IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

A theoretical study of the stability and electronic properties of a GaAs/Te/InAs interface

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1998 J. Phys.: Condens. Matter 10 5739

(http://iopscience.iop.org/0953-8984/10/26/003)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.209
The article was downloaded on 14/05/2010 at 16:33

Please note that terms and conditions apply.

J. Phys.: Condens. Matter **10** (1998) 5739–5748. Printed in the UK PII: S0953-8984(98)90354-X

A theoretical study of the stability and electronic properties of a GaAs/Te/InAs interface

R H Miwa† and A C Ferraz‡

† Departamento de Ciências Físicas, Universidade Federal de Uberlândia, CP 593, 38400-902, Uberlândia, MG, Brazil
‡ Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970 São Paulo, SP, Brazil

Received 6 January 1998, in final form 6 April 1998

Abstract. We report first-principles studies of the stability and electronic properties of a layer of Te atoms at an InAs/GaAs(001) interface. The calculations are performed within the LDA approximation. Our results indicate that the formation of half a monolayer of Te atoms is energetically unstable against phase segregations, indicating that the Te atoms do not reduce the GaAs/InAs interface energy. However, a GaAs/Te(0.5)/InAs interface can be formed on the basis of a kinetic process. The Te atoms occupying As sites have strongly covalent character, and give rise to a half-filled band at 0.15 eV below the conduction band. The calculated valence-band offset, with the inclusion of half a monolayer of Te atoms, presents a good agreement with experimental results.

1. Introduction

Heteroepitaxial growth is best achieved when the lattice parameters are almost matched, and as a consequence the growth proceeds by means of an ideal layer-by-layer 2D mechanism that allows the formation of heterostructures with a monolayer precision. On the other hand, the heteroepitaxial growth of compounds with large mismatch usually leads to an undesirable 3D growth mode. It is found experimentally [1] that the 2D growth mode of InAs on GaAs(001) can be induced by adding a Te monolayer before InAs deposition, drastically changing the growth mode of the InAs/GaAs system. In one proposed model of impurity-assisted 2D growth, the dopant element (Te atoms) acts as a surfactant, floating at the surface and reducing the surface free energy during the growth process. Recently, another model was proposed, confirming the action of the Te of matching the 2D growth of InAs on GaAs; however, the 2D growth is stabilized by the half-monolayer of Te atoms that remain at the interface. This model is supported by experimental indications that only an excess of half a monolayer of Te atoms floats at the InAs surface [2].

In the present work we report first-principles studies of the electronic and structural properties of a layer of Te atoms at an InAs/GaAs(001) interface. Our results indicate that the Te atoms, occupying As sites, have covalent character, and are more strongly bonded to GaAs layers than to InAs layers. The inclusion of the Te atoms at the interface gives rise to a half-filled electron band. Also the valence-band offset (VBO) of this structure was calculated.

0953-8984/98/265739+10$19.50 © 1998 IOP Publishing Ltd

2. The method of calculation

Our calculations are performed within the framework of density functional theory (DFT), within the local density approximation (LDA) using the Ceperley–Alder correlation [3] as parametrized by Perdew and Zunger [4]. The electron–ion interaction was treated by using norm-conserving, *ab initio* fully separable pseudopotentials [5], and the wave functions were expanded in a plane-wave basis set with a kinetic energy cut-off of 12 Ryd.

We adopted the Car–Parrinello approach [6] to simultaneously relax the electronic and ionic degrees of freedom, as in the modified computer code due to Stumpf and Scheffler [7].

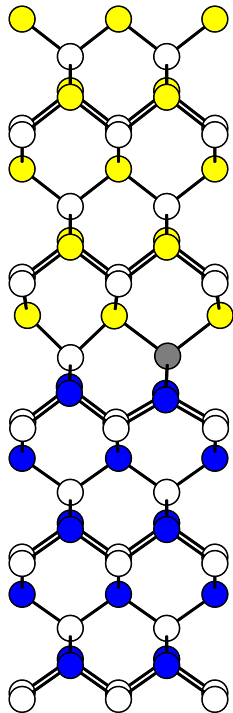

Figure 1. The large unit cell, with periodicity $n = 5$ and $x_{\mathrm{Te}} = 0.5$, for the GaAs/Te/InAs interface. Open circles represent As atoms, solid circles Ga atoms, light-grey circles In atoms, and dark-grey circles Te atoms.

