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Metallization and Schottky-barrier formation for Se-passivated GaAs(1 0 0) interfaces

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Abstract

Using a molecular dynamics DFT-LDA code, we have analyzed the Schottky-barrier formation of a Se-passivated GaAs(1 0 0)-2 × 1 reconstruction. In our approach we consider, first, the energetically most favorable interfaces formed by the deposition of either one or two Ga atoms per surface unit cell; then, we analyze the electron density of states and calculate the interface Fermi level and the Schottky-barrier height. We show that the height depends essentially on the very same interface geometry. In particular, the effect of exchanging Ga and Se atoms at the interface (an intermixing process) yields a normal Schottky-barrier height, while the normal passivated surface yields an ohmic contact.

Keywords: Schottky-barrier; GaAs; Metallization; Electronic calculations

1. Introduction

The metal–semiconductor Schottky-barrier formation has been explained using different mechanisms attributed either to the induced density of interface states (IDIS) [1–3] or to the defects existing at the very same interface [4].

When experimental conditions can be controlled to reduce the interface defect density of states (DOS) to below $10^{13}\,cm^{-3}$, it is commonly accepted that the Schottky-barrier height is determined by the IDIS. In this model, the interface Fermi level is controlled by the electron DOS associated with the chemical bonds formed between the semiconductor last layers and the deposited metal atoms [5,6]. This line of thought suggests that the Schottky-barrier height can be controlled by modifying the interface dangling bonds; the simplest approach to this procedure being to passivate the semiconductor surface before depositing the metal film [7].

Some of us have explored these ideas by analyzing different covalent and ionic semiconductors [8]. In particular, we studied the following passivated semiconductors: H/Si(1 1 1), Sb/Si(1 1 1), S/Si(1 0 0), S/Ge(1 0 0), H/GaAs(1 1 0), As/GaAs(1 1 0) and Sb/GaAs(1 0 0); a full analysis of these cases showed trends that can be summarized in the following conclusions:

(a) The main effect of a passivating monolayer is to reduce the barrier height ϕ_{bn}.
(b) This effect depends on the intralayer electronegativity and the semiconductor ionicity. The barrier height appears to be reduced when the intralayer electronegativity or the semiconductor ionicity are increased.

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In this paper, we analyzed the metal–semiconductor contact of GaAs(1 0 0) surface passivated with a Se-monolayer. This passivation has been analyzed elsewhere [9] and, here, we use the corresponding geometry as starting surface on which a Ga-overlayer is deposited for studying how the Schottky-barrier is formed.

The GaAs(1 0 0) surface is important from a technological point of view, and the effect of its passivation on the Schottky-barrier height formed with a metal contact a subject of interest for designing devices with the appropriate properties [10].

In Section 2, we present our model and method of calculation, while in Section 3, we discuss our main results. Conclusions are presented in Section 4.

2. Model and method of calculation

Our starting point is the Se-passivated GaAs(1 0 0)-2×1 reconstruction shown in Fig. 1. This structure has been determined by means of DFT-LDA calculations, looking for the best fitting to photoemission and STM-data [9]. In this structure, we find two different kinds of Se atoms on the surface unit cell: the simple Se atom of the last layer is bonded to two Ga atoms of the second layer, while two Se atoms replace the third As-layer of the crystal.

In our first approach to the Schottky-barrier formation of this geometry, we deposit a Ga atom per surface unit cell and look for the most stable geometries using a DFT-LDA molecular dynamics code. In a second step, two Ga atoms per surface unit cell are deposited on the surface and again the most stable geometries are sought. In Section 3, we will present these geometries and the corresponding DOS that allow us to find out how the barrier height evolves with the metal coverage.

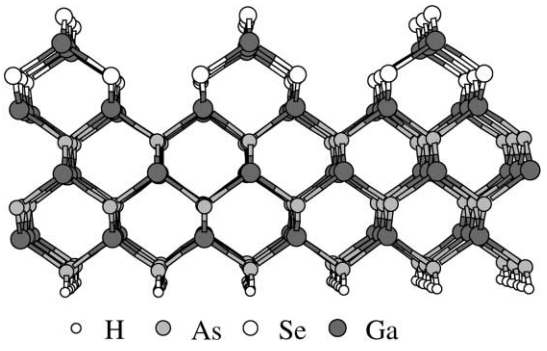

Fig. 1. Ball-and-stick model of the Se-passivated GaAs(1 0 0)-2×1 reconstruction.

