

A first-principles study of the structural and electronic properties of III–V/thermal oxide interfaces

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ABSTRACT

A theoretical study of the structural and electronic properties of the interfaces between a set of III–V compound semiconductors of technological interest and their native oxides is reported. First-principles techniques have been applied to model the reaction of oxidation of the GaAs(001)–β2(2 × 4) surface and to generate a set of representative models of the atomic structure of a thermally grown GaAs/native oxide interface. The obtained models have been extended to the InAs/ and In_{0.5}Ga_{0.5}As/native oxide interfaces case. The impact of indium on both the structural changes occurring during the oxidation of the substrate and the resulting electronic properties has been quantified.

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1. Introduction

The rapid scaling of complementary metal–oxide–semiconductor (CMOS) devices to ever smaller dimensions is currently leading the microelectronic industry to introduce major changes in the design of the transistors. Among them, the replacement of the SiO₂ insulating layer with a gate oxide of higher dielectric constant and the introduction of a metallic electrode have been (and are still) challenging issues. To meet the requirements of the next technological nodes, the silicon channel will soon have to be replaced by an alternative semiconductor [1,2]. Due to their high electron mobility, III–V compounds such as GaAs and InAs are ideal candidates to replace Si as the active material in the transistor channel [3]. However, an effective electrical passivation of the III–V materials remains an unsolved problem which prevents the development of functional MOS devices. In fact, III–V/oxide interfaces are affected by high density of defect states in the band gap which pin the Fermi level and are responsible for the poor electrical performances of the device [4,5].

Even though a lot of effort has been dedicated over the last thirty years to understand the formation of oxide on III–Vs [6],

the impact of the local atomic order and of the chemical bonding on the III–V oxides are still not well described and understood [7].

Through this paper, we aim to provide some understanding of the structure of the III–V/oxide interface at the atomic scale and to shed light on the nature of the defects generated during the oxidation process which affect the electrical properties of the interface.

2. Methodology

The simulations were performed within the density functional theory (DFT) method as implemented in the code SIESTA [8,9]. The electron–ion interaction was described by Troullier–Martins norm-conserving pseudopotentials [10] with the following electronic configuration of the elements: H 1s¹, O [1s²] 2s² 2p⁴, Ga [Ar] 3d¹⁰ 4s² 4p¹, As [Ar, 3d¹⁰] 4s² 4p³, and In [Kr] 4d¹⁰ 5s² 5p¹, with the square brackets denoting the core configurations. The electron–electron interaction was treated within the local density approximation (LDA) [11]. A double zeta basis set with polarization orbitals was employed to describe the valence electrons.

It is well known that the calculated energy band gap of bulk semiconductors, within LDA, is pathologically underestimated by about 50% [12]. A method to solve this problem was proposed by Christensen [13] and Segev et al. [14] who included an atom-centered repulsive potential (of Gaussian shape) at the all-electron stage of the pseudopotential generation. This localized potential

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acts mainly on the lowest-energy state 1s and affects higher-lying states through the orthogonality of the wave functions. This method was applied here to bulk GaAs and InAs, and extensive tests were performed to ensure that the modified pseudopotentials yield band structures in close agreement with experiments while preserving the ability to produce atomic structures and energies that are as accurate as those obtained with regular pseudopotentials. This correction was then used to compute the electronic properties of the III–V/native oxide interface.

The obtained energy band gaps of bulk GaAs and InAs are calculated to be 1.30 and 0.44 eV, which are in agreement within the 12% and 5% with experimental values (1.49 and 0.42 eV, respectively). The V_0 (70 for Ga, 40 for In and 20 for As, in Ha) and r_0 (0.06 Bohr for Ga, In and As) parameters defining the added potential were chosen to keep a proper ordering of the conduction bands [13] and to minimize the impact on both the bulk lattice constant and the structural properties to less than 1% with respect to the unmodified pseudopotential cases.

To model the GaAs(001)– $\beta 2(2 \times 4)$ reconstructed surface, a repeated slab geometry consisting of nine layers of GaAs was terminated by a layer of hydrogen atoms in a bridging and terminal configurations. This construction ensures a proper passivation of the bottom of the slab, as illustrated in reference [15]. The slabs were separated by a vacuum region of ~ 14 Å. An energy cutoff of 250 Ry and a $4 \times 2 \times 1$ Monkhorst–Pack grid for the sampling of the Brillouin zone were adopted for the structural relaxations and a $8 \times 4 \times 1$ grid for the computation of the density of states (DOS). This ensures the convergence of both the structural and electronic properties computed.

