Journal of Solid Mechanics Vol. 13, No. 4 (2021) pp. 503-512
DOI: 10.22034/jsm.2021.1920891.1672

Anisotropic and Isotropic Elasticity Applied for the Study of Elastic Fields Generated by Interfacial Dislocations in a Heterostructure of InAs/(001)GaAs Semiconductors

R. Makhloufi [1], A. Boussaha [2], R. Benbouta [1,*], L. Baroura [3]

[1]*Mechanical Engineering Department, Faculty of Technology, LICEGS Laboratory, University of Batna 2 Mostafa Ben Boulaid, Batna, Algeria*
[2]*Mechanical Engineering Department, Faculty of Technology, University of Batna 2 Mostafa Ben Boulaid, Batna, Algeria*
[3]*Mechanical Engineering Department, University of Constantine 1, Algeria*

Received 1 August 2021; accepted 9 October 2021

ABSTRACT

This work is a study of the elastic fields' effect (stresses and displacements) caused by dislocations networks at a heterostructure interface of a InAs / GaAs semiconductors thin system in the cases of isotropic and anisotropic elasticity. The numerical study of this type of heterostructure aims to predict the behavior of the interface with respect to these elastic fields satisfying the boundary conditions. The method used is based on a development in Fourier series. The deformation near the dislocation is greater than the other locations far from the dislocation.

Keywords : Elastic fields; InAs/GaAs; Anisotropic; Isotropic; Semiconductors.

1 INTRODUCTION

THE production of new miniaturized semiconductors is highly demanded by the electronics industry for their important physical and chemical properties [1, 2]. The manufacturing of this semiconductor creates mechanical stresses which generate failure and reliability problems because of the elastic fields (displacements, stresses) caused by different types of dislocation networks at the interfaces in anisotropic and isotropic elasticity cases. This leads to studies allowing to know the effects of these elastic fields on the interface of the heterostructure. The heterojunction formed by two different semiconductors as for InAs / GaAs is of great interest practically because of the association of specific properties (electrical and opto-electronic properties of the two semiconductors and to overcome the difficult problems to solve with only one material. The heteroepitaxial system of III-V InAs/GaAs semiconductors (001) attracted interests and researches for these promising optoelectronic properties [3, 4]. Yonemoto et al. [5] studied the adsorption - desorption behavior on the surface of the InAs wetting layer cultivated on (001) GaAs substrate. A stress calculation method was proposed by improving the force and moment equilibrium method to

---

[*] Corresponding author. Tel.: +213 33812143, Fax.: +213 33812143.
E-mail address: r_benbouta@yahoo.fr (R. Benbouta)

calculate stress in semiconductor layers such as InGaAs/GaAs multilayers [6]. Derardja et al. [7] treated, taking into account the anisotropic elasticity specific to each crystal, the elastic fields relating to a layer / substrate system and to an ultra thin bi-crystal when the network of dislocations is hexagonal. The stress relaxation processes in InAs heteroepitaxy on substrates was studied by Akihiro et al. [8]. The Stranski-Krastanov SK growth pattern occurs in the InAs/GaAs (001) system with a 7.2% parametric disagreement reported by Leonard et al. [9]. An optimization of the morphological and optical characteristics of BQs InAs / GaAs quantum dots as a function of the nominal thickness of InAs epitaxied by chemical jets on a GaAs substrate (001) was studied by Jihene Zribi [10]. Stress relaxation of ultrafine InAs layers on InGaAs substrates during heteroepitaxy plays a central role in the growth and engineering of III - V single crystals [11].

In this work we studied the elastic behavior of a thin bimetallic strip whose interface is lined with a parallel network of dislocations of parametric disagreement. The analytical method used is a formulation in Fourier series in which the analytical expressions of its coefficients was determined numerically with an accuracy which was checked with respect to the series convergence. It is necessary to have models, which can describe in explicit form the elastic fields for different cases in the cases of isotropic and anisotropic elasticity. We also examined the contrast of different results.

2 BASIC FORMULATIONS

Based on a double Fourier series formulation proposed by Bonnet [12], the elastic fields (displacements and stresses) [13], were calculated in the case of isotropic and anisotropic elasticity.

2.1 Formulation in the isotropic case

In the isotropic case, the deformation is assumed to be plane and periodic along the Ox_1 axis. The displacement field u_k components can be written:

$$u_k = \sum_{n=-\infty}^{\infty} U_k^{(n)} \exp^{\left(\frac{2\pi i n}{\Lambda} x_1\right)} \quad \text{for } n \neq 0 \tag{1}$$

The period Λ of the network is determined by $\Lambda = \frac{b}{\varepsilon}$. Where ***b*** is the modulus of the Burgers vector and ε the misfit $\varepsilon = \frac{2(a^+ - a^-)}{a^+ + a^-}$. We take $\omega = \frac{2\pi}{\Lambda}$. Eq. (1) becomes $u_k = \sum_{n=-\infty}^{\infty} U_k^{(n)} \exp^{(in\omega x_1)}$. Where the $U_k^{(n)}$ depends only on x_2.