In our calculations, we have used the Fireball'96-code [11,12] that has been shown to provide rather fast and accurate molecular dynamics calculations of the geometries and electronic properties of semiconductors interfaces. This method uses localized orbitals generated by solving the atomic problem within the DFT-LDA and the pseudopotential approximations. Norm-conserving pseudopotentials are used, as well as the Ceperly–Adler form of the exchange-correlation potential as parameterized by Perdew and Zunger [13]. We also mention that the forces on each atom are calculated by means of a variation of the Hellmann–Feynman theorem, and that molecular dynamics are used to obtain the lowest-energy atomic configuration. We also mention that in our calculations, we have used a finite slab of six GaAs-layers passivated on one side with hydrogens having the appropriate charges, and, on the other side, with the Se-overlayer mentioned above.

3. Results and discussion

Our main results for the case of one Ga atom per surface unit cell on the Se/GaAs(1 0 0)-2×1 reconstruction are summarized in Fig. 2. Parts (a)–(c) of the figure show three different geometries corresponding to:

(a) The Ga atom adsorbed on top of the Se atom of the last layer.
(b) The Ga atom displaced with respect to the previous position, forming bonds with two Se atoms, one in the last layer, the other in the crystal third layer.
(c) The Ga atom located in the middle of the trench forming two bonds with two Se atoms of the crystal third layer.

Our calculations yield the following chemisorption energies: (a) 1.42 eV, (b) 1.89 eV, and (c) 1.66 eV. These results show that the Ga-preferential adsorption sites correspond to positions where atoms form two bonds (cases (b) and (c)) with Se atoms, and that the

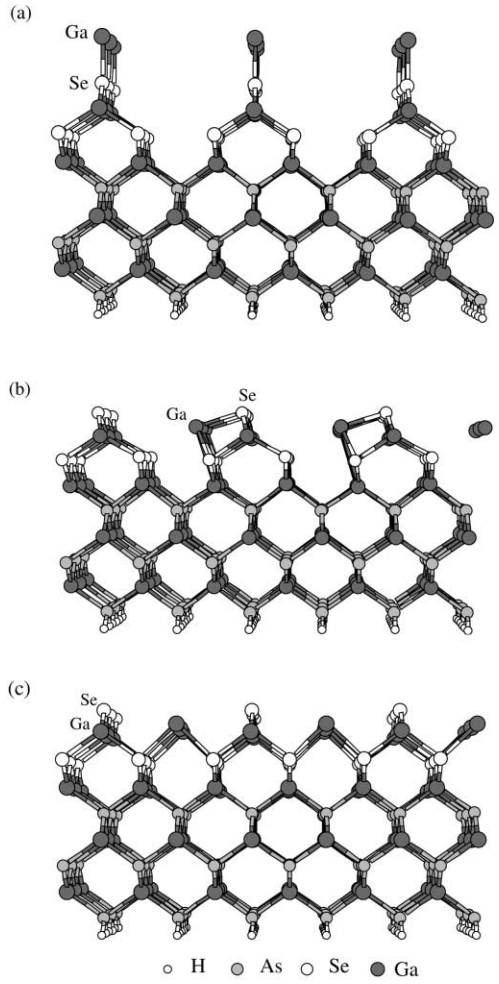

Fig. 2. Ball-and-stick model of the most favorable geometries obtained when depositing one Ga atom per surface unit cell on the Se-passivated GaAs(1 0 0)-2 × 1 reconstruction.

most energetically chemisorption site is the one shown in Fig. 2b.

We analyze the Schottky-barrier formation by calculating the electron DOS for each case and the corresponding interface Fermi energy.

In Fig. 3a–c, we show the local-DOS (LDOS) calculated for the adsorbed Ga atom and the last layer Se atom, the interface Fermi level and the semiconductor energy gap. This energy gap has been determined by calculating the LDOS in third and fourth layers of the semiconductor, a region where the bulk properties are practically recovered. In the three cases, we find similar results: the LDOS shows an energy gap coin-

