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Interfacial stress field generate by a biperiodic hexagonal network of misfit dislocations in a thin bicristal InAs/(111)GaAs

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The elastic interactions generated by the presence of a biperiodic network, more precisely hexagonal, of misfit dislocations in the interfacing of a thin bicristal have been simulated numerically while considering an anisotropic elasticity for each crystal. The representation of the normal equi-stress near the dislocation segments and near of the triple node of hexagonal cell permits to detect the stress concentration zone du to elastic field for InAs/(111)GaAs system, because, in the category of semiconductors, this is an ideal system which exhibit the presence of edge dislocations type parallels to the free surfaces by S.T.M.[1].

Keywords : Misfit dislocations, thin films, interfaces, anisotropic elasticity.

Campo interfacial de tensiones generado por una red biperiódica hexagonal de dislocaciones en un bicristal delgado de InAs/(111)GaAS

Las interacciones elásticas generadas por la presencia de una red biperiódica, de dislocaciones en la interfase de un bicristal han sido simuladas numéricamente, considerando elasticidad anisotropa para cada cristal. La representación de las tensiones próximas a las dislocaciones y del nodo triple de la celda hexagonal, permite detectar la zona de concentración de tensiones debido al campo elástico para el sistema InAS/(111) GaAS, ya que, en los semiconductores, éste es un sistema ideal que muestra la presencia de dislocaciones paralelas a las superficies libres por S.T.M.[1].

Palabras clave: Dislocaciones, películas finas, interfases, elasticidad anisótropa.

1. INTRODUCTION

The combination of two different semiconductors is always challenging in term of understanding both the chemical composition and the effect of the misfit strain during growth. For semiconductors, some authors had study STM images which exhibit the presence of an hexagonal mesh of edge dislocations parallel to the free surfaces, the results are recent, cf InAs/(001)GaAs (Belk & col. 1997), InAs/(111)GaAs (Yamaguchi & col. 1997). Because of the image contrasts of a dislocation can be computed from its displacement field U_k, the aim of this work is to propose a computer simulation of the normal equi-stress near the dislocation segments and near of the triple node of the hexagon cell, for an ultrathin bicristal formed by InAs on (111) GaAs, using a method of determination of biperiodic elastic fields based on a double Fourier series analysis (Bonnet 1992), adapted to the complex geometry of the mesh and to specific boundary conditions of the problem, with the assumption that the two crystals are elastically anisotropic but different as species.

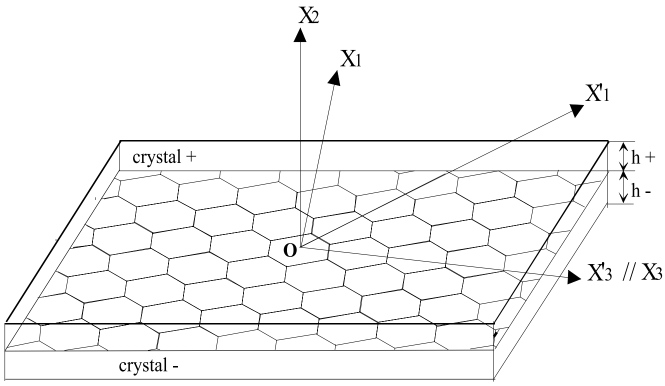

Figure 1. Hexagonal network of misfit dislocations. At the interface of two thin foils.

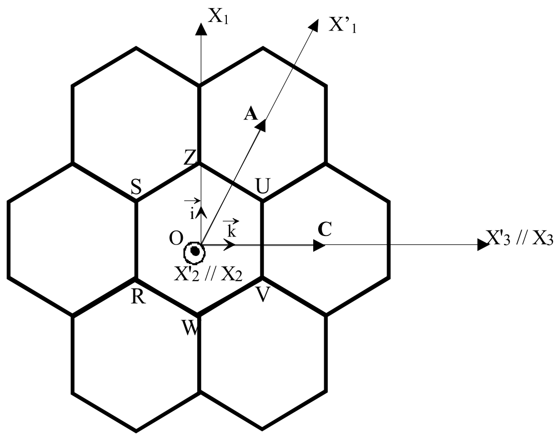

Figure 2. A regular hexagonal network of misfit dislocations oriented Clockwise UVWRSZ around the center O of a hexagon. OA and OC are the period vectors. The Cartesian frame work used is $OX_1X_2X_3$.

