connecting constraints and strains:

$$\sigma_{ij} = C_{ijkl} \cdot \varepsilon_{kl} \quad (5)$$

where

$$\sigma_{kl} = \frac{1}{2} (u_{k,l} + u_{l,k}) \quad (i, j, k, l = 1, 2, 3) \quad (6)$$

Substituting (5) in to (4), we get:

$$\sigma_{ij} = 1/2(C_{ijkl} \cdot u_{k,l}) + 1/2(C_{ijkl} \cdot u_{l,k}) \quad (7)$$

As the 3rd and 4th index of elastic constants can be interchanged, so that we have:

$$\sigma_{ij} = 1/2(C_{ijkl} \cdot u_{k,l}) + 1/2(C_{ijlk} \cdot u_{l,k}) \quad (8)$$

Since that the dumb indices  $k$  and take the same values, so both terms on the right are equal.

$$\sigma_{ij} = C_{ijkl} \cdot u_{k,l} \quad (9)$$

Steady-state constraints in the distortion region are written:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \quad (10)$$

$$\Rightarrow C_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} = 0 \quad (11)$$

By substituting (4) into (11), we obtain three differential equations which can be written as follows:

$$C_{j1k1}(-4\pi^2 g^2 n^2) U_k^{(n)} + (C_{j1k2} + C_{j2k1})(2i\pi n g) U_{k,2}^{(n)} + C_{j2k2} U_{k,22}^{(n)} = 0 \quad (12)$$

The general solution of these equations is given by:

$$U_k^{(n)}(x_2) = \lambda'_{\alpha k} \cdot \exp(2.i.\pi.g.n.p_{\alpha}.x_2) \quad (13)$$

where  $\lambda'_{\alpha k}$  and  $p_{\alpha}$  are complex constants.

Eq. (12) can be put in the following matrix form:

$$\begin{pmatrix} C_{11} + (C_{16} + C_{61})p_{\alpha} + C_{66}p_{\alpha}^2 & C_{16} + (C_{12} + C_{66})p_{\alpha} + C_{62}p_{\alpha}^2 & C_{15} + (C_{14} + C_{65})p_{\alpha} + C_{64}p_{\alpha}^2 \\ C_{61} + (C_{66} + C_{21})p_{\alpha} + C_{26}p_{\alpha}^2 & C_{66} + (C_{62} + C_{26})p_{\alpha} + C_{22}p_{\alpha}^2 & C_{65} + (C_{64} + C_{25})p_{\alpha} + C_{24}p_{\alpha}^2 \\ C_{51} + (C_{56} + C_{41})p_{\alpha} + C_{46}p_{\alpha}^2 & C_{56} + (C_{52} + C_{46})p_{\alpha} + C_{42}p_{\alpha}^2 & C_{55} + (C_{54} + C_{45})p_{\alpha} + C_{44}p_{\alpha}^2 \end{pmatrix} \begin{pmatrix} \lambda'_{\alpha 1} \\ \lambda'_{\alpha 2} \\ \lambda'_{\alpha 3} \end{pmatrix} = 0$$

This system is similar to that obtained by Eshelby et al. (1953) in the case of a straight dislocation placed in homogeneous spaces in anisotropic elasticity. It has for each  $p_{\alpha}$ ,  $\lambda'_{\alpha k}$  nontrivial solutions if the determinant of  $A_{jk}$  is zero:

$$\det(A_{jk}) = |C_{j1k1} + (C_{j1k2} + C_{j2k1}) \cdot p_{\alpha} + C_{j2k2} \cdot p_{\alpha}^2| = 0 \quad (14)$$

These yields a sixth degree equation in  $p_{\alpha}$  ( $\alpha = 1, \dots, 6$ ) as follows,

$$K_0 + K_1 \cdot p + K_2 \cdot p^2 + K_3 \cdot p^3 + K_4 \cdot p^4 + K_5 \cdot p^5 + K_6 \cdot p^6 = 0 \quad (15)$$

where:  $K_0, K_1, K_2, K_3, K_4, K_5$  and  $K_6$  are functions of elastic constants  $C_{ij}$ .