The calculations were performed with large unit cells of 40 atoms (periodicity $n = 5$) and 24 atoms (periodicity $n = 3$). Figure 1 shows the tetragonal unit cell used for the superlattice ($n = 5$) along the (001) direction, and a 2×1 reconstruction at the interface. The primitive cell is characterized by a tetragonal ratio of deformation, $\eta = c/a$, where c and a are the lattice parameters parallel and perpendicular to the growth direction (001). Here we adopt Keating's valence-force-field method [8] to find η; therefore we have neglected the chemical contribution in this process. We found $\eta = 3.152\,85$ (unrelaxed $\eta = 3.000$) for periodicity $n = 3$, and 5.255 10 (unrelaxed $\eta = 5.000$) for periodicity $n = 5$, which correspond to a tetragonal deformation of 5% in both structures. Plane waves with kinetic energies up to 12 Ryd (18 Ryd) were included in the calculations, and two (eight) special k-points were used in the Brillouin zone integrations during the obtaining of self-consistency. The lattice parameter used in all of the calculations is 5.581 Å, which corresponds to the calculated

equilibrium distance for a 12 Ryd cut-off. We consider three possible configurations of Te atoms at the interface, each one corresponding to a given coverage x_{Te} of Te atoms: the configuration without Te atoms corresponds to $x_{\mathrm{Te}} = 0$, the configuration with one Te atom corresponds to $x_{\mathrm{Te}} = 0.5$, half a monolayer, and the configuration with two Te atoms, a full monolayer, corresponds to $x_{\mathrm{Te}} = 1$. The Te atoms were placed substitutionally at As sites at the interface. The Te atoms and their nearest and next-nearest neighbours were allowed to relax towards the energy-minimum geometry until the force on the atoms was less than 25 meV Å^{-1}. The structure with $x_{\mathrm{Te}} = 0$ was also relaxed.

3. Results and discussion

We first analyse the stability of the $x_{\mathrm{Te}} = 0.5$ and $x_{\mathrm{Te}} = 1$ interfaces against phase segregation, by comparing the formation energies of different interfaces. The formation energy is defined as [9, 10]

$$E_n^{\mathrm{form}}(x_{\mathrm{Te}}) = E_n^{\mathrm{het}}(x_{\mathrm{Te}}) - \sum_i n_i \mu_i \tag{1}$$

where $E_n^{\mathrm{het}}(x_{\mathrm{Te}})$ is the total energy of a GaAs/InAs heterostructure with periodicity n and a concentration x_{Te} of Te atoms at the interface, n_i is the number of the atoms of species i, and μ_i represents the chemical potential for this species. In thermodynamic equilibrium, the chemical potentials of the elements are in equilibrium with those of the respective bulk phases, i.e.

$$\mu_{\mathrm{GaAs}} = \mu_{\mathrm{Ga}}^{\mathrm{bulk}} + \mu_{\mathrm{As}}^{\mathrm{bulk}} \tag{2}$$

$$\mu_{\mathrm{InAs}} = \mu_{\mathrm{In}}^{\mathrm{bulk}} + \mu_{\mathrm{As}}^{\mathrm{bulk}} \tag{3}$$

where μ_{GaAs} (μ_{InAs}) is the chemical potential of GaAs bulk (InAs bulk). As InAs is constrained to have the GaAs lattice parameter parallel to the substrate, the InAs bulk is tetragonally distorted along the (001) direction. Using the relations (2) and (3), the formation energy (equation (1)) can be written as

$$E_n^{\mathrm{form}}(x_{\mathrm{Te}} = 0) = E_n^{\mathrm{het}}(x_{\mathrm{Te}} = 0) - n_{\mathrm{Ga}}\mu_{\mathrm{GaAs}} - n_{\mathrm{In}}\mu_{\mathrm{InAs}} \tag{4}$$

$$E_n^{\mathrm{form}}(x_{\mathrm{Te}} = 0.5) = E_n^{\mathrm{het}}(x_{\mathrm{Te}} = 0.5) - n_{\mathrm{Ga}}\mu_{\mathrm{GaAs}} - n_{\mathrm{In}}\mu_{\mathrm{InAs}} + \mu_{\mathrm{As}} - \mu_{\mathrm{Te}} \tag{5}$$

$$E_n^{\mathrm{form}}(x_{\mathrm{Te}} = 1) = E_n^{\mathrm{het}}(x_{\mathrm{Te}} = 1) - n_{\mathrm{Ga}}\mu_{\mathrm{GaAs}} - n_{\mathrm{In}}\mu_{\mathrm{InAs}} + 2\mu_{\mathrm{As}} - 2\mu_{\mathrm{Te}}. \tag{6}$$

