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Displacement Fields Influence Analysis Caused by Dislocation Networks at a Three Layer System Interfaces on the Surface Topology

A. Boussaha *, R. Makhloufi, S. Madani

Laboratory LAMSM, Mechanical Engineering Department, Faculty of Technology, University of Batna 2 Mostafa Ben Boulaid, Batna, Algeria

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ABSTRACT

This work consists in a numerically evaluation of elastic fields distribution, caused by intrinsic dislocation networks placed at a nano metric tri-layers interfaces, in order to estimate their influence on the surface topology during hetero-structure operation. The organization of nanostructures is ensured by the knowledge of different elastic fields caused by buried dislocation networks and calculated in the case of anisotropic elasticity. The influence of elastic fields generated by induced square and parallel dislocation networks at *CdTe* / *GaAs* / (001) *GaAs* tri-layer interfaces was investigated. By deposition, the nanostructures organization with respect to the topology was controlled.

Keywords: Interface; Network; Nano metric; Dislocation; Elastic field; Anisotropic elasticity.

1 INTRODUCTION

IN recent years, the challenge of reducing the size of microelectronics components led to major research efforts on structures synthesis, ranging in size from a few nanometers to a few tenths of nanometers. The components small size induces new properties. For example, the extreme confinement of the charges outside the nanostructures induces new quantum properties interesting for the production of original components and 3D nanostructures of semiconductors could constitute the basic building blocks of future transistors with nano metric dimensions. The smaller their dimensions, the more it will be possible to integrate large number transistors on a single integrated circuit, as to increase the computers calculation power. The *CdTe/GaAs/GaAs* system study will be very interesting to analyze the influence of deposits on grain boundaries (specifically on dislocation networks periodicity) during hetero-epitaxy. For this purpose, a thin bi-crystal strip whose dislocation network is unidirectional, accommodating a parametric mismatch is superposed on a substrate with a dislocations square lattice. Wang et al. [1] treated the displacement and stress fields associated to a bi-periodic misfit dislocation network located along a single interface in a multilayered composite in the case of anisotropic elasticity, relying on the formalism of Stroh using a matrix approach. In the three-layer case, Wang Hu Yi et al. [2] proposed a method based on imaging to solve the problem and they obtained the stress field in the anisotropic case. Makhloufi et al. [3] studied the problem of a

*Corresponding author. Tel.: +213 33812143; Fax: + 213 33812143.
E-mail address: a_boussaha66@yahoo.com (A. Boussaha).

Cu/Cu/(001)Fe three-layer material under the effect of two unidirectional dislocation networks placed at the hetero interface (*Cu*)/(*Cu*) and the hetero interface (*Cu*)/(001)*Fe*. Madani et al. [4] have studied the stress and the necessary stress fields, generated by a square network of screw dislocations located between a *Si* thin layer bonded to a *Si* semi-infinite medium substrate, in anisotropic elasticity. The results obtained are compared with those obtained in isotropic elasticity. Another work by Madani et al. [5], studied the possibility of ordering long-range self-assembled nanostructures on a *GaAs* substrate, by means of elastic fields induced on the surface by periodic dislocation networks not deeply buried. The stress and the necessary stress fields generated by a square network of screw dislocations situated between a *GaAs* thin layer bonded to a *GaAs* semi-infinite medium substrate were calculated using anisotropic elasticity. H.Y.Wang et al. [6], using the image decomposition technique; were able to solve the problem of a mixed dislocation in an anisotropic three-layer. In their analysis of anisotropic nanoparticles deposited on a semi-substrate in the presence of dislocation networks located at the interfaces, Hideo Koguchi et al [7] studied the different interactions on multilayer materials.

In this work, computations were carried out by numerical simulation to determine the fields of the displacements as well as the iso values for an anisotropic three-layer material under the effect of two networks of dislocations placed at the interfaces. The first computation deals with a parallel dislocation network at the first interface between the *CdTe/GaAs* hetero structure, and the second deals with a square dislocation network between the *GaAs/GaAs*. Graphs were drown to analyze the material behavior.