The field of displacements as defined must satisfy the differential equation of elasticity obtained by combining the equilibrium equations of a volume element with the linear equations of Hooke.

$$(\lambda + \mu)u_{i,ik} + \mu u_{i,ik} = (\lambda + \mu)\frac{\partial^2 u_i}{\partial x_i \partial x_k} + \mu \frac{\partial^2 u_k}{\partial x_i \partial x_i} \tag{2}$$

where λ and μ are the Lamé coefficients of the deformed medium. For *i*, *k* = 1, 2, 3 and by inserting Eq. (1) into Eq. (2), we get for each harmonic n of non-zero rank a system of equations.

$$(\lambda + 2\mu)(-n^2\omega^2)u_1 + (\lambda + 2\mu)(-in\omega)u_{2,2} + \mu u_{2,2} = 0 \tag{3}$$

$$(\lambda + \mu)(-in\omega)u_{12,} + (\lambda + 2\mu)u_{2,2} + \mu(-n^2\omega^2)u_2 = 0 \tag{4}$$

$$\mu(-n^2\omega^2)u_3 + \mu u_{3,22} = 0 \tag{5}$$

The fields of displacement components are:

$$u_1=\sum_{n=-\infty}^{\infty}\begin{bmatrix}\left(A+Bn\omega x_2\right)\exp^{(-n\omega x_2)}\\ +i\left(C+Dn\omega x_2\right)\exp^{(in\omega x_2)}\end{bmatrix}\exp^{(in\omega x_1)} \tag{6}$$

$$u_2=\sum_{n=-\infty}^{\infty}\begin{bmatrix}\left(A+(3-4\mu)B+n\omega x_2\right)\exp^{(-n\omega x_2)}\\ -i\left(C-(3-4\mu)D+Dn\omega x_2\right)\exp^{(in\omega x_2)}\end{bmatrix}\exp^{(in\omega x_1)} \tag{7}$$

$$u_3=\sum_{n=-\infty}^{\infty}\left[E\exp^{(-n\omega x_2)}+F\exp^{(in\omega x_2)}\right]\exp^{(in\omega x_1)} \tag{8}$$

For the expression of the stress field in the case of plane strain:

$$\sigma_{ij}=\lambda\delta_{ij}u_{k,k}+\mu(u_{i,j}+u_{j,i})$$

By elimination the parameter λ and using the classical relation (Hirth and Loth), we get the following constraints:

$$\sigma_{21}=\mu(u_{1,2}+u_{2,1})$$
$$\sigma_{22}=\frac{2\mu}{1-2\mu}\left[(1-\mu)u_{2,2}+\nu\left(u_{1,1}+u_{3,3}\right)\right]$$
$$\sigma_{23}=\mu(u_{2,3}+u_{3,2})$$

In our work, we considered the fact that a periodic series of dislocations produces in each medium a displacement field $\boldsymbol{u_k}$ and a stress field $\boldsymbol{\sigma_{ij}}$ whose components can be developed in a double Fourier series. The field of displacements u is bi-periodic parallel to the hetero-interface, in media noted respectively with the signs + and -.

The boundary conditions relating to a thin bimetallic strip valid for the isotropic and anisotropic case are summarized as follow:

a) Condition on the linearity of the interfacial relative displacement:

$$\Delta u_k=u_k^+-u_k^-=\sum_{n=1}^{\infty}\frac{-b_k}{\pi n}\sin(n\omega x_1)$$
$$\Delta u_k=u_k^+-u_k^-=\sum_{n=-\infty}^{\infty}\frac{ib_k}{2\pi n}\exp(in\omega x_1)$$

b) Condition on the stresses continuity σ_{2k} at the interface

$$\sigma_{2k}^+ +\sigma_{2k}^- \quad \text{for} \quad x_2=0$$

c) Condition of the stresses nullity σ_{2k} at free surfaces

$$\sigma_{2k}^+\Big|_{x_2=h}=0$$
$$\sigma_{2k}^-\Big|_{x_2=h}=0$$

To explicitly find each of the Fourier coefficients, the components of the displacement field $U_k^{(n)}$ of the displacement field (1), it is necessary to solve Eqs. (6), (7) and (8). It remains to solve a linear system of twelve equations with twelve complex unknowns $A^+,B^+,C^+,D^+,E^+,F^+,A^-,B^-,C^-,D^-,E^-,F^-$. This system splits into two independent sub-systems. The first contains only the unknowns E^+, F^+, E^-, F^-.The solutions are purely complex. The component of the displacement field parallel to the dislocations therefore depends on the Burgers vector ***b***, the coefficient *v* and the ratio *k* of the shear moduli. The other system of equations has eight unknowns $A^+, B^+, C^+, D^+, A^-, B^-, C^-, D^-$. It is written in the form of a matrix product, where the column matrix $X\left(A^+, B^+, C^+, D^+, A^-, B^-, C^-, D^-\right)$ contains these eight complex unknowns written in the same order from top to bottom $AX = B$.