The maximum values for μ_{As} and μ_{Te} correspond to the As and Te chemical potentials of the respective bulk elemental phases:

$$\mu_{\mathrm{As}} \leqslant \mu_{\mathrm{As}}^{\mathrm{bulk}} \tag{7}$$

$$\mu_{\mathrm{Te}} \leqslant \mu_{\mathrm{Te}}^{\mathrm{bulk}}. \tag{8}$$

Defining the heat of formation of the GaAs (bulk) as

$$\Delta H_{\mathrm{GaAs}} = \mu_{\mathrm{GaAs}} - \mu_{\mathrm{Ga}}^{\mathrm{bulk}} - \mu_{\mathrm{As}}^{\mathrm{bulk}} \tag{9}$$

we obtain the range of the As chemical potential, μ_{As}:

$$\mu_{\mathrm{As}}^{\mathrm{bulk}} + \Delta H_{\mathrm{GaAs}} \leqslant \mu_{\mathrm{As}} \leqslant \mu_{\mathrm{As}}^{\mathrm{bulk}}. \tag{10}$$

The lower limit for the Te chemical potential is given by the chemical potential of Te atoms adsorbed on an InAs(001) surface, $\mu_{\mathrm{Te}}^{\mathrm{InAs(001)}}$:

$$\mu_{\mathrm{Te}}^{\mathrm{bulk}} + \mu_{\mathrm{Te}}^{\mathrm{InAs(001)}} \leqslant \mu_{\mathrm{Te}} \leqslant \mu_{\mathrm{Te}}^{\mathrm{bulk}}. \tag{11}$$

We have used for the heat of formation of GaAs the calculated value obtained by Qian and co-workers [9], -0.74 eV/atom, which is in good agreement with experimental results [11]. Our calculated value for the chemical potential of Te adsorbed on the InAs(001) surface is equal to -1.14 eV/atom. The ranges of the As and Te chemical potentials are given relative to the respective bulk phases; that is, $\mu_{\mathrm{As}} \rightarrow \mu_{\mathrm{As}} - \mu_{\mathrm{As}}^{\mathrm{bulk}}$ and $\mu_{\mathrm{Te}} \rightarrow \mu_{\mathrm{Te}} - \mu_{\mathrm{Te}}^{\mathrm{bulk}}$, and these ranges define the different interface structures which are energetically stable against phase segregation.

From equation (4) we found $E_{n=3}^{\mathrm{form}}(x_{\mathrm{Te}} = 0) = 0.05$ eV/interface and $E_{n=5}^{\mathrm{form}}(x_{\mathrm{Te}} = 0) = 0.02$ eV/interface, indicating that the $x_{\mathrm{Te}} = 0$ abrupt interface is thermodynamically unstable against phase segregation. On increasing the periodicity from $n = 3$ to $n = 5$, which is tantamount to reducing the GaAs/InAs interface density, the contribution due to the charge transfer to the interface formation energy, $E_n^{\mathrm{form}}(x_{\mathrm{Te}} = 0)$, will become smaller (in absolute value). Therefore, the formation energy as a function of the periodicity indicates a positive energy contribution due to the charge transfer in the GaAs/InAs interface, as proposed by Ohno [12] in a theoretical study of $(\mathrm{GaAs})_1/(\mathrm{InAs})_1$ monolayer superlattices. He has suggested that the instability of this structure can be attributed to the unfavourable electronic charge transfer in the GaAs/InAs interface, which gives a positive energy contribution.