2 PROBLEM EXPOSURE

The problem corresponds to bringing into contact two thin layers; a thin bi-crystal on a semi-infinite medium substrate. This case is illustrated in Fig. 1 where a composite *A/B/C* is schematized in detail and in which *A* and B are two thin layers, and *C* is a semi-infinite medium. The three media are separated by two planar interfaces with two dislocation networks at *CdTe/GaAs* and *GaAs/GaAs* and $1/g$ grating period. The three mediums are elastically anisotropic and characterized by their elastic constants and their thicknesses h^+, h^- and h^*.

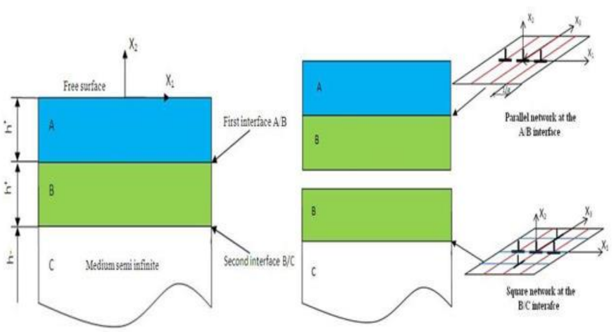

Fig.1
Three-layer material *CdTe/GaAs/GaAs* under the effect of unidirectional and square dislocations networks. $1/g$ is the period.

3 DISPLACEMENTS AND STRESS BOUNDARY CONDITIONS

We must take into consideration conditions at the limits situated at the interfaces of this three-layer material.

The displacement linearity relative to the *CdTe / GaAs* interface of a thin bi-crystal is expressed by: [8]

$$\left[U_k^* - U_k^+\right]_{x_2=h^+} = -\frac{b'_k}{\pi}\sum_{n=1}^{\infty}\left(1/n\right).\sin\left(n.\omega x_1\right) \quad k=1,2,3 \tag{1}$$

(*) Represents the upper layer (*A*) and (+) represents the middle layer (*B*).

The displacement linearity relative to *GaAs/GaAs* interface is expressed by [13]:

$$\left[U_k^+ - U_k^-\right]_{x_2=0} = -\frac{b_k}{\pi}\sum_{n=1}^{\infty}\left(1/n\right).\sin\left(n.\omega x_1\right) \quad k=1,2,3 \qquad \omega = 2\pi g \tag{2}$$

where (+) represents the middle layer (*B*), (-) represents the substrate (*C*) and *b* the Burger's vector.

The continuity of normal stresses at the interface and the balance of the two crystals are defined as following (Fig. 2).

$$\left[\ \sigma_{2k}^{+}\ \right]_{x_2=0}=\left[\ \sigma_{2k}^{-}\ \right]_{x_2=0} \qquad \left[\ \sigma_{2k}^{*}\ \right]_{x_2=h^+}=\left[\ \sigma_{2k}^{+}\ \right]_{x_2=h^+} \tag{3}$$

At the free surface level of the three-layer material in equilibrium, allow to consider that the normal stress is zero at the surface for $x_2=h^*$ (Fig. 2):

$$\left[\ \sigma_{2k}^{*}\ \right]_{x_2=h^*}=0 \tag{4}$$

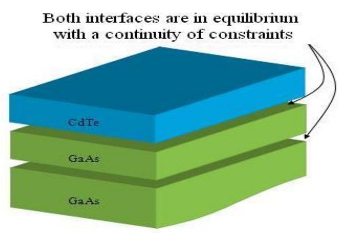

Fig.2
Stress boundary conditions.