2. GEOMETRY OF HEXAGONAL NETWORK OF MISFIT DISLOCATIONS

In figure (1), we consider the heterointeface papered with a regular hexagonal network of misfit dislocations between two ultrathin layers having finite thickness, different nature and elastically anisotropic, which are noted crystal(+) and crystal(-), the elastic constants of this crystals are denoted by C_{ijkl}^+ and C_{ijkl}^- respectively.

3. FORMAL SOLUTION OF DISPLACEMENT AND STRESS FIELD

3.1. Displacement field

The displacement field being biperiodic for either crystal (+) or (-), the generalised solution of elasticity equations of Navier, is given in [8b] by :

$$U_k = \sum_{G\neq 0} u_k^{(G)}(x2)\exp 2\pi\, i.G.R \qquad (1)$$

The displacements (1) must satisfy the differential equations of the classical elasticity theory, in one part:

$$\sigma_{ij} = C_{ijkl} U_{k,l} \qquad (2)$$

And static equilibrium of stresses condition, in the other part :

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \qquad (3)$$

After combination of (1) with (2) and (3), the general expression of displacements $u_k^{(G)}$**Error! Bookmark not defined.**must have the form :

$$u_k^{(G)} = \sum_{\alpha=1}^{6} P_\alpha^{(G)} \lambda_{\alpha k}^{(G)} .\exp 2\pi .i.P_\alpha^{(G)}.x_2 \qquad (4)$$

Replacing (4) in (1) leads to :

$$U_k = \sum_{G\neq 0} \sum_{\alpha=1}^{6} P_\alpha^{(G)} \lambda_{\alpha k}^{(G)} .\exp 2\pi .i.(p_\alpha^{(G)}.x_2 + G.R) \qquad (5)$$

- Σ : represents a double sum over the possible values of the couple (m,n), taken inside a domain D defined in [7], not including the couple (0,0).
- $P_\alpha^{(G)}$ are complex constant unknowns of global system for (α =1,2,3) assigned by a sign (+) or (-) as may be depending on crystal (+) or (-). The total number of six complex unknowns are found from boundary conditions at the interface, so they depend on the Burgers vectors and on the geometry of the network.
- $\lambda_{\alpha k}^{(G)}$ are complex coefficients depending only on the C_{ij} of the crystal considered, they are calculated for each α from the solutions of the linear homogeneous system (6) obtained after combining and developing expressions (1) and (3).

$$\begin{bmatrix} \psi_{11}+\varphi_{11}p_\alpha + C_{1212}p_\alpha^2 & \psi_{21}+\varphi_{21}p_\alpha + C_{2212}p_\alpha^2 & \psi_{31}+\varphi_{31}p_\alpha + C_{3212}p_\alpha^2 \\ \psi_{12}+\varphi_{12}p_\alpha + C_{1222}p_\alpha^2 & \psi_{22}+\varphi_{22}p_\alpha + C_{2222}p_\alpha^2 & \psi_{32}+\varphi_{32}p_\alpha + C_{3222}p_\alpha^2 \\ \psi_{13}+\varphi_{13}p_\alpha + C_{1232}p_\alpha^2 & \psi_{23}+\varphi_{23}p_\alpha + C_{2232}p_\alpha^2 & \psi_{33}+\varphi_{33}p_\alpha + C_{3232}p_\alpha^2 \end{bmatrix} \begin{bmatrix} \lambda_{\alpha 1} \\ \lambda_{\alpha 2} \\ \lambda_{\alpha 3} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad (6)$$

with :

$$\psi_{jk}^{(G)} = C_{j1k1}G_1^2 + C_{j3k3}G_3^2 + (C_{j1k3} + C_{j3k1})\, G_1 G_3$$

$$\varphi_{jk}^{(G)} = (C_{j1k2} + C_{j2k1})\, G_1 + (C_{j2k3} + C_{j3k2})\, G_3$$

The coefficients $\lambda_{\alpha k}^{(G)}$ must also be calculated so as to verify the relation $\lambda_{\alpha 1}^2 + \lambda_{\alpha 2}^2 \lambda_{\alpha 3}^2 = 1$.

- $P_\alpha^{(G)}$ are complex roots obtained by solving the sextic polynomial which is the expression of the determinant of system (6), this determinant must be equalled to zero for obtaining non trivial solutions.