In this equation, the matrices *A* and *B* are respectively an 8 × 8 complex square matrix and a column matrix. The equation was solved analytically and we obtained the explicit expressions of the field of displacements for the two mediums:

$$u_1^+ = \sum_{n=-\infty}^{\infty} \left[\begin{array}{l} b_2\left(a_{re}^+ + n\omega b_{re}^+ x_2\right)e^{-n\omega x_2} + \left(c_{re}^+ + n\omega d_{re}^+ x_2\right)e^{n\omega x_2}\dfrac{\cos(n\omega x_1)}{n\pi\Delta} - b_1\left(a_{im}^+ + n\omega b_{im}^+ x_2\right)e^{-n\omega x_2} \\ +\left(c_{im}^+ + n\omega d_{im}^+ x_2\right)e^{n\omega x_2}\dfrac{\sin(n\omega x_1)}{n\pi\Delta} \end{array} \right]$$

$$u_2^+ = \sum_{n=-\infty}^{\infty} \left[\begin{array}{l} b_1\left(a_{im}^+ + n\omega x_2 + 3 - 4v^+\right)b_{im}^+)e^{-n\omega x_2} + \left(c_{im}^+ - d_{im}^+(-n\omega x_2 + 3 - 4v^+)\right)e^{n\omega x_2}\dfrac{\cos(n\omega x_1)}{n\pi\Delta} - \\ b_2\left(a_{re}^+ + n\omega x_2 + 3 - 4v^+\right)b_{re}^+)e^{-n\omega x_2} + \left(c_{re}^+ + d_{re}^+(-n\omega x_2 + 3 - 4v^+)\right)e^{n\omega x_2}\dfrac{\sin(n\omega x_1)}{n\pi\Delta} \end{array} \right]$$

$$u_3^+ = -\frac{b_3}{\pi}\sum_{n=-\infty}^{\infty} \left[\left(f_{im}^+ e^{n\omega x_2} + e_{im}^+ e^{-n\omega x_2}\right)\frac{\sin(n\omega x_1)}{nv}\right]$$

$$u_1^- = \sum_{n=-\infty}^{\infty} \left[\begin{array}{l} b_2\left(a_{re}^- + n\omega b_{re}^- x_2\right)e^{-n\omega x_2} + \left(c_{re}^- + n\omega d_{re}^- x_2\right)e^{n\omega x_2}\dfrac{\cos(n\omega x_1)}{n\pi\Delta} - b_1\left(a_{im}^- + n\omega b_{im}^- x_2\right)e^{-n\omega x_2} \\ +\left(c_{im}^- + n\omega d_{im}^- x_2\right)e^{n\omega x_2}\dfrac{\sin(n\omega x_1)}{n\pi\Delta} \end{array} \right]$$

$$u_2^- = \sum_{n=-\infty}^{\infty} \left[\begin{array}{l} b_1\left(a_{im}^- + n\omega x_2 + 3 - 4v^+\right)b_{im}^+)e^{-n\omega x_2} - \left(c_{im}^- - d_{im}^-(-n\omega x_2 + 3 - 4v^-)\right)e^{n\omega x_2}\dfrac{\cos(n\omega x_1)}{n\pi\Delta} - \\ b_2\left(a_{re}^- + n\omega x_2 + 3 - 4v^-\right)b_{re}^-)e^{-n\omega x_2} + \left(c_{re}^- + d_{re}^-(-n\omega x_2 + 3 - 4v^-)\right)e^{n\omega x_2}\dfrac{\sin(n\omega x_1)}{n\pi\Delta} \end{array} \right]$$

$$u_3^- = -\frac{b_3}{\pi}\sum_{n=-\infty}^{\infty} \left[\left(f_{im}^- e^{n\omega x_2} + e_{im}^- e^{-n\omega x_2}\right)\frac{\sin(n\omega x_1)}{nv}\right]$$