4 MATHEMATICAL FORMULATION

4.1 Displacements field

The final expression of the displacement field can be written [9]:

$$\begin{aligned} u_k = & \sum_{n\succ 0}\left(\frac{1}{\pi.n}\right)\sum_{\alpha=1}^{3}[\{\cos[n.\omega(x_1+r_\alpha x_2)].Re[(-i.X_\alpha^{(n)}.\lambda_{\alpha k}).exp(-n.\omega.s_\alpha.x_2)+(-i.Y_\alpha^{(n)}.\bar{\lambda}_{\alpha k}).exp(n.\omega.s_\alpha.x_2)]\} \\ & +\{\sin[n.\omega(x_1+r_\alpha x_2)]\times Re[(X_\alpha^{(n)}.\lambda_{\alpha k}).exp(-n.\omega.s_\alpha.x_2)+(Y_\alpha^{(n)}.\bar{\lambda}_{\alpha k}).exp(n.\omega.s_\alpha.x_2)]\} \\ & \alpha=1,3\ ; \qquad k=1,2,3 \end{aligned} \tag{5}$$

According to the superposition principle [9], the elastic field of a square dislocation network can be solved in a simple way. The family (II) is deduced from the family (I) by a + $\pi/2$ rotation around the Ox_2 axis (Fig. 3).

Then, point $M'(-x_3,x_2,x_1)$ corresponds to point $M(x_1,x_2,x_3)$ and the total displacement field becomes:

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}=\begin{bmatrix} u_1(M)+u_3(M') \\ u_2(M)+u_2(M') \\ u_3(M)-u_1(M') \end{bmatrix} \tag{6}$$

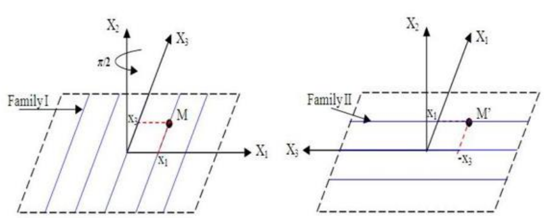

Fig.3
Dislocations parallel networks superposition.

4.2 Stress field

Similarly the final stress field expression can be written:

$$\sigma_{ij} = 2.g\sum_{n\succ 0}\sum_{\alpha=1}^{3}[\{\cos[n.\omega\,(x_1 + r_\alpha x_2)].\mathrm{Re}[X_\alpha^{(n)}.L_{\alpha ij}.\exp(-n.\omega s_\alpha x_2) + Y_\alpha^{(n)}\overline{L}_{\alpha ij}.\exp(n.\omega s_\alpha x_2)\}$$
$$+\{\sin[n.\omega(x_1 + r_\alpha x_2)] + \mathrm{Re}[i\,X_\alpha^{(n)}.L_{\alpha ij}.\exp(-n.\omega s_\alpha x_2) + i\,Y_\alpha^{(n)}.\overline{L}_{\alpha ij}.\exp(n.\omega s_\alpha x_2)\} \qquad (7)$$
$$avec \quad L_{\alpha kl} = \lambda_{\alpha j}\left[C_{klj1} + p_\alpha C_{klj2}\right] \qquad i,j=1,2,3 \quad 1=1,2 \quad \alpha=1,3$$

Similarly, square network total stress field is calculated by:

$$\left[\sigma_{ij}^{(I+II)}(M)\right] = \begin{bmatrix} \sigma_{11}^I(M)+\sigma_{33}^I(M') & \sigma_{12}^I(M)+\sigma_{23}^I(M') & \sigma_{13}^I(M)-\sigma_{13}^I(M') \\ \sigma_{12}^I(M)+\sigma_{23}^I(M') & \sigma_{22}^I(M)+\sigma_{22}^I(M') & \sigma_{23}^I(M)-\sigma_{12}^I(M') \\ \sigma_{13}^I(M)-\sigma_{13}^I(M') & \sigma_{23}^I(M)-\sigma_{12}^I(M') & \sigma_{33}^I(M)+\sigma_{11}^I(M') \end{bmatrix} \qquad (8)$$