In writing that :

$$\overline{p_\alpha^{(G)}} = p_{\alpha+3}^{(G)}, Q_\alpha^{(G)} = P_{\alpha+3}^{(G)} \text{ and } \overline{\lambda_{\alpha k}^{(G)}} = \lambda_{(\alpha+3)k}^{(G)} \text{ for } \alpha = 1,3.$$

The expression (5) becomes :

$$U_k = \sum_{G\neq 0}\Big(\sum_{\alpha=1}^{3} P_\alpha^{(G)}\lambda_{\alpha k}^{(G)} \exp 2\pi .i(G.R + p_\alpha^{(G)}.x_2) + Q_\alpha^{(G)}\lambda_{\alpha k}^{(G)} \exp 2\pi .i(G.R + p_\alpha^{(G)}.x_2) + \sum_{\alpha=4}^{6} P_\alpha^{(G)}\lambda_{\alpha k}^{(G)} \exp 2\pi .i(G.R + p_\alpha^{(G)}.x_2) + Q_\alpha^{(G)}\lambda_{\alpha k}^{(G)} \exp 2\pi .i(G.R + p_\alpha^{(G)}.x_2)\Big).$$

Knowing that U_k is necessary a real quantity, The expression (5) becomes :

$$U_k = 2.\mathrm{Re}\sum_{G} \sum_{\alpha=1}^{3} [P_\alpha^{(G)}\lambda_{\alpha k}^{(G)} \exp 2\pi .i(G.R + p_\alpha^{(G)}.x_2) + Q_\alpha^{(G)}\overline{\lambda_{\alpha k}^{(G)}} \exp 2\pi .i(G.R + \overline{p_\alpha^{(G)}}.x_2)] \qquad (7)$$

Re means "real part of ".

3. 2. Stress field

Using Hook's law in anisotropic elasticity theory expressed by (2),

$$\sigma_{kl} = C_{kl i1}\frac{\partial U_i}{\partial x_1} C_{kl i2}\frac{\partial U_i}{\partial x_2} C_{kl i3}\frac{\partial U_i}{\partial x_3} \qquad (8)$$

From derivation of equation (7) via (8), we obtain :

$$\sigma_{kl} = 4\pi .\mathrm{Re}\left\{\sum_{G}\sum_{\alpha=1}^{3} i.L_{\alpha kl}^{(G)} P_\alpha^{(G)} \exp\theta + i.\overline{L_{\alpha kl}^{(G)}} Q_\alpha^{(G)} \exp\bar{\theta}\right\} \qquad (9)$$

With :

$$L_{\alpha kl}^{(G)} = (C_{kl j1}G1 + C_{kl j3}G3 + p_\alpha^{(G)} C_{kl j2})\lambda_{\alpha j}^{(G)}$$

$$\overline{L_{\alpha kl}^{(G)}} = (C_{kl j1}G1 + C_{kl j3}G3 + \overline{p_\alpha^{(G)}} C_{kl j2}\overline{\lambda_{\alpha j}^{(G)}}) \qquad (10)$$

$$\theta = (GR + P_\alpha^{(G)}\, x2) \quad \text{and} \quad \bar{\theta} = (GR + \overline{P_\alpha^{(G)}}\, x2)$$

4. BOUNDARY CONDITIONS AND GLOBAL SYSTEM

4.1. Displacements conditions

Knowing the discontinuity of displacement field U crossing the heterointerface, the relative displacement $\Delta U = |u_k^+ - u_k^-|_{x2=0}$ is zero at the centre of the cell and varies linearly along interface, from centre of each hexagon see fig (2), thus ΔU is varying linearly with x_1 and x_3 and takes a maximal value along dislocation segments UV and ZU, this is means that ΔU is equal to half value of Burgers vector adjoining these segments . We can express ΔU analytically inside the unit cell UVWRSZ, using the geometric transformations developed in appendix B cf. Ref [7] as :

$$\Delta u = u^+ - u^- = b^{(ZU)}\left(\frac{x_1'}{a}\right) + b^{(UV)}\left(\frac{x_3'}{c}\right) \qquad (11)$$

$b^{(ZU)}$ and $b^{(UV)}$ being Burgers vectors respectively for segments of dislocation ZU and UV. The displacement inside one hexagon cell being biperiodic, when we develop ΔU into a double Fourier series on all the vectors G relative to the frame $Ox'_1x'_2x'_3$, as indicate in [7], we obtain :

$$\Delta U = \left|U_k^+ - U_k^-\right|_{x_2=0} = \sum_{G}\frac{-iT_k^{(G)}}{2}.\exp 2\pi\, i.G.R \qquad (12)$$

The vector $T^{(G)}$ with components (T_1,T_2,T_3) describe the geometry of the network, it has been obtained from cumbersome integrations, it depends on the non-zero reciprocal vector G(m,n) and is defined in appendix B ref.[9] as for an irregular hexagon.