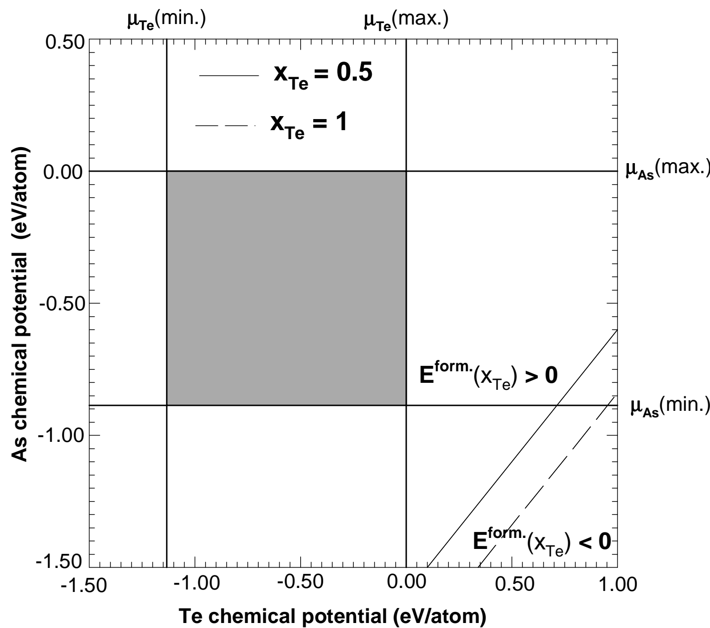

Figure 2. The phase diagram of the formation energy of the GaAs/Te/InAs interface. The ranges of the chemical potentials of As and Te, as related to their respective bulk values, are indicated by the hatched region.

Next we consider the formation energy of the $x_{\mathrm{Te}} = 0.5$ and $x_{\mathrm{Te}} = 1$ interfaces, using equations (5) and (6), for the formation of structures with periodicity $n = 3$. The formation energy difference between the $x_{\mathrm{Te}} = 0.5$ and $x_{\mathrm{Te}} = 1.0$ interfaces that was obtained was 0.18 eV/interface, indicating that the $x_{\mathrm{Te}} = 0.5$ structure is energetically more favourable. By increasing the dimension of the cell to the periodicity $n = 5$, we also verified that the $x_{\mathrm{Te}} = 0.5$ interface is energetically more favourable than the $x_{\mathrm{Te}} = 1.0$ interface, by 0.24 eV/interface. From these results we can infer a convergence

of 0.06 eV/interface to the interface formation energy, as a function of the periodicity ($n = 3 \rightarrow 5$). The individual changes in the absolute values of the formation energies were equal to 0.01 eV/interface for the $x_{\mathrm{Te}} = 0.5$ interface and 0.07 eV/interface for the $x_{\mathrm{Te}} = 1.0$ interface. These formation energy differences can be explained if we consider the increase of the interface charge density with the Te-atom concentration, inducing an interface–interface electrostatic interaction, which is reduced when the cell periodicity is increased. The results are summarized in figure 2. The range of the As and Te chemical potentials indicates that the $x_{\mathrm{Te}} = 0.5$ and $x_{\mathrm{Te}} = 1$ abrupt interfaces are thermodynamically unstable against phase segregation, forming some mixed interface, as proposed by Kley and Neugebauer [10] in their theoretical study of the GaAs/ZnSe interface. The thermodynamic instability of the $x_{\mathrm{Te}} = 0.5$ interface indicates that the presence of the Te atoms does not reduce the GaAs/InAs interface energy as was proposed by Rodrigues *et al* [2]. In that study the surfactant action of the Te atoms during the epitaxial growth of InAs on GaAs(001) was analysed, and it was verified that 0.57 ± 0.07 of a monolayer of the Te atoms remains at the GaAs/InAs interface, embedded between the GaAs and InAs, and reducing the interface energy. Our results, showing the increase of the interface formation energy with Te concentration, $x_{\mathrm{Te}} = 0.5 \rightarrow 1$, indicate that the $x_{\mathrm{Te}} = 0.5$ interface is energetically more favourable against phase segregation than the $x_{\mathrm{Te}} = 1$ interface.

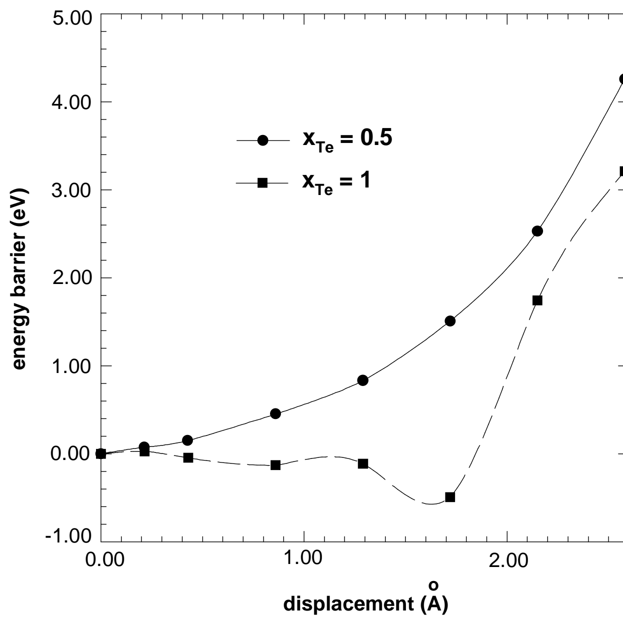

Figure 3. The energy barrier to the atomic displacements of the Te atom along the (111) direction.