5 BOUNDARY CONDITIONS

The complex constants (X_α^*, Y_α^*, X_α^+, Y_α^+ and Y_α^-) are the linear system solutions with 30 real equations obtained by combining the displacements and the stresses expressions with the boundary conditions:

a) The first discontinuity condition for $x_2 = 0$ in displacement at the first interface level *CdTe/GaAs* is expressed as follow:

$$Re\sum_{\alpha=1}^{3} -(X_\alpha^+\lambda_{\alpha k}^+ + Y_\alpha^+\overline{\lambda}_{\alpha k}^+) + Y_\alpha^-\overline{\lambda}_{\alpha k}^- = b_k$$
$$Re\,i\sum_{\alpha=1}^{3} -(X_\alpha^+\lambda_{\alpha k}^+ + Y_\alpha^+\overline{\lambda}_{\alpha k}^+) - Y_\alpha^-\overline{\lambda}_{\alpha k}^- = 0$$

b) The second condition represents the discontinuity for $x_2 = h$ at the second interface between *GaAs/GaAs*:

$$Re\sum_{\alpha=1}^{3} -(X_\alpha^*\lambda_{\alpha k}^* + Y_\alpha^*\overline{\lambda}_{\alpha k}^*) + (X_\alpha^+\lambda_{\alpha k}^+ + Y_\alpha^+\overline{\lambda}_{\alpha k}^+) = b'_k$$
$$Re\,i\sum_{\alpha=1}^{3} (X_\alpha^*\lambda_{\alpha k}^* + Y_\alpha^*\overline{\lambda}_{\alpha k}^*) - (X_\alpha^+\lambda_{\alpha k}^+ + Y_\alpha^+\overline{\lambda}_{\alpha k}^+) = 0$$

c) The third continuity condition for $x_2 = h^+$ at the *GaAs/GaAs* interface:

$$Re\sum_{\alpha=1}^{3} X_\alpha^* L_{\alpha 2k}^* E_1(C_1+iS_1) + (Y_\alpha^*\overline{L}_{\alpha 2k}^* E_2)(C_1+iS_1) -$$
$$(X_\alpha^+ L_{\alpha 2k}^+ E_3)(C_2+iS_2) - (Y_\alpha^+\overline{L}_{\alpha 2k}^+ E_4)(C_2+iS_2) = 0$$
$$Rei\sum_{\alpha=1}^{3} X_\alpha^* L_{\alpha 2k}^* E_1(S_1-iC_1) + (Y_\alpha^*\overline{L}_{\alpha 2k}^* E_2(S_1-iC_1)$$
$$-(X_\alpha^+ L_{\alpha 2k}^+ E_3)(S_2-iC_2) - (Y_\alpha^+\overline{L}_{\alpha 2k}^+ E_4(S_2-iC_2) = 0$$

d) The fourth condition is the stress continuity condition at $x_2 = 0$ at the *CdTe/GaAs* interface:

$$Re\sum_{\alpha=1}^{3} (X_\alpha^+ L_{\alpha 2k}^+ + Y_\alpha^+\overline{L}_{\alpha 2k}^+) - Y_\alpha^-\overline{L}_{\alpha 2k}^- = 0$$

$$Re\, i \sum_{\alpha=1}^{3} -(X_{\alpha}^{+} L_{\alpha 2k}^{+} + Y_{\alpha}^{+} \overline{L}_{\alpha 2k}^{+}) - Y_{\alpha}^{-} \overline{L}_{\alpha 2k}^{-} = 0$$

e) Similarly, the fifth condition concerns the zero normal stress at the free surface for $x_2 = h^*$:

$$Re\, i \sum_{\alpha=1}^{3} (X_{\alpha}^{*} L_{\alpha 2k}^{*} E_5 + Y_{\alpha}^{*} \overline{L}_{\alpha 2k}^{*} E_6)\, EC - (X_{\alpha}^{*} L_{\alpha 2k}^{*} E_5 + Y_{\alpha}^{*} \overline{L}_{\alpha 2k}^{*} E_6)\, ES = 0$$

$$Re \sum_{\alpha=1}^{3} (X_{\alpha}^{*} L_{\alpha 2k}^{*} E_5 + Y_{\alpha}^{*} \overline{L}_{\alpha 2k}^{*} E_6)\, EC + (X_{\alpha}^{*} L_{\alpha 2k}^{*} E_5 + Y_{\alpha}^{*} \overline{L}_{\alpha 2k}^{*} E_6)\, ES = 0$$

