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Research Paper

Modeling at The Nanometric Scale of Interfacial Defects of A Semiconductor Heterostructure in The Isotropic And Anisotropic Cases For The Study of The Influence of Stresses

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ABSTRACT

This work aims to determine the effect of stresses caused by dislocation networks placed at the interface of a semiconductor heterostructure of the thin GaAs/Si system. In this case, we use a mathematical modeling by Fourier series expansion to numerically simulate the stresses for the two cases of isotropic and anisotropic elasticity in order to predict the mechanical behavior of the heterostructure in the presence of interfacial dislocations while respecting well-defined stress boundary conditions. The elastic stress relaxation is reached for a layer thickness threshold of the GaAs deposit on the Si substrate not exceeding 5 nm.

Keywords: Nanometric; Heterostructure; GaAs/Si; Isotropic; Anisotropic; Elastic fields.

1 INTRODUCTION

THE evaluation of elastic fields generated by dislocation networks in semiconductor heterostructures has become essential. To design and manufacture better semiconductors, the electronics industry uses heterostructures with greater reliability in their various properties. Among the heterostructures which have been the object of study of the mechanical behavior of thin films of nanometric thickness deposited on a substrate to solve the problems of the constraints observed in the manufacture of components used in microelectronics, mention may be made of semiconductor heterostructures GaAs/Si and InAs/GaAs which are very interesting in research for their physical and optoelectronic properties [1].

Nakajima [2] calculated for the GaAs/Si heterostructure by proposing a theoretical model while considering that the interface is coherent between the thin layers.

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Mao et al. [3] treated the effect of dislocations on the deformation of GaAs/Si samples by varying the thickness deposited by means of Raman scattering and hall measurement at different temperatures.

Ünlü [4] to model semiconductor heterostructures at the microscopic and nanometric scale to assess the effect of deformation on electronic and optical properties using GaAs/Si (001) as a model.

Makhloufi et al. [5] studied the possibility of epitaxy of thin layers of InAs on GaAs.

Boussaha et al. [6] determined the fields of the displacements as well as the iso values for an anisotropic three-layer CdTe/GaAs/GaAs(001) material under the effect of two dislocation networks placed at the interfaces.

Vincent [7] presented a development of theoretical models and numerical methods for the study at the nanometric scale of plastic deformation assisted by dislocations and by grain boundary type interfaces.

An isotropic domain calculation of the stress fields, for which analytical expressions have already been proposed by Gutkin and al. [8] for the case of the InAs / (001) GaAs system.

Our study is reserved for the GaAs/Si heterostructure in order to determine the effect of tensile and compressive stresses on its mechanical behavior.

Kim et al. [10] considered in their study the potential effect for GaAs/Si tandem cells showed a 1.28 V open circuit voltage.

Lovegine et al. [11] studied the integration of III.V GaAs semiconductors on Si for the fabrication of tandem solar cells obtained by the ether oepitaxy mode of GaAS on Si.

The integration of GaAs on Si without defects is one of the challenges for researchers in order to have an association with a very good quality interface unlike the interface of the InAs/GaAs system [5] and to combine the many advantages of Si, with the high mobility and direct gap properties of GaAs, to increase the speed of processors, to add new optical functionalities in microsystems, but also to produce photovoltaic cells with high efficiency and low cost.

2 GEOMETRY OF PROBLEM

The geometry of the problem represented in figure 1 below, shows the unidirectional network of dislocations generated between the layers of the GaAs/Si heterostructure.

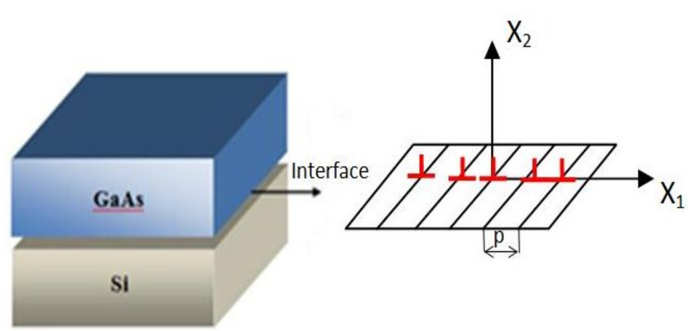

Fig. 1

Geometry of the thin GaAs/Si bicrystal: 1/g is the period. The crystal stiffness's are C^{+}_{ijkl} and C^{-}_{ijkl}, with thicknesses h^{+} and h^{-}.