The explicit expressions of the stress field for the two media are:

$$\sigma_{11}^+ = 2\omega\mu^+ \sum_{n=-\infty}^{\infty} \left[\begin{array}{l} b_1\{\left(a_{im}^+ - b_{im}^+(n\omega x_2 - v^+)\right)e^{-n\omega x_2} + \left(c_{im}^+ + d_{im}^+(n\omega x_2 + v^+)\right)e^{n\omega x_2}\}\dfrac{\cos(n\omega x_1)}{n\pi\Delta} \\ -b_2\{\left(a_{re}^+ - b_{re}^+(n\omega x_2 - 2v^+)\right)e^{-n\omega x_2} + \left(c_{re}^+ + d_{re}^+(n\omega x_2 + 2v^+)\right)e^{n\omega x_2}\}\dfrac{\sin(n\omega x_1)}{n\pi\Delta} \end{array} \right]$$

$$\sigma_{22}^+ = 2\omega\mu^+ \sum_{n=-\infty}^{\infty} \left[\begin{array}{l} b_1\{\left(a_{im}^+ + b_{im}^+(n\omega x_2 + 2 - 2v^+)\right)e^{-n\omega x_2} + \left(c_{im}^+ + d_{im}^+(n\omega x_2 + 2 + 2v^+)\right)e^{n\omega x_2}\}\dfrac{\cos(n\omega x_1)}{n\pi\Delta} \\ -b_2\{\left(a_{re}^+ - b_{re}^+(n\omega x_2 - 2v^+)\right)e^{-n\omega x_2} + \left(c_{re}^+ + d_{re}^+(n\omega x_2 - 2 + 2v^+)\right)e^{n\omega x_2}\}\dfrac{\sin(n\omega x_1)}{n\pi\Delta} \end{array} \right]$$

$$\sigma_{21}^+ = 2\omega\mu^+ \sum_{n=-\infty}^{\infty} \left[\begin{array}{l} b_2\{\left(-a_{re}^+ - b_{re}^+(n\omega x_2 + 1 - 2v^+)\right)e^{-n\omega x_2} + \left(c_{re}^+ + d_{re}^+(n\omega x_2 + 1 + 2v^+)\right)e^{n\omega x_2}\}\dfrac{\cos(n\omega x_1)}{n\Delta} \\ -b_1\{\left(a_{im}^+ - b_{im}^+(n\omega x_2 + 1 - 2v^+)\right)e^{-n\omega x_2} + \left(c_{im}^+ + d_{im}^+(n\omega x_2 - 1 + 2v^+)\right)e^{n\omega x_2}\}\dfrac{\sin(n\omega x_1)}{n\Delta} \end{array} \right]$$

$$\sigma_{23}^{+}=2\omega\mu^{+}\sum_{n=-\infty}^{\infty}\left[b_2\left(f_{re}^{+}e^{-n\omega x_2}-e_{re}^{+}e^{-n\omega x_2}\right)\frac{\cos(n\omega x_1)}{n\Delta}-b_1\left(f_{im}^{+}e^{-n\omega x_2}-e_{im}^{+}e^{-n\omega x_2}\right)\frac{\sin(n\omega x_1)}{n\Delta}\right]$$

$$\sigma_{11}^{-}=2\omega\mu^{-}\sum_{n=-\infty}^{\infty}\begin{bmatrix}b_1\{\left(a_{im}^{-}-b_{im}^{-}(n\omega x_2-v^{-})\right)e^{-n\omega x_2}+\left(c_{im}^{-}+d_{im}^{-}(n\omega x_2+v^{-})\right)e^{n\omega x_2}\}\dfrac{\cos(n\omega x_1)}{n\Delta}\\-b_2\{\left(a_{re}^{-}-b_{re}^{-}(n\omega x_2-2v^{-})\right)e^{-n\omega x_2}+\left(c_{re}^{-}+d_{re}^{-}(n\omega x_2+2v^{-})\right)e^{n\omega x_2}\}\dfrac{\sin(n\omega x_1)}{n\Delta}\end{bmatrix}$$

$$\sigma_{22}^{-}=2\omega\mu^{-}\sum_{n=-\infty}^{\infty}\begin{bmatrix}b_1\{\left(a_{im}^{-}+b_{im}^{-}(n\omega x_2+2-2v^{-})\right)e^{-n\omega x_2}+\left(c_{im}^{-}+d_{im}^{-}(n\omega x_2+2+2v^{-})\right)e^{n\omega x_2}\}\dfrac{\cos(n\omega x_1)}{n\Delta}\\-b_2\{\left(a_{re}^{-}-b_{re}^{-}(n\omega x_2-2v^{-})\right)e^{-n\omega x_2}+\left(c_{re}^{-}+d_{re}^{-}(n\omega x_2-2+2v^{-})\right)e^{n\omega x_2}\}\dfrac{\sin(n\omega x_1)}{n\Delta}\end{bmatrix}$$