So to solve the problem, it is necessary to calculate the six roots of the polynomial Eq. (15). These roots are complex (Eshelby et al., 1953) since the energy density must always be positive. Since the coefficients of the polynomial are real, the roots occur in complex conjugate pairs:  $p_{\alpha}$  ( $\alpha = 1, 3$ ), only the roots with positive imaginary part are chosen. These roots are written as:

$$p_{\alpha}^{(n)} = p_{\alpha}^r(n) \pm ip_{\alpha}^i(n)$$

With:

$$\alpha = 1, 2, 3 \text{ and } p_{\alpha}^i(n) > 0 \quad (16)$$

For each of the six roots  $p_{\alpha}$  given in (16), we solve the following system to determine the complex solutions  $\lambda'_{\alpha k}$ .

$$\begin{pmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{pmatrix} \begin{pmatrix} \lambda'_{\alpha 1} \\ \lambda'_{\alpha 2} \\ \lambda'_{\alpha 3} \end{pmatrix} = 0 \quad (17)$$

where:

$$F_{11} = C_{11} + 2C_{16}p + C_{66}p^2$$

$$F_{22} = C_{66} + 2C_{26}p + C_{22}p^2$$

$$F_{33} = C_{55} + 2C_{45}p + C_{44}p^2$$

$$F_{12} = F_{21} = C_{61} + (C_{66} + C_{12})p + C_{26}p^2$$

$$F_{13} = F_{31} = C_{51} + (C_{14} + C_{56})p + C_{46}p^2$$

$$F_{23} = F_{32} = C_{56} + (C_{25} + C_{46})p + C_{42}p^2$$

The  $\lambda'_{\alpha k}$  thus obtained depend on the  $C_{ij}$  and are complex.

They are of the form:

$$\lambda'_{\alpha k}^{(n)} = \lambda_{\alpha k}^r(n) \pm i\lambda_{\alpha k}^i(n) \quad (18)$$

The theory states that the displacements and constraints depend only on the relative values of  $\lambda'_{\alpha k}^{(n)}$  with ( $k = 1, 3$ ).

Therefore, the general solution of each of Eq. (12) is given by:

$$U_k^{(n)}(x_2) = \sum_{\alpha=1}^6 C_{\alpha}^{(n)} \cdot \lambda_{\alpha k} \cdot \exp(2.i.\pi.g.n.p_{\alpha}.x_2) \quad (19)$$

where  $C_{\alpha}^{(n)}$  are complex constants that can be determined using the boundary conditions. Substituting the expression of  $U_k^{(n)}(x_2)$  thus obtained in Eq. (19), we get:

$$U_k^{(n)}(x_2) = \sum_{\alpha=1}^3 \frac{X_{\alpha}^{(n)} \cdot \lambda_{\alpha k}}{2.i.\pi.n} \cdot \exp(2.i.\pi.g.n.p_{\alpha}.x_2) + \frac{Y_{\alpha}^{(n)} \cdot \bar{\lambda}_{\alpha k}}{2.i.\pi.n} \cdot \exp(2.i.\pi.g.n.\bar{p}_{\alpha}.x_2) \quad (20)$$

Combining (2) with (20) we can rewrite the displacement field as follows:

$$u_k = \sum_{n \neq 0} \sum_{\alpha=1}^3 \frac{X_{\alpha}^{(n)} \cdot \lambda_{\alpha k}}{2.i.\pi.n} \cdot \exp[(2.i.\pi.g.n.(x_1 + p_{\alpha}.x_2))] + \frac{Y_{\alpha}^{(n)} \cdot \bar{\lambda}_{\alpha k}}{2.i.\pi.n} \cdot \exp[(2.i.\pi.g.n.(x_1 + \bar{p}_{\alpha}.x_2))] \quad (21)$$

where the complex constants  $X_{\alpha}^{(n)}$  et  $Y_{\alpha}^{(n)}$  are determined using boundary conditions relative to the problem. To get better numerical performances only positive integer values of  $n$  are used in the summation in (21).

$$u_k = \sum_{n \neq 0} \sum_{\alpha=1}^3 C_{\alpha k}^{(n)} \cdot \exp[2.i.\pi.g.n.(x_1 + r_{\alpha}.x_2)] \Rightarrow C_{\alpha k}^{(-n)} = \bar{C}_{\alpha k}^{(n)} \quad (22)$$