In the isotropic case, the classical differential equation of elasticity is written [9]:

$$(\lambda+\mu)u_{i,ik}+\mu u_{k,ii}=0 \quad (1)$$

λ and μ are the Lamé coefficients of the deformed medium.

The deformation is assumed to be plane and periodic along the Ox_1 axis. The expression of the stress field in the case of plane strain is:

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

After elimination of the parameter λ, using the classical relation (Hirth and Loth):

$$\lambda + 2\mu = 2\mu \frac{1-\upsilon}{1-2\upsilon} \tag{3}$$

With the Poisson's ratio υ.

The stress equations necessary for the calculations are:

$$\sigma_{21} = \mu(u_{1,2} + u_{2,1}) \tag{4}$$

$$\sigma_{22} = \frac{2\mu}{1-2\mu}\left[(1-\mu)u_{2,2} + \nu(u_{1,1} + u_{3,3})\right] \tag{5}$$

$$\sigma_{23} = \mu(u_{2,3} + u_{3,2}) \tag{6}$$

In the anisotropic case we must switch from the starting system to the working system by the passage matrix a_{ij}:

$$a_{ij}=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

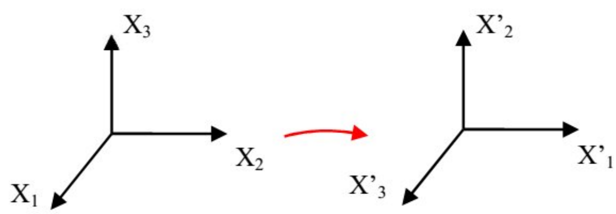

Fig. 2

Diagram of the two starting and working markers.

a_{ij} is the matrix which allows the transition from the starting frame to the working frame.

The matrix of the elastic constants C_{ij} for an anisotropic material having 36 elements in the reference of the crystal is written:

$$C_{ij}=\begin{pmatrix} C_{11} & \ldots\ldots & C_{16} \\ \cdot & \cdot & \cdot \\ C_{61} & \ldots\ldots & C_{66} \end{pmatrix}$$

The matrix Cij is symmetric; therefore, the linear behavior of a material is then described in the general case by 21 independent coefficients.

After transformation, one obtains the matrix of the elastic constants C'_{ij} in the work reference:

$$C'_{ij} = T^{T}.C_{ij}.T \tag{7}$$

"T" is a (6x6) matrix obtained after transformation of the passage matrix aij

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

And:

$$T^T = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

3 EXPRESSION OF STRESSES AND BOUNDARY CONDITIONS

The mathematical formulation that deals with the anisotropic case is different from the isotropic case, we must consider that the two media are supposed to obey the general Hooke's law:

$$\sigma_{ij} = C_{ijkl}\,\varepsilon_{kl} \tag{8}$$

Ou :

$$\varepsilon_{kl} = \frac{1}{2}\left(u_{k,l} + u_{l,k}\right) \quad (i, j, k, l = 1,2,3) \tag{9}$$

After substituting (9) for (8), we get:

$$\sigma_{ij} = \frac{1}{2}(C_{ijkl}\,u_{k,l}) + \frac{1}{2}(C_{ijkl}\,u_{l,k}) \tag{10}$$

Since the dumb indices *k* and *l* will take the same values, therefore the two terms $\frac{1}{2}(C_{ijkl}\,u_{k,l})$ and $\frac{1}{2}(C_{ijkl}\,u_{l,k})$ are equal. We obtain:

$$\sigma_{ij} = C_{ijkl}\,u_{k,l} \tag{11}$$

The state of equilibrium of the stresses in the region of the distortions is written:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{12}$$