$$\sigma_{21}^{-}=2\omega\mu^{-}\sum_{n=-\infty}^{\infty}\begin{bmatrix}b_2\{\left(-a_{re}^{-}-b_{re}^{-}(n\omega x_2+1-2v^{-})\right)e^{-n\omega x_2}+\left(c_{re}^{-}+d_{re}^{-}(n\omega x_2+1+2v^{-})\right)e^{n\omega x_2}\}\dfrac{\cos(n\omega x_1)}{n\Delta}\\-b_1\{\left(a_{im}^{-}-b_{im}^{-}(n\omega x_2+1-2v^{-})\right)e^{-n\omega x_2}+\left(c_{im}^{-}+d_{im}^{-}(n\omega x_2-1+2v^{-})\right)e^{n\omega x_2}\}\dfrac{\sin(n\omega x_1)}{n\Delta}\end{bmatrix}$$

$$\sigma_{23}^{-}=2\omega\mu^{-}\sum_{n=-\infty}^{\infty}\left[b_2\left(f_{re}^{-}e^{-n\omega x_2}-e_{re}^{-}e^{-n\omega x_2}\right)\frac{\cos(n\omega x_1)}{n\Delta}-b_1\left(f_{im}^{-}e^{-n\omega x_2}-e_{im}^{-}e^{-n\omega x_2}\right)\frac{\sin(n\omega x_1)}{n\Delta}\right]$$

2.2 Formulation in the anisotropic case

In the case of anisotropic elasticity and during the epitaxy of two materials, where the two lattice parameters are different, an interface composed of a periodic network of dislocations will appear to relax the constraints of parametric disagreement "misfit dislocations ".

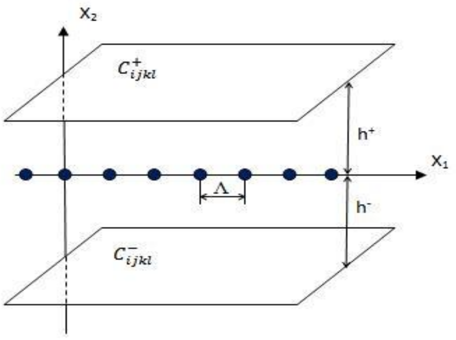


Fig.1
Thin bicrystal strip +/-, with a network of dislocations at the interface, *h* thickness, C^{+}_{ijkl} elastic constants and Λ period.

with the assumption that the interface is plane and the displacement field is periodic (period Λ). The linearity of the relative displacement can be described by the following expression:

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

As the relative displacement $u_k\,(x_1)$ is periodic along ox_3, it can be developed as Fourier series:

$$\Delta u_k\,(x_1)=\sum_{n=1}^{+\infty}\left(\frac{-b_k}{\pi n}\right)\sin(2i\,\pi gnp_\alpha x_1)$$

This displacement field can be written as:

$$u_k = \sum_{n \neq 0} U_k^n(x_2) \exp\left(\frac{2\pi n x_1}{\Lambda}\right)$$

u_k must satisfy the generalized Hooke's law, linking stresses and strains $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$,$U_k^n(x_2)$ is written as follows:

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

where X_α^n and Y_α^n represent complex constants which will be determined using the boundary conditions related to the problem [14].

For more numerical performance, it is convenient to write the equation of the field of displacements in a form where the summation takes only into account the positive values of the integer *n* which can be written as [15]:

$$\begin{aligned} u_k = \sum_{n \succ 1} \left(\frac{1}{\pi n}\right) \sum_{\alpha=1}^{3} [\{\cos[n\omega(x_1 + r_\alpha x_2)].\mathrm{Re}[(-iX_\alpha^n \lambda_{\alpha k})\exp(-n\omega s_\alpha x_2) + (-iY_\alpha^n \bar{\lambda}_{\alpha k})\exp(n\omega s_\alpha x_2)]\} \\ + \sin[n\omega(x_1 + r_\alpha x_2)].\mathrm{Re}[(X_\alpha^n \lambda_{\alpha k})\exp(-n\omega s_\alpha x_2) + (Y_\alpha^n \bar{\lambda}_{\alpha k})\exp(n\omega s_\alpha x_2)]\} \qquad k = 1,2,3 \end{aligned}$$

In the same way for the stress field, we have:

$$\begin{aligned} \sigma_{ij} = 2g \sum_{n \succ 0} \sum_{\alpha=1}^{3} [\{\cos[n\omega(x_1 + r_\alpha x_2)] + \mathrm{Re}[(X_\alpha^n L_{\alpha ij})\exp(-n\omega s_\alpha x_2) + (Y_\alpha^n \bar{L}_{\alpha ij})\exp(n\omega s_\alpha x_2)]\} \\ + \sin[n\omega(x_1 + r_\alpha x_2)] + \mathrm{Re}[(iX_\alpha^n L_{\alpha ij})\exp(-n\omega s_\alpha x_2) + (iY_\alpha^n \bar{L}_{\alpha ij})\exp(n\omega s_\alpha x_2)]\} \end{aligned}$$

with $L_{\alpha ij} = \lambda_{\alpha j}[C_{klj1} + p_\alpha C_{klj2}],\ i,j = 1,2,3\ et\ 1 = 1,2$

3 DESCRIPTION OF THE PROBLEM AND BASIC FORMULATION

Fig. 2. Shows the Misfit for a layer-to-layer heterostructure.