So the double sum (22) becomes:

$$2 \sum_{n>0} \sum_{z=1}^3 \text{Re}(C_{zk}^{(n)}) \cdot \cos[2 \cdot \pi \cdot g \cdot n(x_1 + r_z \cdot x_2)] + \text{Re}(i \cdot C_{zk}^{(n)}) \cdot \sin[2 \cdot \pi \cdot g \cdot n(x_1 + r_z \cdot x_2)] \quad (23)$$

Setting  $\omega = 2 \cdot \pi \cdot g$ , we obtained the final expression of  $u_k$ :

$$U_k = \sum_{n>0} \left( \frac{1}{\pi \cdot n} \right) \sum_{z=1}^3 \{ \cos[n \cdot \omega \{x_1 + r_z \cdot x_2\}] \times [(-i \cdot X_z^{(n)} \cdot \lambda_{zk}) \cdot \exp(-n \cdot \omega \cdot s_z \cdot x_2) + (-i \cdot Y_z^{(n)} \cdot \bar{\lambda}_{zk}) \cdot \exp(n \cdot \omega \cdot s_z \cdot x_2)] \} + \{ \sin[n \cdot \omega \{x_1 + r_z \cdot x_2\}] \times \text{Re}[(X_z^{(n)} \cdot \lambda_{zk}) \cdot \exp(-n \cdot \omega \cdot s_z \cdot x_2) + (Y_z^{(n)} \cdot \bar{\lambda}_{zk}) \cdot \exp(n \cdot \omega \cdot s_z \cdot x_2)] \} \quad (k=1,2,3) \quad (24)$$

From Eq. (24) and the Hooke's:

$$\sigma_{kl} = C_{klj} \cdot \varepsilon_{ij} \quad (25)$$

We get the constraint field

$$\sigma_{kl} = C_{klij} \cdot u_{i,j} = C_{kli1} \cdot u_{i,1} + C_{kli2} \cdot u_{i,2} + C_{kli3} \cdot u_{i,3} \quad (26)$$

Since  $u_i$ , in our case does not depend on  $x_3$ , Eq. (26) can be reduced to:

$$\sigma_{kl} = C_{kli1} \cdot u_{i,1} + C_{kli2} \cdot u_{i,2} \quad (27)$$

where:

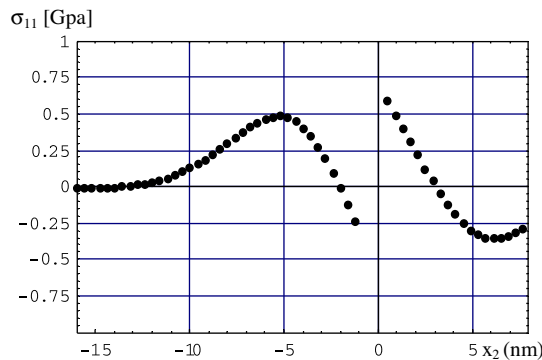
$$\sigma_{kl} = C_{k1l1} \cdot u_{1,1} + C_{k2l1} \cdot u_{2,1} + C_{k1l2} \cdot u_{1,2} + C_{k2l2} \cdot u_{2,2} \quad (28)$$

We finally obtain the following expression:

$$\sigma_{ij} = 2 \cdot g \sum_{n>0} \sum_{z=1}^3 \{ \cos[n \cdot \omega \{x_1 + r_z \cdot x_2\}] + \text{Re}[X_z^{(n)} \cdot L_{zij} \cdot \exp(-n \cdot \omega \cdot s_z \cdot x_2) + Y_z^{(n)} \cdot \bar{L}_{zij} \cdot \exp(n \cdot \omega \cdot s_z \cdot x_2)] \} + \{ \sin[n \cdot \omega \{x_1 + r_z \cdot x_2\}] + \text{Re}[i \cdot X_z^{(n)} \cdot L_{zij} \cdot \exp(-n \cdot \omega \cdot s_z \cdot x_2) + i \cdot Y_z^{(n)} \cdot \bar{L}_{zij} \cdot \exp(n \cdot \omega \cdot s_z \cdot x_2)] \} \text{ avec } L_{zkl} = \lambda_{zj} [C_{klj1} + p_z C_{klj2}] \quad i, j = 1, 2, 3, \quad l = 1, 2 \quad (29)$$