After developing these conditions, we get a system of equations, which can be written, in the form of a matrix product:

$$AX = B \tag{9}$$

where the column matrix X (A^+, A^-, B^+, B^-, C^+, C^-, D^+ and D^-) contains unknown complex, the system is solved numerically using an analytical approach based on double Fourier series [10].

To illustrate the internal elastic fields of the three-layer material, a numerical application was studied on *CdTe/GaAs/GaAs* epitaxial system.

6 APPLICATIONS AND FINAL RESULTS

Table 1., shows the materials (*CdTe*) and (*GaAs*) characteristics [9, 11 and 12].

Burgers vector and the network period are calculated by the following expressions [13]:

$$b = \frac{a_{CdTe} + a_{GaAs}}{2\sqrt{2}} \qquad \Lambda = \frac{a_{CdTe}\, a_{GaAs}}{\left(a_{CdTe} - a_{GaAs}\right)\sqrt{2}}$$

The parametric disagreement is given by:

$$\varepsilon = 2\frac{\left|a_{CdTe} - a_{GaAs}\right|}{a_{CdTe} + a_{GaAs}} = 18.81\%$$

In 1994, R.Bonnet and M.Loubradou [14] proposed a so-called "continuous" approach, to describe the atomic positions around misfit dislocations present along a plane interface between two anisotropic heterogeneous mediums. This approach application for the heterojunction (001)*CdTe*/(001)*GaAs* shows that the results are very close to M.E.T.H.R images.

Table 1
CdTe and *GaAs* crystalline parameters.

Designation	*CdTe*	*GaAs*
Lattice parameters a (*nm*)	0.4681	0.56533
Elastic constants C_{ij} (*Gpa*)	$C_{11} = 53.5$ $C_{12} = 36.9$ $C_{44} = 20.2$	$C_{11} = 118$ $C_{12} = 53.5$ $C_{44} = 59.4$
Burgers vector b (*nm*)	0.3997	
Period Λ (*nm*)	25	

6.1 Relative interfacial displacement for the CdTe / GaAs interface

Fig. 4 shows that the linear relative interfacial displacement described for each u_k component of a *CdTe/GaAs* bilayer material under the effect of intrinsic dislocations is a saw tooth curve. The curve obtained by numerical computation is superposed with the analytic curve over several periods because of the convergence of the Fourier series far from the centre of the dislocation. The "saw tooth" curve represents the connecting condition of the two media at the interface.

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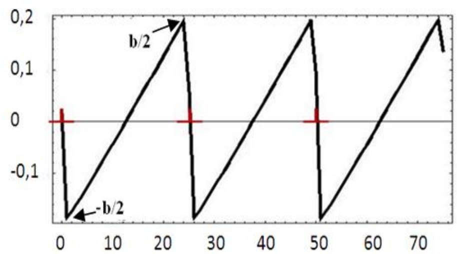


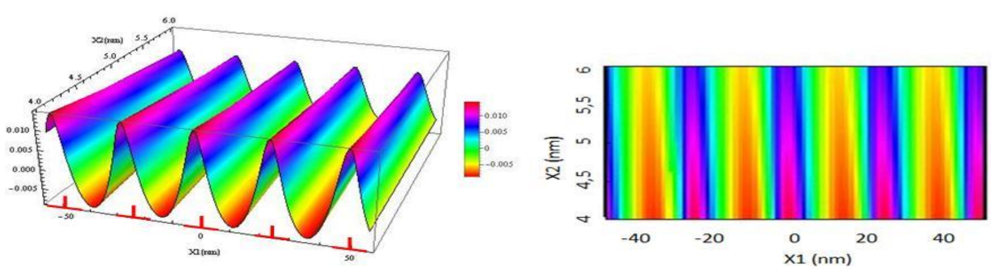
Fig.4
Displacement relative to the interface of the *CdTe/GaAs* system.