The convergence of the formation energy with respect to the cut-off energy was also considered. The calculation was performed in a cell with periodicity $n = 3$, using two special k-points for the Brillouin zone integration, and a cut-off energy of 18 Ryd. Our results indicate a formation energy difference, between the $x_{\mathrm{Te}} = 0.5$ and $x_{\mathrm{Te}} = 1$ interfaces, equal to 0.26 eV/interface, also indicating that the $x_{\mathrm{Te}} = 0.5$ interface is energetically more favourable. Finally we considered the convergence of our results for the interface formation energy with respect to the number of special k-points used in the Brillouin zone integration.

Using a cell with periodicity $n = 3$, a cut-off energy of 18 Ryd, and eight special k-points, we have established that the $x_{\text{Te}} = 0.5$ interface is energetically more favourable than the $x_{\text{Te}} = 1$ interface by 0.18 eV/interface. Therefore we can conclude that the interface formation energy presents a good convergence with respect to the cell size, cut-off energy, and number of k-points used in the Brillouin zone integration.

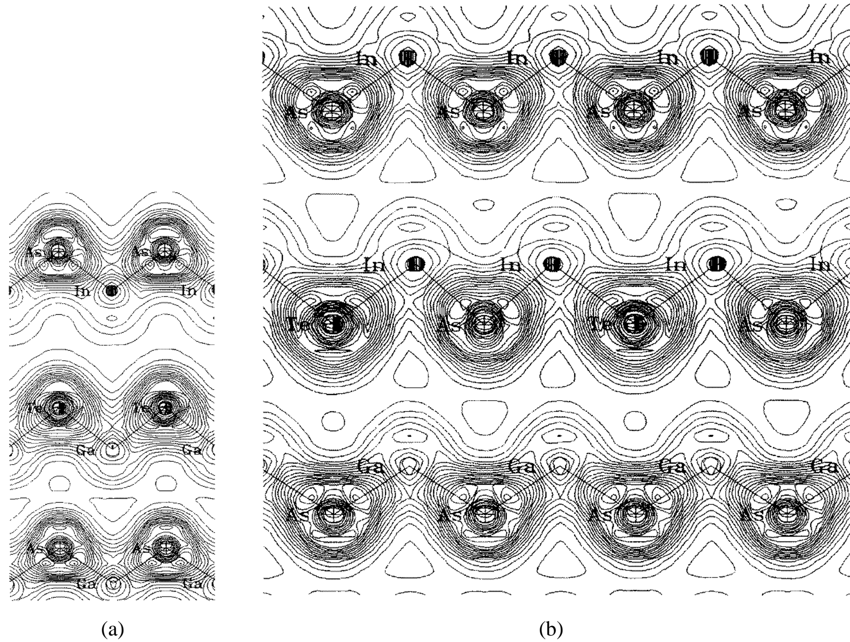

Figure 4. The total electron charge density of the GaAs/Te(0.5)/InAs interface. (a) The $(\bar{1}10)$ plane and (b) the (110) plane.

We also examine the total energy as a function of the atomic displacement of the Te atoms along the (111) threefold direction, for the $x_{\text{Te}} = 0.5$ and $x_{\text{Te}} = 1$ interfaces. Figure 3 presents the results obtained for the total energy difference, or the value of the energy barrier, defined as

$$E^{\text{barr}}(x_{\text{Te}}) = E^{\text{disp}}(x_{\text{Te}}) - E^{0}(x_{\text{Te}}) \tag{12}$$