**Table 1** Data of thin bicrystal Cu/(001) Fe.

Designation	Cu	Fe
Lattice parameters a (nm)	0.361	0.355
Burgers vector $b$ (nm) of network	0.253	
Period of dislocation network $1/g$ (nm)	15.10	
Anisotropic elastic constants (Gpa)	$C_{11} = 168.4$	$C_{11} = 232$
	$C_{12} = 121.4$	$C_{12} = 136$
	$C_{44} = 75.4$	$C_{44} = 117$



#### 4. Application

The matrix Cu/Fe, Table 1, was recently the subject of intense research in the field of physics by Hyeok Shim and Whan Cho (2007) to fully exploit the electronic and magnetic properties as well as the structural and chemical characterization of the interface between layers of copper and iron (Myagkov et al., 2009).

The Burgers vector  $b = (a_{Cu} + a_{Fe})/2 \cdot 2^{1/2}$  and the period of the network  $1/g = (a_{Cu} \cdot a_{Fe}) / (a_{Cu} - a_{Fe}) \cdot 2^{1/2}$  are respectively calculated according to Bonnet (2000). The anisotropic elastic constants and lattice parameters are given by Myagkov et al. (2009) and Charles (2005).

Firstly we present in Fig. 4 the evolution of stresses  $\sigma_{11}$  and  $\sigma_{22}$  with respect to  $x_2$  within the material Cu/(001) Fe under the effect of a corners interfacial dislocation network whose Burgers vector is parallel to the  $Ox_1$  axis, for a value of  $x_1 = 1/2 \cdot g$  and an overall thickness of the bicrystal equal to 24 nm ( $h^+ = 8$  nm and  $h^- = 16$  nm) and the number of harmonics equal to 1000.

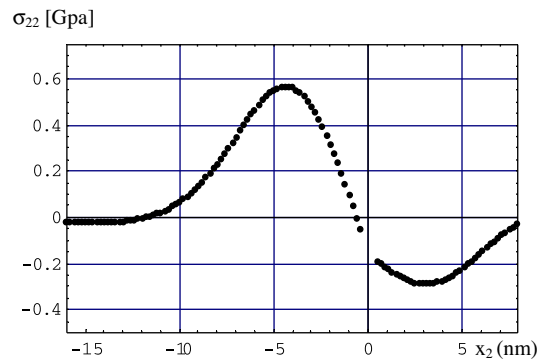
Regarding the constraints field, Fig. 4 shows that:

1. For the chosen value of  $x_1$ , we obtain a discontinuity of constraints  $\sigma_{(l)}$  across the interface.
2. Constraints  $\sigma_{(l)}$  are continuous across the interface and null at the free surfaces in accordance with the boundary conditions.
3. The distortion is much greater near the center of the dislocation than far from it. To better see the effect of the heterogeneity of the material on the evolution of the constraints, we present on the same Fig. 5 curves of constraints  $\sigma_{(l)}$  and  $\sigma_{(l)}$ . Different applications are presented for the thin homogeneous crystals Cu/(001) Cu and Fe/(001) Fe, where the total thickness of the bicrystal is kept constant ( $h^+ = 8$  nm and  $h^- = 16$  nm) for a value of  $x_1 = 1/2 \cdot g$ .

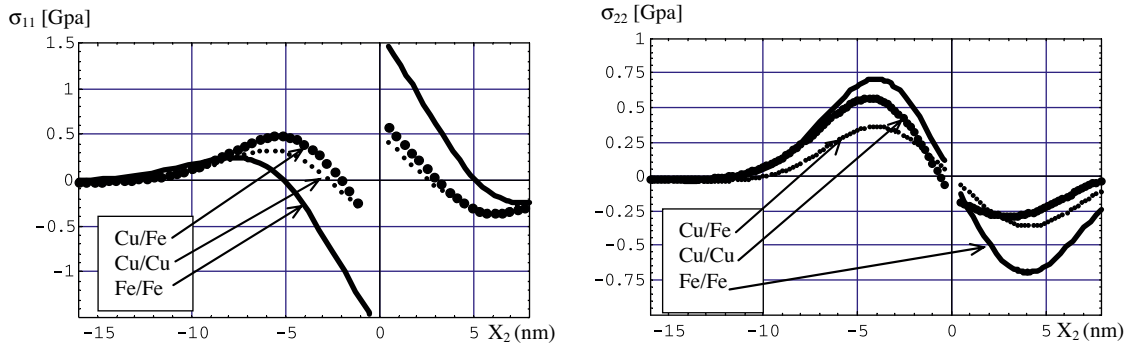
It is noteworthy that the stress values  $\sigma_{11}$  and  $\sigma_{22}$  are more important for material Fe/(001) Fe than for the heterogeneous system Cu/(001) Fe.