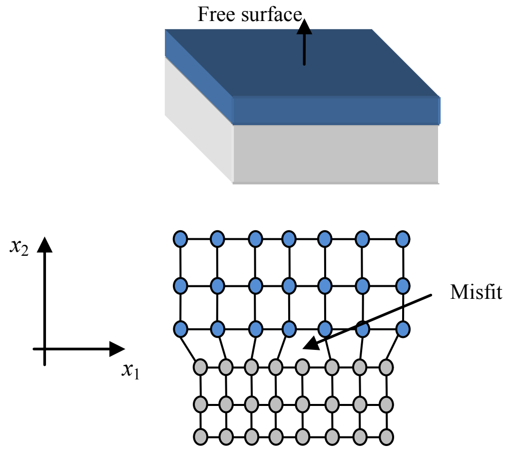


Fig.2
Geometry of the thin bimetal InAs / (001) GaAs with a dislocation network at the interface $x_2 = 0$.

4 InAs / (001) GaAs SYSTEM

Epitaxy of thin films of InAs on GaAs is possible. Thin epitaxial films have a good interface quality.

Table 1
General characteristics of InAs/GaAs isotropic bicrystals [16, 17].

Settings	InAs	GaAs
a	0.6058	0.56533
v	0.30	0.25
μ	29.18	46.27
b	0.41405	
p	5.984	

Table 2
General characteristics of InAs/GaAs anisotropic bicrystals [17, 18].

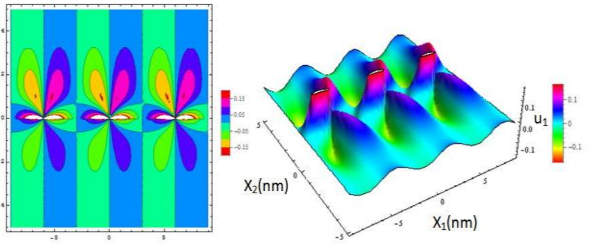
Settings	InAs	GaAs
a	0.6058	0.56533
C_{22}	86.5	118
C_{22}	48.5	53.5
C_{22}	39.6	59.4
b	0.41405	
p	5.984	

The relative elasticity constants $\boldsymbol{C_{ij}}$ for each crystal are taken in the reference Cartesian frame $Ox_1x_2x_3$. The unidirectional network is studied by considering that the dislocations are distributed on both sides of the origin O of the Cartesian coordinate system $Ox_1x_2x_3$, knowing that a dislocation is located at the origin of the axes. The Burgers vector $\boldsymbol{b}$ is oriented parallel to the Ox_1 axis. The deposited layer of the InAs single crystal is chosen on the positive side while the GaAs is chosen on the negative side and therefore represents a substrate.

5 RESULTS AND DISCUSSION

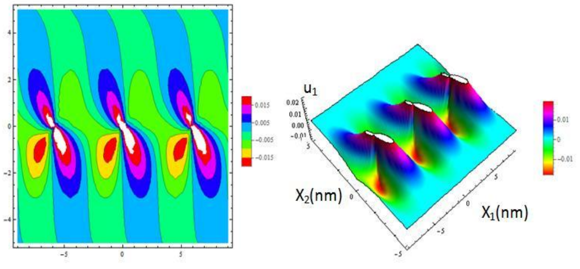
5.1 Displacement fields iso values

We illustrated displacement fields' iso values around dislocations belonging to the unidirectional network in the isotropic and anisotropic elasticity cases.



(2D) (3D)

Fig.3
Iso values of the displacement fields u_1 of the InAs / (001) GaAs bicystals induced by a network of interfacial dislocations where $\boldsymbol{b}$ // Ox_1; isotropic case.



(2D) (3D)

Fig.4
Iso values of the displacement fields u_1 of the InAs / (001) GaAs bicystals induced by a network of interfacial dislocations where $\boldsymbol{b}$ // Ox_1; anisotropic case.

The contrast of the heterogeneous system (Fig. 3 and Fig. 4) indicates values varying from -0.15*nm* up to +0.15*nm*. These results provide information on the heterogeneity effect, which will be visible in the representation of the stress distribution. For the 5*nm* thick deposited InAs layer, the result appears as an ascending ripple mechanism along Ox_1. Already described in the literature as a 3D growth mode specific to InGaAs layers which is in accordance with the behavior of Fourier series. In the anisotropic case, the contrast indicates for the heterogeneous system, values varying from -0.015 *nm* up to +0.015 *nm*. The 3D representation of the displacement fields in both isotropic and anisotropic elasticity cases indicates that the deposited layer is in tension while the substrate is in compression. These calculations show in particular the fields' displacement extrema. We also notice that the symmetry of the displacement fields respects the linear symmetry of the dislocation network.