6.2 Parallel network influence on the displacement fields

Fig. 5 shows the simulated upper surface topology, under the effect of a parallel dislocation network, for *a* $b//Ox_1$ Burger vector orientation and h=2 *nm* thickness.

The topology appears as an ascending ripple along x_1, reflecting the behavior of the Fourier series. The periodic morphology is repeated every 25 *nm*.

The iso-values of the displacement fields around the parallel network dislocations of the first interface range from -0.01*nm* to +0.01*nm* for the *CdTe/GaAs* hetero-structure with the *CdTe* upper layer thickness equal 2 *nm*.



a- 3D b- 2D

Fig.5
CdTe/GaAs heterostructure topology in 2D and 3D under the effect of an interfacial parallel dislocation network for b // Ox_1: (Λ = 25 *nm*, h = 2 *nm*).

6.2.1 Square network ISO values placed at the GaAs/GaAs interface

The iso-values of the displacement fields u_1 around one dislocation and several dislocations, of the square network, are presented in Figs. 6-9 for *GaAs/GaAs*(001) hetero-structure accommodating a parametric disagreement under the effect of a square network for a burgers vector orientation b // x_1.

The displacement fields (positive and negative) are located between the dislocation lines. The $u_1$values vary from -0.1*nm* to +0.3 *nm* for *GaAs/GaAs* and the displacement fields' extremes (positive and negative) are located between dislocation lines. The displacement field's symmetry is in agreement with the linear symmetry of the edge dislocation square network. The 3D representation shows the fields of displacements u_1.

The first dislocation placed at x_1=0 and the second at x_1=25 *nm* corresponding to a period, allows us to note a clear deformation at the dislocation cores heart with an amplitude between -0.1*nm* and 0.3 *nm*.

To check the network periodicity over several periods, we simulated the iso values over 100 *nm* distance on the x_1 axis where the periodicity is respected.

By calculating the displacement fields u_1, for edge dislocations network *GaAs*(001)/*GaAs*(001) molecular bonding, with a 10 *nm* period and 7 *nm* thickness bonded layer, the values show that the extrema of the surface displacement fields are not located above the dislocation lines (Fig. 10).

This behavior explains the positioning of the elastic energy extrema. The curve is plotted over four periods (Fig. 11).

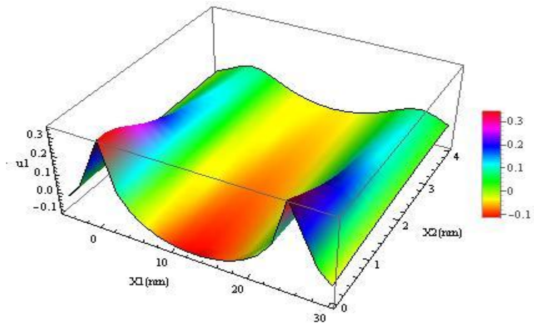


Fig.6
Displacement fields u_1 Iso-values of the *GaAs* medial layer versus the layers thickness for $h^+ = 4$ *nm* under the effect of interfacial dislocations for b_1 // x_1.