where $E^{\text{disp}}(x_{\text{Te}})$ is the total energy of the x_{Te} interface with a Te atom displaced along the (111) direction, and $E^{0}(x_{\text{Te}})$ is the total energy of the interface with the Te atoms in the on-site positions. The calculations are performed by fixing the displaced atom along the (111) direction, and allowing the nearest- and the next-nearest-neighbour atoms to relax. We must stress that these results give only an estimate of the energy barrier, because, as a result of the small size of the supercell in the plane perpendicular to the (001) direction, there ensues an interaction between the displaced Te atoms. However, the results clearly indicate very different behaviours of the shapes of the energy barriers for the $x_{\text{Te}} = 0.5$ and $x_{\text{Te}} = 1$ interfaces. The $x_{\text{Te}} = 0.5$ interface does not present any metastable position along the (111) direction, resulting in an energy barrier of 4.26 eV corresponding to a displacement of 2.60 Å from the zinc-blende position. However, the $x_{\text{Te}} = 1$ interface displays a very different energy barrier, indicating that the Te atoms are not energetically stable in the on-site positions; but a minimum energy is found at a displacement of 1.72 Å along the (111) direction, which corresponds to an energy barrier of -0.46 eV. This can be understood as

indicating the possibility of formation of a Ga(In)Te alloy or some amorphous structure in the $x_{Te} = 1$ interface. These results are in agreement with the increase of the formation energy with increasing Te-atom concentration, $x_{Te} = 0.5 \rightarrow 1$, in the interface. On the other hand, since, from our finding, there is no metastable configuration for the $x_{Te} = 0.5$ interface, we can infer that the formation of a GaAs/Te(0.5)/InAs interface, as proposed by Rodrigues *et al* [2], can be attributed to a kinetic process, where half a monolayer of Te atoms is fixed in the GaAs/InAs interface, although the interface is unstable against phase segregation. The formation of half a monolayer of Te atoms in the GaAs/InAs interface, indicated by kinetic arguments, was verified theoretically [13] using a sequence of processes of adsorption and exchange of As_2 molecules on a GaAs(001) surface, covered by a monolayer of Te atoms.

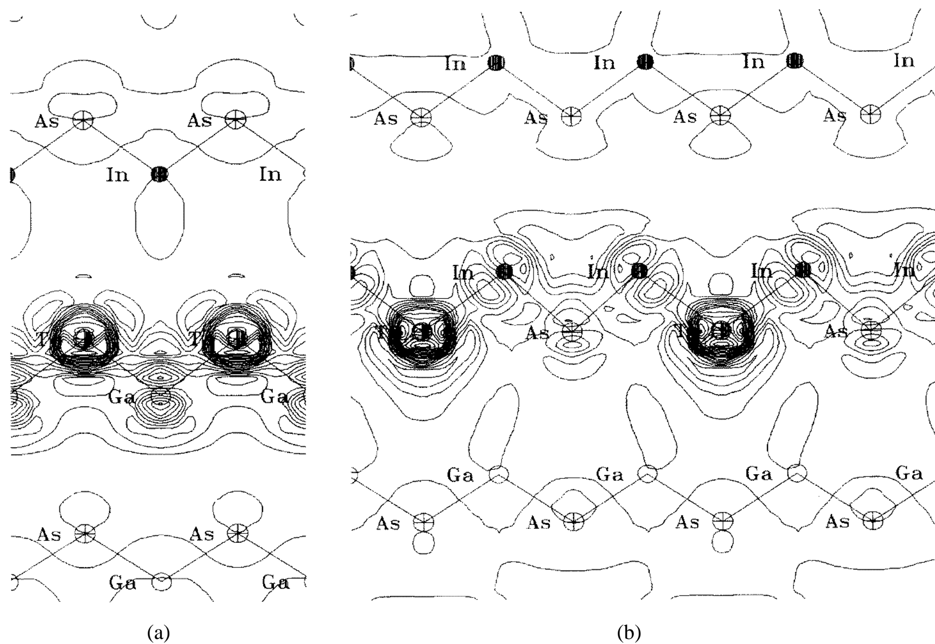

Figure 5. The total charge-density difference between the GaAs/Te/InAs interfaces with $x_{Te} = 0.5$ and $x_{Te} = 0.0$. (a) The $(\bar{1}10)$ plane and (b) the (110) plane.

The major contribution to the energy reduction comes from the relaxation of the Te atoms and their nearest neighbours, and this lowers the total energy by 0.86 eV/interface. Further relaxation of next-nearest neighbours reduces the total energy by 0.11 eV/interface. The atomic relaxation around the Te atoms leads to Te–Ga and Te–In distances equal to $d_{Te-Ga} = 2.59$ Å and $d_{Te-In} = 2.72$ Å; these values are similar to the sums of the covalent radii, indicating a covalent character of the bonds. The same atomic relaxation was obtained using a cell with periodicity $n = 3$. This covalent character can also be seen in figure 4, where we plot the total charge density on the plane that contains Te atoms, bonding with Ga and In atoms. The similarity between the charge densities at As and Te sites is noticeable; additionally, figure 4 indicates that the charge density in the Te–Ga bond is higher than that in the Te–In bond, indicating that the Te atoms are more strongly bonded to the GaAs layers (the substrate) than the InAs layers.