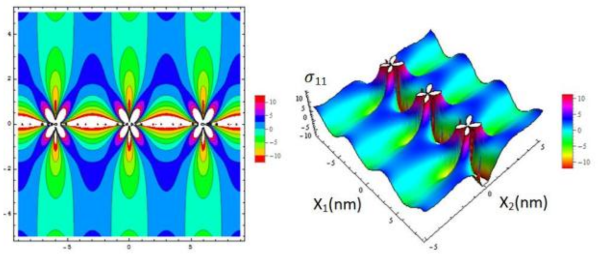
The theoretical method of development by Fourier series for the case of the heterojunction InAs / (001) GaAs a clear difference between anisotropy and isotropy was detected knowing that the single crystals of InAs and GaAs are very anisotropic. Their respective Zener factors are $A = 2.084$ for InAs and $A = 1.82$ for GaAs calculated by the following expression:

$$A = \frac{2C_{44}}{C_{11} - C_{12}}$$

The applied elastic field is felt differently in the two cases due to the effect of anisotropy.

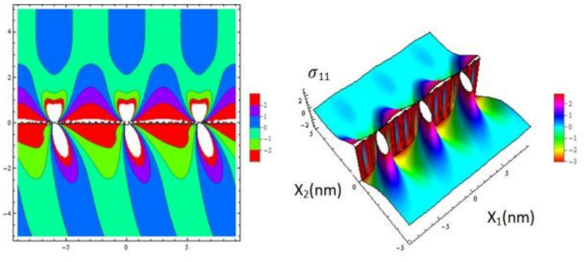
5.2 Stress fields iso values

The stress distributions are shown in Fig. 5-8 for a thin bimetal InAs/(001) GaAs and for two dislocations with a Burgers vector $\boldsymbol{b} = 0.41405$ *nm* parallel to Ox_1.



(2D) (3D)

Fig.5
Iso-stresses σ_{11} of the InAs / (001) GaAs bicystals induced by a network of interfacial dislocations where $\boldsymbol{b}$ // Ox_1; isotropic case.



(2D) (3D)

Fig.6
Iso-stresses σ_{11} of the InAs / (001) GaAs bicystals induced by a network of interfacial dislocations where $\boldsymbol{b}$ // Ox_1; anisotropic case.

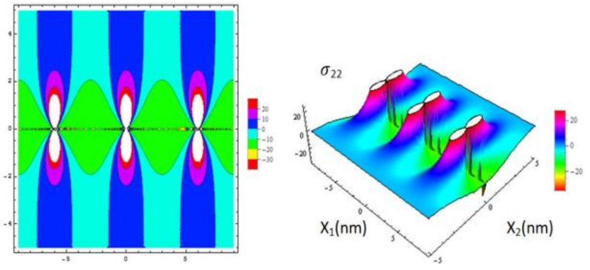
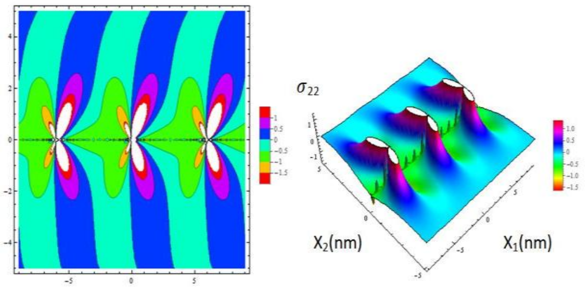


Fig.7
Iso-stresses σ_{22} of the InAs / (001) GaAs bicystals induced by a network of interfacial dislocations where $\boldsymbol{b}$ // Ox_1; isotropic case.

(2D) (3D)



(2D) (3D)

Fig.8
Iso-stresses σ$_{22}$ of the InAs / (001) GaAs bicystals induced by a network of interfacial dislocations where ***b*** // *Ox*$_1$; anisotropic case.

The iso- stresses σ_{11} correspond to -10 *GPa* up to +10 *GPa* for the isotopic case (Fig. 5) and from -3 *GPa* up to +3 *GPa* in the anisotropic case (Fig. 6). For the iso-stresses σ_{22} correspond to -30 *GPa* up to +30 *GPa* for the isotopic case (Fig. 7) and from -1.5 *GPa* up to +1.5 *GPa* in the anisotropic case (Fig. 8). We notice positive peaks and negative peaks which mean that there is a positive tensile stress in the first case, and conversely, we are in compression if the stress is negative.

6 CONCLUSION

Determining the elastic field's effect of nanometric materials is important in both experimental applications and theoretical modeling. In this context we solved the problem of a thin system composed of InAs / GaAs semiconductors in the cases of isotropic and anisotropic elasticity. We analyzed the results contrast for different parameters. We analyzed the contrast of the results for different parameters like the deposited layer thickness, the burger vector orientation and the network dislocation in order to apprehend the tensile and compressive stresses relaxation.