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} = 0 \tag{13}$$

This field of displacements can be written in this form:

$$u_k = \sum_{n\neq 0} U_k^n(x_2)\,exp\left(\frac{2\pi n x_1}{\Lambda}\right) \tag{14}$$

u_k must satisfy Hooke's generalized law, linking stresses and deformations:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \tag{15}$$

$U_k^n(x_2)$ can be written as follows:

$$U_k^n(x_2) = \sum_{\alpha=1}^{3}\frac{X_\alpha^n \lambda_{\alpha k}}{2i\pi n}\exp(2i\pi g n p_\alpha x_2) + \sum_{\alpha=1}^{3}\frac{Y_\alpha^n \bar{\lambda}_{\alpha k}}{2i\pi n}\exp(2i\pi g n \bar{p}_\alpha x_2) \tag{16}$$

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

So, by substituting (16) in (14) we have the equation of the field of displacements

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

(17)

By deriving the field from displacement, we get the stress field and the fact that a periodic series of intrinsic dislocations produces in each medium a stress field σ_{ij} whose components can be developed in Fourier series which is written:

$$\sigma_{ij=}2g\sum_{n>0}\sum_{\alpha=1}^{3}[\{\cos\,[n\omega(x_1+r_\alpha x_2)]+ \mathrm{Re}\left[(X_\alpha^n L_{\alpha ij})\exp(-n\omega s_\alpha x_2)+(Y_\alpha^n\bar{L}_{\alpha ij})exp(n\omega s_\alpha x_2)\right]\}+\sin[n\omega(x_1+r_\alpha x_2)]+ \mathrm{Re}\left[(\mathrm{i}X_\alpha^n L_{\alpha ij})\exp(-n\omega s_\alpha x_2)+(\mathrm{i}Y_\alpha^n\bar{L}_{\alpha ij})\exp(n\omega s_\alpha x_2)\right]\}$$

$$\text{with}\quad L_{\alpha ij}=\lambda_{ij}\left[C_{klj1}+p_\alpha C_{klj2}\right]\qquad i,j=1,2,3\ \text{et}\ l=1,2 \tag{18}$$

g: network period
n: harmonic number
x_1: the periodicity axis
x_2: the axis of heteroepitaxy

$$\omega=\frac{2\pi}{g}$$

$$p_\alpha=r_\alpha+is_\alpha$$

$p_\alpha=r_\alpha+is_\alpha$ Represent the complex roots where:
r_α Real part of p_α
s_α: imaginary part of p_α

$$\sigma_{ij}=C_{ijkl}\varepsilon_{kl}$$

where C_{ijkl} is a fourth order tensor. To pass to a second order tensor we use the simplified notation of Voigt:

$$\sigma_m=C_{mn}\varepsilon_n \tag{19}$$

X_α^n Complex constants which represent the solutions of the fields of displacements and stresses
Y_α^n: Complex constants which represent the solutions of the fields of displacements and stresses
$L_{\alpha ij}$: Complex constants
$\overline{L_{\alpha ij}}$ conjugate of $L_{\alpha ij}$
λ_{ij}: Complex constants

The determination of the complex constants X_α^n and Y_α^n ($\alpha=1,2$ et 3) for the positive layer deposited on the negative layer representing the substrate is done by applying the boundary conditions (Fig. 3) to the field suitable constraints which are:

- The continuity of the normal stresses at the interface:

$$\left[\sigma_{2k}^{+}\right]_{x_2=0}=\left[\sigma_{2k}^{-}\right]_{x_2=0}\qquad k=1,2\text{ and }3 \tag{20}$$

- The free surfaces of the bimetallic thin strip being in equilibrium:

$$\left[\sigma_{2k}^{+}\right]_{x_2=h^+}=0\quad\text{and}\quad\left[\sigma_{2k}^{-}\right]_{x_2=-h^-}=0\qquad k=1,2\text{ and }3 \tag{21}$$