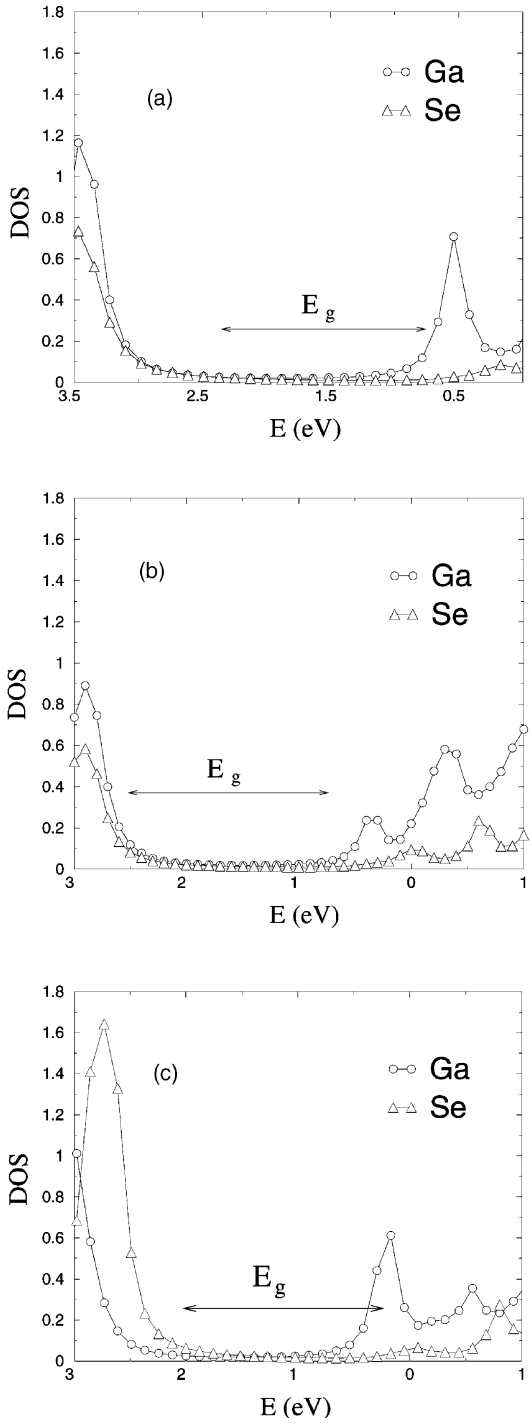

Fig. 3. LDOS on the Ga and the Se atoms of the geometries shown in Fig. 2a–c. The Fermi level defines the zero of energy. E_g defines the semiconductor energy gap.

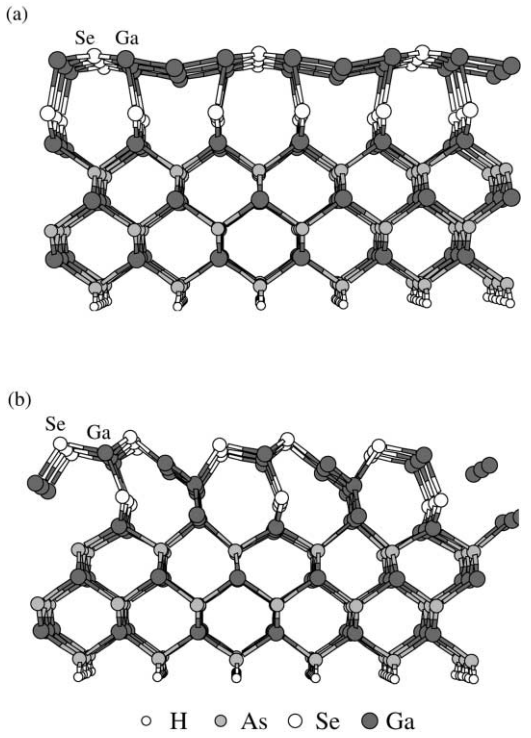

Fig. 4. Ball-and-stick model of the most favorable geometries obtained when depositing two Ga atoms per surface unit cell on the Se-passivated GaAs(1 0 0)-2 × 1 reconstruction.

ciding practically with the semiconductor energy gap, in such a way that the Fermi level is practically located in the semiconductor conduction band bottom. Notice also the Ga-induced DOS around the conduction band bottom, responsible of the new IDIS pinning the Fermi level at the top of the semiconductor energy gap. In our results, the Fermi level appears a little above the energy gap top due to the finite slab used in our calculations; we can expect, however, that for a semiinfinate semiconductor the interface Fermi level would be pinned at the semiconductor conduction band bottom.

Our main results for two Ga atoms deposited on the Se–GaAs(1 0 0)-2 × 1 reconstruction are summarized in Fig. 4.

In Fig. 4a, we find a geometry in which the Se atoms of the GaAs/Se(1 0 0)-2 × 1 reconstruction are still bonded to the Ga atoms of the fourth layer; on top of this we find a layer formed by three Ga atoms and one Se atom per surface unit cell. This structure presents a substantial modification of the original GaAs/Se(1 0 0)-2 × 1 surface, the two new Ga atoms forming with the Se and Ga atoms of the first and second layers of the passivated structure an almost flat layer. Fig. 4b presents another structure we have found in our molecular dynamics calculations: in this geometry, one out of the two Se atoms of the third layer of the GaAs/Se(1 0 0)-2 × 1 reconstruction is substituted for a Ga atom; then, there appears a rather irregular layer formed by two Ga and two Se atoms. In our calculations, the chemisorption energies of Fig. 4a and b are 5.13 and 5.96 eV per two Ga atoms, respectively, showing that case (b) is more favorable energetically.