The iso value results of the displacement fields around the dislocations belonging to the unidirectional network provide information on the heterogeneity effect. The curves symmetry with respect to the x_2 axis is very visible, because of the dislocation network periodicity which reflects the behavior of the Fouries series. For the anisotropic case, the contrast indicates for the heterogeneous system values varying from -0.015 *nm* up to +0.015 *nm*. The displacement fields in both isotropic and anisotropic elasticity indicate that the deposited layer is in tension while the substrate is in compression. The iso stress results show positive and negative peaks, it means that there is a positive tensile stress in the first case, and conversely, we have a compression if the stress is negative.

REFERENCES

[1] Makhloufi R., Brioua M., Benbouta R., 2016, The effect of the elastic fields caused by a networks of dislocations placed at interfaces of a three-layer material Cu/Cu/(001) Fe in the case of anisotropic elasticity, *Arabian Journal for Science and Engineering* **41**(5): 1955-1960.

[2] Boussaha A., Makhloufi R., Madani S., 2019, Displacement fields influence analysis caused by dislocation networks at a three layer system interfaces on the surface topology, *Journal of Solid Mechanics* **11**(3): 606-614.

[3] Belk J.G., McConville C.F., Sudijono J.L., Jones T.S., Joyce B.A., 1997, Surface alloying at InAs/GaAs interfaces grown on (001) surfaces by molecular beam epitaxy, *Surface Science* **387**(1-3): 213-226.

[4] Youssef S.B., Fnaiech M., Chen F.R., Loubradou M., Bonnet R., 1999, Electron microscopy of nanoledges at the (001) InAs/(001) GaAs interface for an approximate orientation relationship, *Physica Status Solidi (a)* **174**(2): 403-411.

[5] Yonemoto K., Akiyama T., Pradipto A.M., Nakamura K., Ito T., 2020, Ab initio study for adsorption-desorption behavior on InAs wetting layer surface grown on GaAs (001) substrate, *Journal of Crystal Growth* **532**: 125369.

[6] Nakajima K., 1994, Calculation of stresses in strained semiconductor layers, *Materials Research Society Symposium Proceedings* **338**: 149-160.

[7] Derardja A., Adami L., Youssef S., Bonnet R., 2004, Anisotropie de la relaxation elastique d'un reseau biperiodique de dislocations enterrées: theorie et application aux bicristaux de semi-conducteurs, *European Journal of Control* **29**(4):123-132.

[8] Ohtake A., Mano T., Sakuma Y., 2020, Strain relaxation in InAs heteroepitaxy on lattice-mismatched substrates, *Scientific Reports* **10**(1): 1-7.

[9] Leonard D., Pond K., Petroff P.M., 1994, Critical layer thickness for self-assembled InAs islands on GaAs, *Physical Review B* **50**(16): 11687.

[10] Zribi J., 2014, *Croissance et Caractérisation des Boîtes Quantiques InAs/GaAs Pour des Applications Photovoltaïques*, Thèse Présentée au Département de Physique en vue de l'Obtention du Grade de Docteur ès Sciences, Université de Sherbrooke.

[11] Eiwwongcharoen W., Nakareseisoon N., Thainoi S., Panyakeow S., Kanjanachuchai S., 2016, Ultrathin epitaxial InAs layer relaxation on cross-hatch stress fields, *CrystEngComm* **18**(31): 5852-5859.

[12] Bonnet R., 1981, Periodic displacement and stress fields near a phase boundary in the isotropic elasticity theory, *Philosophical Magazine A* **43**: 1165 -1187.

[13] Eshelby J.D., Read W.T., Shockley W., 1953, Anisotropic elasticity with applications to dislocation theory, *Acta Materialia* **1**: 251-259.

[14] Bonnet R., 1981, Periodic displacement and stress fields near a phase boundary in the isotropic elasticity theory, *Philosophical Magazine A* **43**(5): 1165-1187.

[15] Bonnet R., Verger-Gaugry J.L., 1992, Couche épitaxique mince sur un substrat semi-infini: rôle du désaccord paramétrique et de l'épaisseur sur les distortions élastiques, *Philosophical Magazine A* **66**(5): 849-871.

[16] Bonnet R., Morton A.J., 1987, Contraste en M.E.T. I deux ondes d'une dislocation rectiligne parallèle à la surface libre d'un cristal anisotrope, *Philosophical Magazine A* **56**: 815-830.

[17] Nye J. F., 1969, *Physical Properties of Crystals*, Clarendon Press (Oxford).

[18] Chami A.C., 1988, *Contraintes et Relaxation des Couches de Semi-Conducteurs*, Etude Par Canalisation, Thèse de Doctorat, Université d'Alger.