Figure 5 shows the charge-density difference between the $x_{\mathrm{Te}} = 0.5$ and $x_{\mathrm{Te}} = 0$ interfaces, given by

$$\Delta\rho = \rho(x_{\mathrm{Te}} = 0.5) - \rho(x_{\mathrm{Te}} = 0).$$

The plot shows how far the total charge density is affected by the inclusion of Te atoms. It can be clearly seen that the perturbation of the charge density is localized within the nearest neighbourhood of the interface. Outside that region, $\Delta\rho \approx 0$. This suggests that the number of layers of the unit cell considered is sufficient for studying the structural properties of this interface.

We have also computed the LDA eigenvalues for the $x_{\mathrm{Te}} = 0$ and $x_{\mathrm{Te}} = 0.5$ structures, at the high-symmetry points of the Brillouin zone of the large unit cell. The $x_{\mathrm{Te}} = 0$ structure has a direct LDA band gap, at the $\bar{\Gamma}$ point, of 1.11 eV. The inclusion of the Te atoms has a major consequence for the band structure, namely that a half-filled band appears.

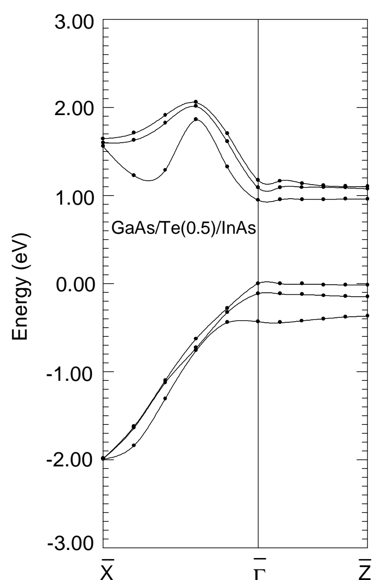

Figure 6. The electronic band structure of the GaAs/Te(0.5)/InAs interface.

The Te half-filled band approximately follows the bottom of the conduction band (figure 6), and exhibits a dispersion of 0.90 eV along the $\bar{\Gamma}\bar{\mathrm{X}}$ direction. This large dispersion is attributed to the strong interaction between Te atoms, as derived from the periodic boundary conditions, in the plane perpendicular to the growth direction. In this case the distance between the Te atoms, perpendicular to the (001) direction, is 3.946 Å. On the other hand, we have obtained a dispersion of 0.05 eV along the $\bar{\Gamma}\bar{\mathrm{Z}}$ direction, which is related to the weak interaction between the Te atoms along to the growth direction. Here, the distance between the Te atoms along the (001) direction is 29.905 Å.

Finally, we have calculated the valence-band offset of the InAs/GaAs interface with the inclusion of half a monolayer of Te atoms. The valence-band offset across the interface can be written as [14]

$$\Delta E^{\mathrm{val}} = \left[E_v - \bar{V}\right]_{\mathrm{AC}} - \left[E_v - \bar{V}\right]_{\mathrm{BC}} + \left[\bar{V}_{\mathrm{AC}} - \bar{V}_{\mathrm{BC}}\right] \tag{13}$$

where $[E_v - \bar{V}]_{\mathrm{AC}}$ is the energy of the top of the valence band in pure AC material with respect to the average potential $\bar{V}$, and the second term is the corresponding quantity for BC

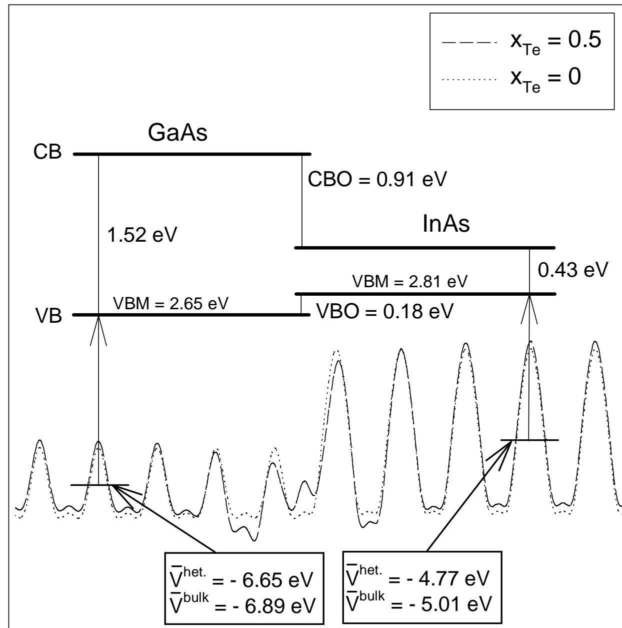

Figure 7. The valence- and conduction-band offsets of the GaAs/Te(0.5)/InAs interface.