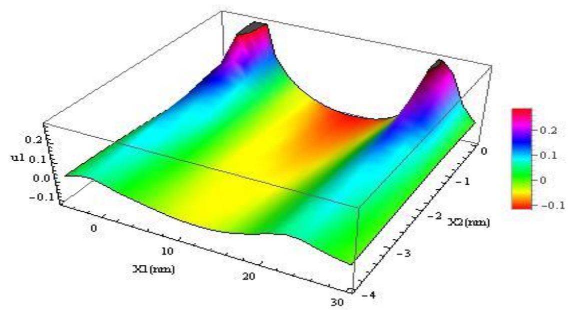


Fig.7
Displacement fields u_1 Iso-values of the *GaAs* lower layer versus the layers thickness for $h^+ = 4$ *nm* under the effect of interfacial dislocations for b_1 // x_1.

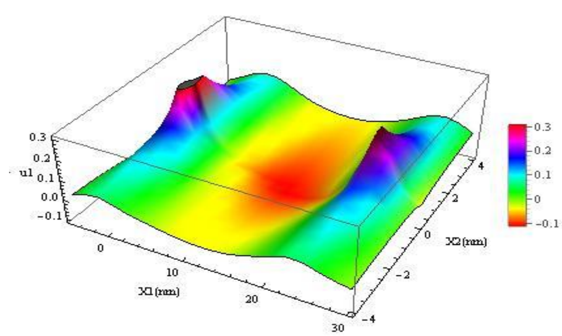


Fig.8
Displacement fields u_1 Iso-values of *GaAs/GaAs* hetero-structure.

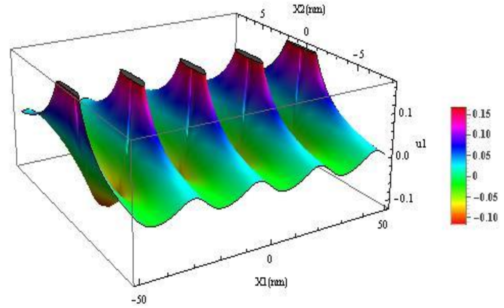


Fig.9
Displacement fields u_1 Iso-values 3D representation of the *GaAs/GaAs* hetero-structure: case of a dislocation network versus the layers thickness for $h^- = 8nm$ and $h^+ = 8nm$ under the interfacial dislocations effect for b_1 // x_1.

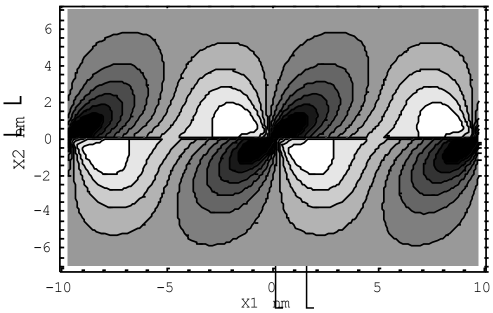


Fig.10
Fields of displacement between two corner dislocations separated by 25 *nm*.

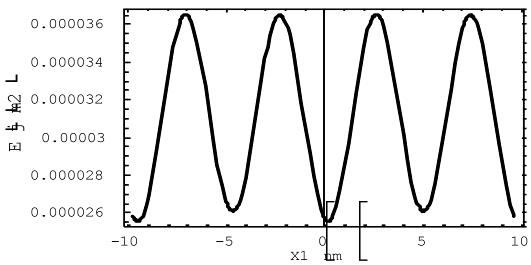


Fig.11
Elastic energy density for a network of edge dislocations, separated from 10 *nm*, for a thickness of 10 *nm*.

7 CONCLUSIONS

In this work, the elastic fields evaluation of a nano-metric three-layer material, determined by analytic formulation in double Fourier series in anisotropic elasticity case, shows its influence on the surfaces morphology. This was confirmed by applications for the *CdTe/GaAs*/(001)*GaAs* case.

Dislocations organized in networks are at the origin of elastic fields.

The surface topological shape understanding is done by the elastic fields study. The insertion of two dislocation networks into a nano metric *CdTe/GaAs/GaAs* tri-layer influences the different surfaces topology.

The results found confirm that the elastic fields are sufficiently important at the surface when the deposited layer is thin. The used method allows the visualization of the zones in tension and compression states.

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