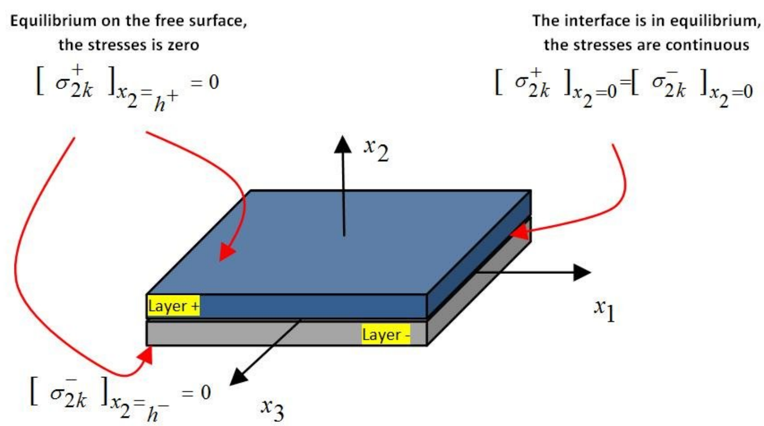

Fig. 3
Boundary conditions in the stress field.

4 APPLICATIONS AND RESULTS

4.1 GaAs/(001)Si system

In this work we have chosen the materials Gallium Arsenide (GaAs) and Silicon (Si) which are the subject of several studies in the field of optoelectronics.

Table1
Parameters of GaAs/ Si materials [12,13]

Parameters	**GaAs**	**Si**
Lattice parameters a(nm)	0.56533	0.5428
ν	0.25	0.23
μ (Gpa)	46.27	66.28
Burgers vector b (nm)	0.3838	0.3997
Burgers vector of network b (nm)	0.3917	
Period of dislocation network g (nm)	9.7	
ω	0.65	
Anisotropic elastic constants C_{ij} (Gpa)	C_{11} = 118 C_{12} = 53.5 C_{44} = 59.4	C_{11} = 165.7 C_{12} = 63.9 C_{44} = 79.6

We take : $\omega = \frac{2\pi}{g}$

In the following, we present the results of the stress simulation in the upper free layer of the GaAs/Si heterostructure in both isotropic and anisotropic cases.

4.2 Isotropic GaAs/Si case

Figures 4, 5, 6 and 7 illustrate, in the isotropic elastic case, the iso- constraints curves of a network of edge dislocations located at the interface of two GaAs and Si facets.

The representation of the iso- constraints σ_{11} and σ_{22} in 2D and 3D varying between 5 Mpa and 10 Mpa clearly shows the importance of the deformation around the dislocation along the X_2 axis for a total thickness of the heterostructure of 10 nm and a vector of burgers b = 0.3917 nm oriented along the direction of periodicity of the X_1 dislocations.

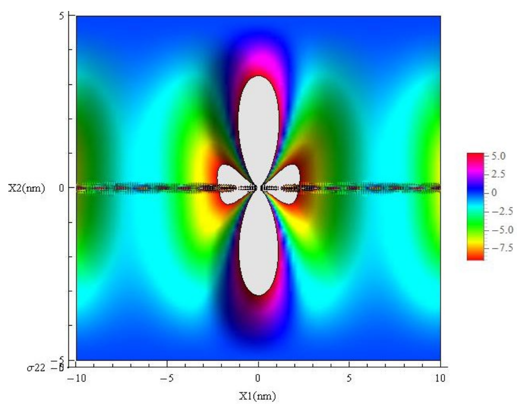

Fig. 4
Iso-constraints σ_{22} in 2D GaAs / (001) Si: isotropic case.

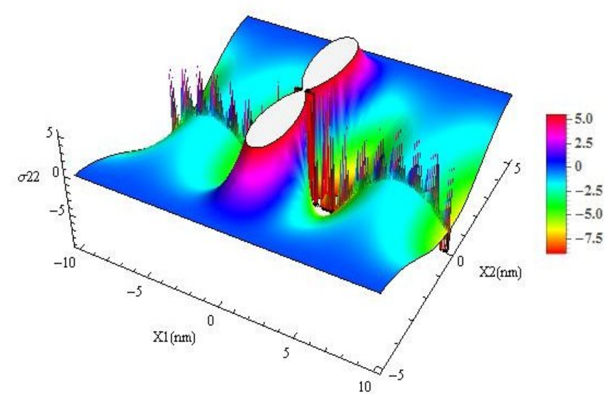

Fig. 5
Iso-constraints σ_{22} in 3D GaAs / (001) Si: isotropic case.