material. These two terms refer to the bulk properties of InAs and GaAs materials; since we are using the lattice parameter of GaAs for InAs, there will be a bias towards this compound. $[\bar{V}_{\mathrm{AC}} - \bar{V}_{\mathrm{BC}}]$ represents the interfacial dipole, or the difference between the average potential on either side of the AC/BC interface and that far away from it, and is attributed to the charge transfer in the GaAs/InAs interface. The value obtained, $\Delta E^{\mathrm{val}} = 0.18$ eV, is in very good agreement with the experimental result [15]: 0.17 eV. Figure 7 shows the valence-band offset of the GaAs/Te(0.5)/InAs interface, and the planar average of the effective potentials of the $x_{\mathrm{Te}} = 0.5$ and $x_{\mathrm{Te}} = 0$ interfaces. The conduction-band offset was obtained by adding the experimental values for the gaps of GaAs and InAs.

4. Conclusions

In summary, our calculations show that the inclusion of Te atoms in a GaAs/InAs abrupt interface does not reduce the formation energy. Therefore, the stability of layer-by-layer epitaxial growth of InAs on a GaAs(001) surface, using Te atoms as a surfactant element, cannot be attributed to the Te atoms of the GaAs/InAs interface. However, the formation of a GaAs/Te(0.5)/InAs interface could be based on a kinetic process.

The inclusion of half a monolayer of Te atoms in the GaAs/InAs interface gives rise to a half-filled band with a dispersion of 0.05 eV along the $\bar{\Gamma}\bar{Z}$ direction, and a valence-band offset equal to 0.18 eV, in good agreement with experimental results.

Acknowledgments

We acknowledge the Brazilian agencies CNPq, FINEP, and FAPEMIG for financial support, and LNCC and CENAPAD for computational support.

References

[1] Grandjean N, Massies J and Etgens V H 1992 *Phys. Rev. Lett.* **69** 796
[2] Rodrigues W N, Etgens V H, Sauvage-Simkin M, Rossi G, Sirotti F, Pinchaux R and Rochet F 1995 *Solid State Commun.* **95** 873
[3] Ceperley D M and Alder B I 1980 *Phys. Rev. Lett.* **45** 566
[4] Perdew J P and Zunger A 1981 *Phys. Rev.* B **23** 5048
[5] Kleinmann L and Bylander D M 1982 *Phys. Rev. Lett.* **48** 1425
Gonze X, Stumpf R and Scheffler M 1991 *Phys. Rev.* B **44** 8503
[6] Car R and Parrinello M 1985 *Phys. Rev. Lett.* **55** 2471
[7] Stumpf R and Scheffler M 1994 *Comput. Phys. Commun.* **79** 447
[8] Keating N 1967 *Phys. Rev.* **145** 637
[9] Qian G-X, Martin R and Chadi D J 1989 *Phys. Rev.* B **38** 7649
[10] Kley A and Neugebauer J 1994 *Phys. Rev.* B **50** 8616
[11] *Handbook of Chemistry and Physics* 1958 67th edn, ed R C Weast (Boca Raton, FL: Chemical Rubber Company Press)
[12] Ohno T 1988 *Phys. Rev.* B **38** 13 191
[13] Miwa R H, Ferraz A C, Rodrigues W N and Chacham H 1996 *Proc. 23rd Int. Conf. on the Physics of Semiconductors* ed M Scheffler and R Zimmermann (Singapore: World Scientific) p 1107
[14] Baroni S, Resta R, Baldereschi A and Peresi M 1989 *Spectroscopy of Semiconductor Microstructures (NATO ASI Series B, vol 206)* ed M Fasol, A Fasolino and P Lugli (New York: Plenum) p 251
[15] Rodrigues W N, Etgens V H, Sauvage-Simkin M, Rossi G, Sirotti F, Pinchaux R and Rochet F 1998 to be published