$$T^{(G)} = \sin\frac{[2\pi(n\alpha_1 + m\alpha_2)]}{\pi^2[m + n - 2(n\alpha_1 + m\alpha_2)]}\, \mathrm{X} \left[\frac{(1-2\alpha_2).b^{(ZU)}}{n - 2(n\alpha_1 + m\alpha_2)} + \frac{1-2\alpha_1 .b^{(UV)}}{m - 2(n\alpha_1 + m\alpha_2)}\right] \qquad (13)$$

in which α_1 and α_2 are the internal co-ordinates of the U point in unit cell UVWRSZ (fig2), as: **OU** = α_1 **c** + α_2 **a.**

The cases of zero denominators in (12) for a regular hexagon ($\alpha_1 = \alpha_2 = \pi/6$) are presented in table in [7].

4.2 Stress conditions

The interfacing of a thin bicristal, being in equilibrium, in the reference mark Cartesian $Ox_1x_2x_3$ figs (2), the normal stresses (according to x_2) σ_{2K} are, on the one hand, continuous through the heterointerface, and on the other hand, hopeless to the free surface of each crystal.

- The continuity at the interface gives:

$$\sigma^{+}_{2k} = \sigma^{-}_{2k}\Big|_{x_2=0} = 0 \tag{14}$$

- The nothing at the free surfaces gives:

$$\sigma^{+}_{2k}\Big|_{x_2=+h} = 0 \tag{15}$$

$$\sigma^{-}_{2k}\Big|_{x_2=-h} = 0 \tag{16}$$

4.3 Gotten global system

After transformation of expressions of displacements and constraints (7) and (8) in trigonometric terms and application of boundary conditions (12), (14), (15) and (16), a system of (4x3) equations (17) is obtain with 12 complex unknowns to determine. This system must be solved numerically because of its complexity, a FORTRAN program had established to this effect to determine complex coefficients P^+, P^-, Q^+ and Q^-, holding amount of the necessity to work in double precision, because, for high order of harmonic (m,n), the inversion is very difficult numerically when the exponential terms become very bigger or very smaller. Fields of displacement being discontinuous to the neighbourhood of dislocation cores, the convergence becomes very nit for very big harmonic.

$$\begin{cases} \sum_{\alpha=1}^{3}\left[P^{+}_{\alpha}\lambda^{+}_{\alpha k} + Q^{+}_{\alpha}\overline{\lambda^{+}_{\alpha k}}) - (P^{-}_{\alpha}\lambda^{-}_{\alpha k} + Q^{-}_{\alpha}\overline{\lambda^{-}_{\alpha k}})\right] = -i\dfrac{T_k}{2} \\ \sum_{\alpha=1}^{3} i.\left[P^{+}_{\alpha}L^{+}_{\alpha 2k} + Q^{+}_{\alpha}\overline{L^{+}_{\alpha 2k}}) - (P^{-}_{\alpha}L^{-}_{\alpha 2k} + Q^{-}_{\alpha}\overline{L^{-}_{\alpha 2k}})\right] = 0 \\ i\sum_{\alpha=1}^{3}\left[P^{+}_{\alpha}L^{+}_{\alpha 2k}\exp(2\pi.i.p^{+}_{\alpha}.h^{+}) + Q^{+}_{\alpha}\overline{L^{+}_{\alpha 2k}}\exp(2\pi.i.\overline{p^{+}_{\alpha}}.h^{+})\right] = 0 \\ i\sum_{\alpha=1}^{3}\left[P^{-}_{\alpha}L^{-}_{\alpha 2k}\exp(-2\pi.i.p^{-}_{\alpha}.h^{-}) + Q^{-}_{\alpha}\overline{L^{-}_{\alpha 2k}}\exp(-2\pi.i.\overline{p^{-}_{\alpha}}.h^{-})\right] = 0 \end{cases} \tag{17}$$

5. APPLICATION

The program is written to compute the values of displacement of structural units at the free surface, data used where relative to bicristal prepared by Yamaguchi & col. (1997), which are deposition of InAs on (111) GaAs substrate. The two crystals have same parallel directions and Burgers vectors of misfit dislocations are from 1/2<110> type.