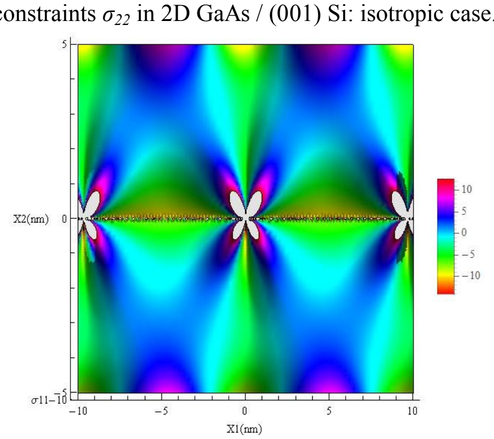

Fig. 6
Iso-constraints σ_{11} in 2D GaAs/(001)Si: isotropic case.

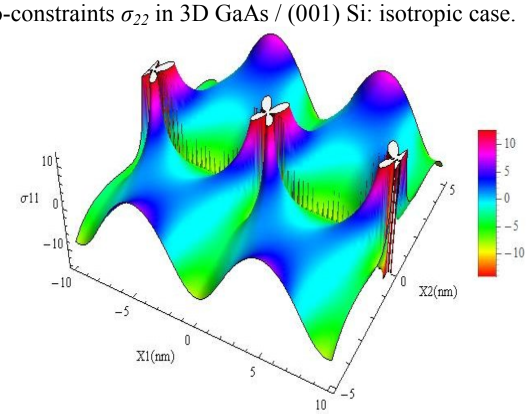

Fig. 7
Iso-constraints σ_{11} in 3D GaAs/(001)Si: isotropic case.

4.3 Anisotropic GaAs/Si case

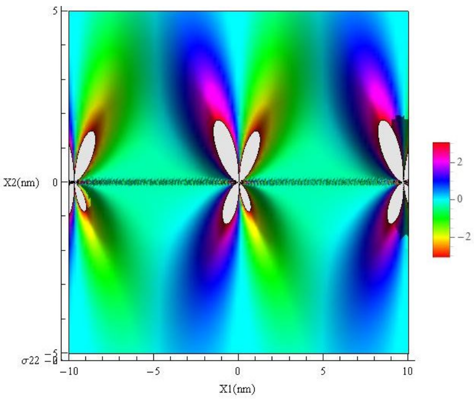

Fig. 8
Iso- constraints σ_{22} in 2D GaAs/(001)Si anisotropic case.

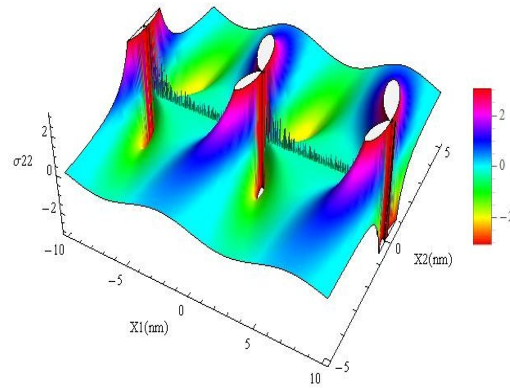

Fig. 9
Iso- constraints σ_{22} in 3D GaAs/(001)Si anisotropic case.

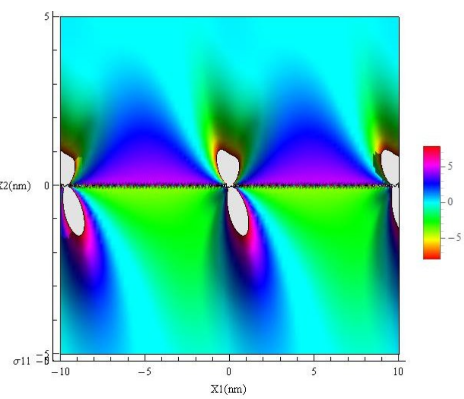

Fig. 10
Iso- constraints σ_{11} in 2D GaAs/(001)Si anisotropic case.