To highlight the effect of anisotropy, we plot, on the same Fig. 6 the results of our present study and those of early studies based on the assumption of isotropy for the core of Cu (001) Fe.

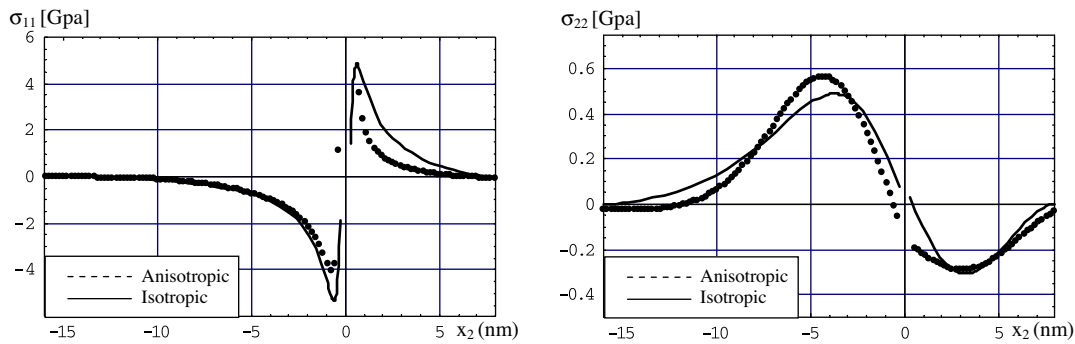
Fig. 6 shows that for the chosen value of  $x_1$  we obtain a discontinuity of stresses  $\sigma_{11}$  through the interface. These constraints  $\sigma_{11}$  evolve in the same crystal from positive values to



**Figure 4** Diagram illustrating the evolution of stresses  $\sigma_{11}$  and  $\sigma_{22}$  of the composite materials Cu/(001) Fe,  $C_{ij}$  anisotropic, period  $1/g = 15.10$  nm,  $n = 1000$ ,  $x_1 = 1/2 \cdot g$ ,  $b//Ox_1$ ,  $h^+ = 8$  nm and  $h^- = 16$  nm.



**Figure 5** Superposition of constraints fields  $\sigma_{11}$  and  $\sigma_{22}$ , of the composite materials Cu/(001) Cu, Fe/(001) Fe and Cu/(001) Fe,  $x_1 = b$  nm and  $x_1 = 1/2 g$  nm,  $b//Ox_1$ ,  $h^+ = 8$  and  $16$  nm.



**Figure 6** Superimposing of constraints fields  $\sigma_{11}$  and  $\sigma_{22}$ ,  $C_{ij}$  anisotropic and isotropic  $C_{ij}$  of the composite materials Cu/(001) Fe,  $x_1 = 1/2 g$ , and  $b//Ox_1$ ,  $h^+ = 8$  nm and  $h^- = 16$  nm.

negative values and vice versa depending on whether there is a tension or compression of the crystal. This explains that in the case of dislocation network, the state of stress changes its sign whether it is near the center of the dislocation or along the period away from it. Note also that the stresses  $\sigma_{22}$  are continuous across the interface and null at the layer's boundary in accordance with the boundary conditions.

The invalidity constraints  $\sigma_{11}$  and  $\sigma_{22}$  very far from the dislocation ( $x_1 = 1/2 g$ ) for a period of that can catch the misfit explain the limitation of the deformation field at the free surfaces.

Our Mathematical code based on the Fourier series in the case of isotropic elasticity gives results that show the difference between the anisotropic and isotropic. It is clear that the dispersions of constraints  $\sigma_{11}$  and  $\sigma_{22}$  in the bicrystal Cu/(001) Fe go through maxima whose values indicate.