We have also analyzed the Schottky-barrier formation by calculating the LDOS on the adsorbed Ga atoms and the last Se atom of both structures. Fig. 5a

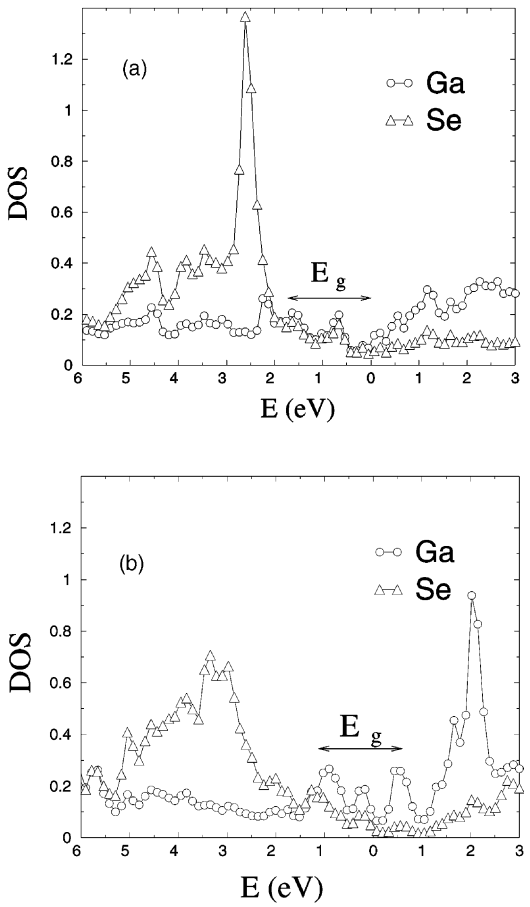

Fig. 5. LDOS on the Ga and the Se atoms of the geometries shown in Fig. 4a and b. The Fermi level defines the zero of energy. E_g defines the semiconductor energy gap.

and b shows the corresponding LDOS and the semiconductor energy gap.

Two results are worth commenting:

(a) For the structure of Fig. 4a, with a Se-layer bonded to a Ga-layer, we find similar results to what we calculated for a Ga atom coverage; this means that we find a Fermi level practically located at the top of the semiconductor energy gap.
(b) For the geometry of Fig. 4b, we find an important change: in this case, for which the Se-layer is replaced by a $Se_{0.5}Ga_{0.5}$ layer, the Schottky-barrier is located around the mid-gap, very much in coincidence with results obtained for clean GaAs surfaces. More precisely, we find a Schottky-barrier, ϕ_{bn}, of $\simeq 0.6$ eV, for an energy gap of $\simeq 1.7$ eV. This should be compared with some calculations [14] for K deposited on GaAs(1 0 0)–As-rich surfaces where the Fermi level is controlled by the semiconductor intrinsic charge neutrality level [2]: in this case, it was found a Schottky-barrier ϕ_{bn} of $\simeq 0.5$ eV for an energy gap of $\simeq 1.5$ eV.

These results show a striking difference between the cases of Fig. 4a and b, and suggest that in the case of passivated surfaces, as far as we keep the basic passivated structure between the semiconductor surface and the external passivating agent, we alter dramatically the Schottky-barrier heights. As shown in many other examples [9], we always found for these cases ohmic contacts for the GaAs–metal interface. However, if after the metal deposition we alter the structure between the semiconductor and the passivating agent, we can restore the ''ideal'' Schottky-barrier as found in the case of Fig. 4b.

4. Conclusions

We have analyzed theoretically the effect of depositing a Ga-overlayer on a Se-passivated GaAs(1 0 0)-2×1 reconstruction. Our molecular dynamics calculations, performed by means of DFT-LDA-selfconsistent calculations, show dramatic effects of the metal overlayer on the GaAs surface. Initially, for a deposition of a Ga atom per surface unit cell we still find the semiconductor keeping its initial identity, with the Ga-adatom deposited on the passivated interface: in this case, we find that the Ga-adatoms create a new LDOS located around the semiconductor energy gap top, and yield an ohmic contact between the metal and the semiconductor.

In a second step, when a deposition of two Ga-adatoms per surface unit cell is considered, a strong modification of the passivated surface is found. In the energetically most favorable structure, we found that some Ga atoms replace the Se atoms of the third layer of the initial GaAs(1 0 0)–Se-2×1 geometry. This structure presents a very different electronic structure: in particular, we found that its Schottky-barrier is similar to the one found for ideal GaAs–metal junctions.

Our results show the extreme importance of characterizing the metal–semiconductor interface geometry to control appropriately the corresponding Schottky-barrier.

Acknowledgements

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