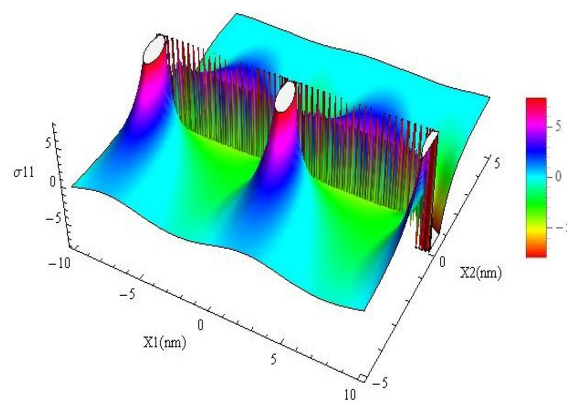

Fig. 11
Iso- constraints σ_{11} in 3D GaAs/(001)Si anisotropic case.

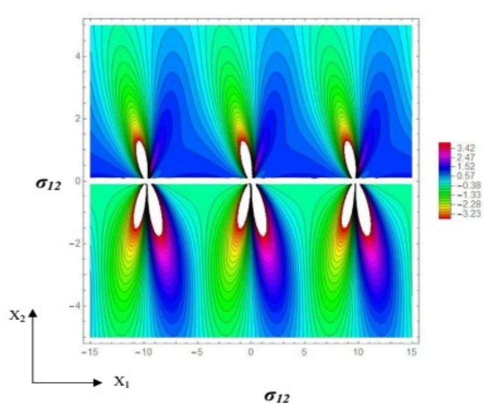

Fig. 12
Iso- constraints σ_{12} in 2D GaAs/(001)Si anisotropic case.

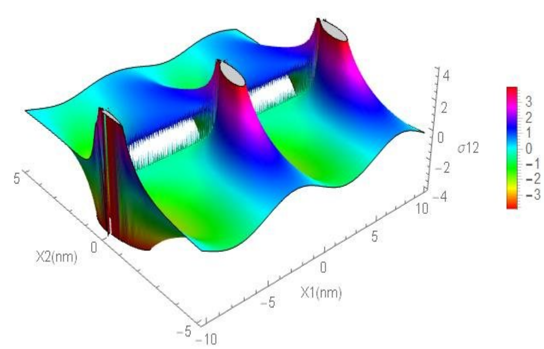

Fig. 13
Iso- constraints σ_{12} in 3D GaAs/(001)Si anisotropic case.

The results obtained from the theory and the simulation calculation shown in figures 8 to 13 in the form of 2D and 3D stress maps are to be understood. The 3D relief of the deformation of the interface between GaAs/(001)Si is due to the unidirectional dislocation network of Misfit which is a function of the deposited thickness for a vector of burgers oriented along Ox_1. The deformation peak is clearly significant in the vicinity of the core of the dislocation which propagates tensile and compressive stresses influencing the mechanical behavior of the heterostructure.

The importance of the elastic quantities on the surface caused by the network of interfacial dislocations causing the phenomenon of undulation represents a determining index on the possibility of using the surface for a possible 3D growth of nanometric layers. This same phenomenon allows an elastic relaxation of the heterostructure being under tensile and compressive stress for a total thickness of 10 nm.

The symmetry of the stress fields in the isotropic case is quite visible contrary to the anisotropic case because of the anisotropy effect.

5 CONCLUSIONS

This work allowed us to examine and simulate, at the nanometric scale, the stress fields generated by unidirectional Misfit dislocation networks in the cases of isotropic and anisotropic elasticity.

After establishing the hypotheses of the chosen model, which is a thin bimetallic strip, representing the GaAs/Si semiconductor heterostructure, and the boundary conditions relating to the problem posed, we obtained results of the stress distribution around a dislocation showing that the deformation is greater near the core of the dislocation.

The importance of the elastic quantities on the surface caused by the network of interfacial dislocations causing the phenomenon of undulation represents a determining index on the possibility of using the surface for a possible 3D growth of nanometric layers. This same phenomenon allows an elastic relaxation of the heterostructure being under tensile and compressive stress for a total thickness of 10 nm.

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