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

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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. © 2019 IAU, Arak Branch. All rights reserved.

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. Makhlouf et al. [3] studied the problem of a

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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 drawn 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 $h^*$.

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]

$$
\left[ U^*_k - U^*_k \right]_{x=0} = \frac{h^+}{\pi} \sum_{n=1}^{\infty} \frac{1}{n \sin(n \omega x_1)} \quad k = 1, 2, 3
$$

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

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

$$
\left[ U^*_k - U^*_k \right]_{x=0} = \frac{h^-}{\pi} \sum_{n=1}^{\infty} \frac{1}{n \sin(n \omega x_1)} \quad k = 1, 2, 3 \quad \omega = 2\pi g
$$
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):

\[
\begin{bmatrix}
\sigma_{2k}^+ \\
\end{bmatrix}
\bigg|_{x_2=0} = 
\begin{bmatrix}
\sigma_{2k}^-
\end{bmatrix}
\bigg|_{x_2=-h^*}
\]

(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):

\[
\begin{bmatrix}
\sigma_{2k}^+
\end{bmatrix}
\bigg|_{x_2=h^*} = 0
\]

(4)

4 MATHEMATICAL FORMULATION

4.1 Displacements field

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

\[
\begin{bmatrix}
u_1 \\
u_2 \\
u_3
\end{bmatrix} = \sum_{\alpha=1}^{1,3} \sum_{n=0}^{3} \left( \frac{1}{\pi n} \right) [\cos(n\omega(x_1 + r_\alpha x_2)) \cdot \text{Re}(-i X_{\alpha}^{(\alpha)} \cdot \lambda_{\alpha k} \cdot \exp(-n\omega s_\alpha x_2) + (-i Y_{\alpha}^{(\alpha)} \cdot \lambda_{\alpha k}) \cdot \exp(n\omega s_\alpha x_2))] + \sin(n\omega(x_1 + r_\alpha x_2)) \cdot \text{Re}((X_{\alpha}^{(\alpha)} \cdot \lambda_{\alpha k} \cdot \exp(-n\omega s_\alpha x_2) + (Y_{\alpha}^{(\alpha)} \cdot \lambda_{\alpha k}) \cdot \exp(n\omega s_\alpha x_2))]
\]

(5)

\[
\alpha = 1, 3 ; \quad k = 1, 2, 3
\]

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:

\[
\begin{bmatrix}
u_1 \\
u_2 \\
u_3
\end{bmatrix} = \begin{bmatrix}
u_1(M) + u_3(M') \\
u_2(M) + u_2(M') \\
u_3(M) - u_1(M')
\end{bmatrix}
\]

(6)

4.2 Stress field

Similarly the final stress field expression can be written:
\[
\sigma_{ij} = 2g \sum_{n=0}^{3} \left\{ \cos[n.\omega(x_1 + r_a x_2)] \right\} \text{Re}[X_a^{(n)} L_{aij} \exp(-n.\omega s_a x_2) + Y_a^{(n)} \overline{L}_{aij} \exp(n.\omega s_a x_2)] \\
+ \left[ \sin[n.\omega(x_1 + r_a x_2)] \right] \text{Re}[i X_a^{(n)} L_{aij} \exp(-n.\omega s_a x_2) + i Y_a^{(n)} \overline{L}_{aij} \exp(n.\omega s_a x_2)] \\
\text{avec } L_{aij} = \lambda_{aij} \left[ C_{kij} + p_a C_{kij} \right] \quad i,j=1,2,3 \quad l=1,2 \quad \alpha = 1,3
\]

Similarly, square network total stress field is calculated by:

\[
\left[ \sigma_{ij}^{(l)} \right] (M) = \begin{bmatrix}
\sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') & \sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') & \sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') \\
\sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') & \sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') & \sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') \\
\sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') & \sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M') & \sigma_{0}^{(l)}(M) + \sigma_{0}^{(l)}(M')
\end{bmatrix}
\]

5 BOUNDARY CONDITIONS

The complex constants (\(X_{\alpha}^*, Y_{\alpha}^*, X_{\alpha}^+, Y_{\alpha}^+\)) 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:

\[
\text{Re} \sum_{a=1}^{3} \left[ - (X_{\alpha}^* \lambda_{ak}^+ + Y_{\alpha}^* \overline{\lambda}_{ak}) + Y_{\alpha}^- \overline{\lambda}_{ak} \right] = b_k
\]

\[
\text{Re} \sum_{a=1}^{3} \left[ - (X_{\alpha}^* \lambda_{ak}^+ + Y_{\alpha}^* \overline{\lambda}_{ak}) - Y_{\alpha}^- \overline{\lambda}_{ak} \right] = 0
\]

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

\[
\text{Re} \sum_{a=1}^{3} \left[ - (X_{\alpha}^* \lambda_{ak}^+ + Y_{\alpha}^* \overline{\lambda}_{ak}) + (X_{\alpha}^+ \lambda_{ak}^+ + Y_{\alpha}^+ \overline{\lambda}_{ak}) \right] = b'_{k}
\]

\[
\text{Re} \sum_{a=1}^{3} \left[ (X_{\alpha}^* \lambda_{ak}^+ + Y_{\alpha}^* \overline{\lambda}_{ak}) - (X_{\alpha}^+ \lambda_{ak}^+ + Y_{\alpha}^+ \overline{\lambda}_{ak}) \right] = 0
\]