The values of the Zener anisotropy factor are (Zener, 1984):

$$A = \frac{2 \cdot C_{44}}{C_{11} - C_{12}} = 3.20 \quad \text{for Cu and} \quad 2.43 \quad \text{for Fe}$$

## 5. Conclusion

By studying the effect of anisotropy on the constraints field created by an intrinsic unidirectional dislocation network with a network period, and knowing that the monocrystals of copper and iron are very anisotropic and whose values of Zener anisotropy factor are high, the results obtained concerning

these constraints fields depend on several essential factors which are the orientation of the Burgers vector  $b$  (oriented according to  $Ox_1$  in our case), the period of the network, the elastic constants  $C_{ij}$  and the thickness of the selected layer.

For the constraints distribution  $\sigma_{11}$  and  $\sigma_{22}$ , note that the constraint  $\sigma_{11}$  changes its sign in layers and that it is important when calculated near the heart of the dislocation ( $b = x_1$ ). We also noted that the  $\sigma_{11}$  constraints discontinuity and the  $\sigma_{22}$  constraints continuity along the interface as well as the values of  $\sigma_{22}$  become null at the level of the free surfaces at a distance equal to some nanometers away from the heart leaving room to a perfect relaxation in accordance with boundary limits which are verified. It is worth noting that the deformation is much bigger near the heart of the dislocation than far from it and the amplitude of the  $\sigma_{22}$  constraints is greater when the thickness is small.

Aiming to compare the elastic behavior, a comparison of the results obtained in isotropic elasticity for the same bicrystal under the same conditions is done. A clear difference is visible between the anisotropic and isotropic cases for the thin bicrystal Cu/(001)Fe leading to conclude that the anisotropy effect is essential for the chosen bicrystal.

## References

- Bonnet, R., 1981. Periodic displacement and stress fields near a phase boundary in the isotropic elasticity theory. *Philos. Mag. A* 43, 1165–1187.

- Bonnet, R., 2000. A two-layer epitaxial composite strained by an array of misfit dislocations accommodating the lattice mismatch. *Phys. Status Solidi A* 177, 219.
- Bonnet, R., 2003. Elastic field of a straight dislocation parallel to interfaces: a new approach. *C R Phys.* 4, 961–966.
- Brioua, M., Benbouda, R., Madani, S., Adami, L., 2005. Numerical simulation of the anisotropic elastic field generated by a misfit dislocations along a NiS<sub>2</sub>/Si/(001) GaAs heterotwin interface. *J. Colloid Interface Sci.* 282, 120–123.
- Charles, K., 2005. Introduction to Solid State Physics. University of California.
- Eshelby, J.D., Read, W.T., Shockley, W., 1953. Anisotropic elasticity with applications to dislocation theory. *Acta Meta.* 1, 251–259.
- Fabien, Leroy, 2003. Thèse de Doctorat de l'université Joseph Fourier – Grenoble 1.
- Hyeok Shim, J., Whan Cho, Y., 2007. Screw dislocation assisted martensitic transformation of a bcc Cu precipitate in bcc Fe. *Appl. Phys. Lett.* 90, 021906-3.
- Jesser, W.A., Matthews, J.W., 1967. Evidence for pseudomorphic growth of iron on copper. *Philos. Mag.* 15, 1097–1106.
- Myagkov, V.G., Bayukov, O.A., Bykova, L.E., Bondarenko, G.N., 2009. The  $\gamma$ -Fe formation in epitaxial Cu(001)/Fe(001) thin films by the solid-state synthesis: Structural and magnetic features. *J. Magn. Mater.* 321, 2260–2264.
- Peralta, P., Schober, A., Laird, C., 1993. Elastic stresses in anisotropic bicrystals. *Mater.Sci. Eng.* 169.
- Peralta, P. et al., 2001. Effects of anisotropy and slip geometry on fatigue fracture of Cu/sapphire bicrystals. *Mater. Sci. Eng. A314*, 55–66.
- Wang, X., Pan, E., Albercht, J.D., 2007. Anisotropic elasticity of multilayered crystals deformed by a biperiodic network of misfit dislocations. *Phys. Rev. B* 76, 134112.
- Wu, W.P. et al., 2011. Structural evolution of misfit dislocation networks at  $\gamma\gamma'$  phase interfaces of Ni-based super-alloys: Molecular dynamics simulation. *Philos. Mag.* 91, 357–372.
- Zener, C., 1984. *Elasticity and Anelasticity of Metals*. Chicago Univ. Press, 16.