The lattice parameters and elastic anisotropic constants are given by Chami (1988) [10], Burgers vector modulus is given by : b = (a_{InAs} + a_{GaAs}) / 2√2 = 5.98 nm, so the components will be as folow : $b^{(UV)}$ = (0; 0; -b) and $b^{(ZU)}$ = (-b√3/2; 0; -b/2). Period vectors OA and OC from hexagonal cell have same length as : a = a_{InAs}. a_{InAs} / │(a_{InAs} - a_{InAs}) √2 │, all this is given in table I . For numerical computation, the summation parameters m and n were stopped at 20 because it gives a good convergence of double Fourier series, and a thickness of h = 5 a_{InAs} / √2 was chosen for representing the displacement field (Bonnet [6]).

6. RESULTS AND DISCUSSIONS

In figures (3a) and (3b), we can see the normlal equi-stress σ_{11} and σ_{22} through the interface near the triple node of the hexagonal cell.

The theoretical contrast varies from -3 GPa to +3 GPa when the values passes from a dark maximum to a white minimum. Hollow of the surface is more accentuated. These features are perfectly find again on the figure 4 of Guenther & col. (1995) for which the hexagonal network of misfit dislocations is perfectly relaxed. The results permits to detect with precision the stress concentration zone du to elastic field, and shows a good analogy with analytical results obtained using an isotropic coefficients.

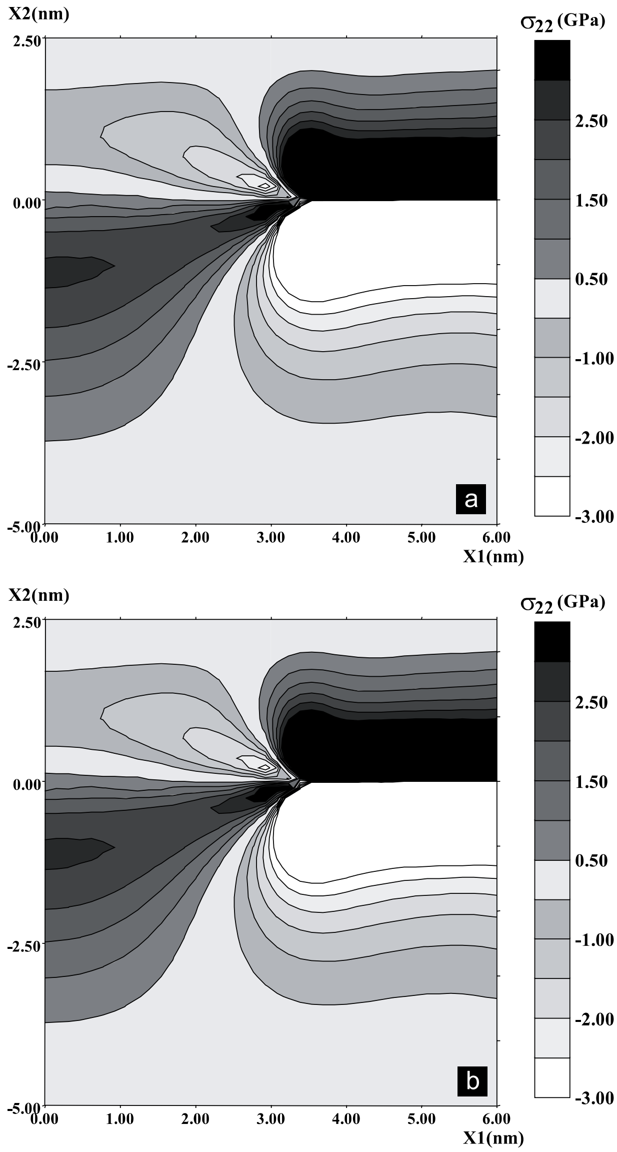

Fig 3. a) equistress σ_{11} near the triple node of hexagon. b) equistress σ_{22} near the triple node of hexagon

7. CONCLUSION

Numerical simulation proposed in this notes shows that, using has method of determination of biperiodic and anisotropic elastic fields based one has double Fourier series analysis (R.Bonnet 1992), it is possible to quantify stress fields aspects characteristics of a deformed free surface by a regular hexagonal network of misfit dislocations. The gotten features are indeed in good agreement with the count of S.T.M images proposed by R.Bonnet (1997) for the same bicrictal and isotropic elastic constants, as well as with observations (fig 4) of Guenther & col. (1995) for Cu / (001)Ru and more rudely, with those of Yamaguchi & col. (1997), see (fig 1c) for InAs / (111)GaAs.

Considering Zeners coefficients value more elevated for the two crystals, to know 1.82 for GaAs and 2.08 for InAs, we can say that the relative relief to the hexagonal shape of the network of DMS have been preserved, and put to part nuances of gray, we are very able to judge the conformity of images gotten relatively.

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