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

\[
\text{Re} \sum_{a=1}^{3} (X_{\alpha}^* L_{a2k}^+ E_{j} (C_{1} + iS_{1} )) + (Y_{\alpha}^* \overline{L}_{a2k} E_{2} )(C_{1} + iS_{1} ) - \\
(X_{\alpha}^+ L_{a2k}^+ E_{3} ) (C_{2} + iS_{2} ) - (Y_{\alpha}^+ \overline{L}_{a2k} E_{4} )(C_{2} + iS_{2} ) = 0
\]

\[
\text{Re} \sum_{a=1}^{3} \left[ (X_{\alpha}^* L_{a2k}^* E_{i} (S_{1} - iC_{1} )) + (Y_{\alpha}^* \overline{L}_{a2k} E_{2} (S_{1} - iC_{1} ) \right) \right.
\]

\[
- (X_{\alpha}^+ L_{a2k}^* E_{3} ) (S_{2} - iC_{2} ) - (Y_{\alpha}^+ \overline{L}_{a2k} E_{4} (S_{2} - iC_{2} ) = 0
\]

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

\[
\text{Re} \sum_{a=1}^{3} \left[ (X_{\alpha}^* L_{a2k}^* + Y_{\alpha}^* \overline{L}_{a2k}^+) - Y_{\alpha}^- \overline{L}_{a2k} = 0
\]
Displacement Fields Influence Analysis Caused....

\[ \text{Re} \left( \sum_{\alpha=1}^{3} - (X_{\alpha} L_{a2k} + Y_{\alpha} \overline{L}_{a2k}) - Y_{\alpha} \overline{L}_{a2k} = 0 \right) \]

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

\[ \text{Re} \left( \sum_{\alpha=1}^{3} (X_{\alpha} L_{a2k} E_5 + Y_{\alpha} \overline{L}_{a2k} E_6) \right) EC - (X_{\alpha} L_{a2k} E_5 + Y_{\alpha} \overline{L}_{a2k} E_6) ES = 0 \]

\[ \text{Re} \left( \sum_{\alpha=1}^{3} (X_{\alpha} L_{a2k} E_5 + Y_{\alpha} \overline{L}_{a2k} E_6) \right) EC + (X_{\alpha} L_{a2k} E_5 + Y_{\alpha} \overline{L}_{a2k} E_6) ES = 0 \]

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

\[ AX = B \]

(9)

where the column matrix \( X (A^+, A^-, B^+, B^-, C^+, C^-, D^+ \text{ and } D^-) \) 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]:

\[ b = \frac{a_{CdTe} + a_{GaAs}}{2\sqrt{2}} \]

\[ \Lambda = \frac{a_{CdTe} a_{GaAs}}{(a_{CdTe} - a_{GaAs}) \sqrt{2}} \]

The parametric disagreement is given by:

\[ \varepsilon = 2 \left( \frac{a_{CdTe} - a_{GaAs}}{a_{CdTe} + a_{GaAs}} \right) = 18.81\% \]

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.

<table>
<thead>
<tr>
<th>Designation</th>
<th>CdTe</th>
<th>GaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice parameters ( a ) (nm)</td>
<td>0.4681</td>
<td>0.56533</td>
</tr>
<tr>
<td>Elastic constants ( C_{ij} ) (Gpa)</td>
<td>( C_{11} = 53.5 )</td>
<td>( C_{11} = 118 )</td>
</tr>
<tr>
<td></td>
<td>( C_{12} = 36.9 )</td>
<td>( C_{12} = 53.5 )</td>
</tr>
<tr>
<td></td>
<td>( C_{44} = 20.2 )</td>
<td>( C_{44} = 59.4 )</td>
</tr>
<tr>
<td>Burgers vector ( b ) (nm)</td>
<td>0.3997</td>
<td></td>
</tr>
<tr>
<td>Period ( \Lambda ) (nm)</td>
<td>25</td>
<td></td>
</tr>
</tbody>
</table>

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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.

The "saw tooth" curve represents the connecting condition of the two media at the interface.

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 $h=2 \text{ nm}$ 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 $-0.01 \text{ nm}$ to $+0.01 \text{ nm}$ for the CdTe/GaAs hetero-structure with the CdTe upper layer thickness equal 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 $-0.1 \text{ nm}$ to $+0.3 \text{ nm}$ 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 $x_1=25 \text{ nm}$ corresponding to a period, allows us to note a clear deformation at the dislocation cores heart with an amplitude between $-0.1 \text{ nm}$ and $0.3 \text{ nm}$.
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).

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**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 $h^+ = 8$nm and $h^- = 8$nm under the interfacial dislocations effect for $b_1 // x_1$. 

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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.

REFERENCES