The ionic relaxations were performed using the conjugate gradient algorithm [16], fixing the bottom two layers as well as the hydrogen atoms, until the atomic forces converge to 20 meV/Å. The ab initio molecular dynamics (MD) simulations [17] were carried out at either a constant or a varying temperature controlled by a Nosé thermostat [18], with a time step of 1 fs.

3. Results and discussion

3.1. GaAs/oxide interface

The oxidation of the GaAs(001) surface has been modeled by performing a set of MD simulations where oxygen atoms have been gradually added on top of the surface. Note that we took advantage of the dissociative process of the adsorption of oxygen on the GaAs(001) surface [15] to minimize the computational burden required for our simulations. We therefore oxidized the GaAs surface by using atomic oxygen instead of molecular ones with the following procedure: firstly, the reconstructed surface has been loaded with oxygen atoms at a temperature ranging in the values of 680–800 K until one, two and three monolayers (MLs) of native oxide are grown on GaAs(001). Subsequently, a simulated annealing treatment at a target temperature of 1400 K for a simulation time of ~ 5.3 ps has been applied. The resulting structures were

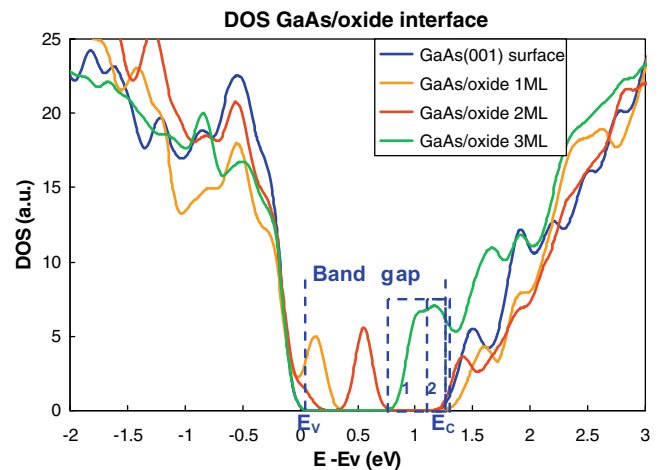


Fig. 2. DOS of the three GaAs/oxide (1, 2, 3ML) interface models and of the GaAs(001)– $\beta 2(2 \times 4)$ surface.

finally quenched to room temperature within 1 ps to be refined by a geometry optimization procedure.

During the reaction, the upcoming O atoms attack the Ga–As bonds of the surface to form mainly bridging Ga–O–As units. The obtained thin oxide films are formed by a random network of Ga–O–As structures (Fig. 1) for which, the computed average bond lengths are 1.82 Å for the As–O and 1.97 Å for the Ga–O bonds. During the dynamics, the native oxide thickens and adopts (for the thickest film we considered) an averaged coordination number of 2.5, 2.9 and 3.7 for the O, As and Ga atoms, respectively.

The electronic properties of the interfaces were investigated by computing the density of electronic states (DOS). Interestingly, the comparison of the DOS profiles of the relaxed GaAs/oxide interfaces with the GaAs(001)– $\beta 2(2 \times 4)$ one (Fig. 2) reveals a clean band gap for the unoxidized surface and the presence of defect electronic states within the gap for all the interfaces considered. Moreover, the distribution of the defect states is located in different regions of the gap for the three interfaces, i.e. close to the valence band, at the middle of gap, and close to the conduction band for the 1, 2 and 3ML models, respectively.

In order to gain a better understanding on the nature of these electronic defects, we integrated their associated electronic charge densities and projected them on the atomic structure of the interfaces. The obtained spatial distribution of the electronic charge is then correlated with the nature of the defect states present in the band gap. As an illustration, two examples of this study are shown in Fig. 3 for the GaAs/oxide 3ML interface: in (a) the charge density (associated to the energy range indicated as 1 in Fig. 2) is localized around an As atom with a dangling bond, while in (b) the computed charge density (associated to the energy range 2 in Fig. 2) is mainly localized on a Ga dangling bond.

In summary, our simulations reveal that the main source of defect levels within the gap is directly associated to structural defects

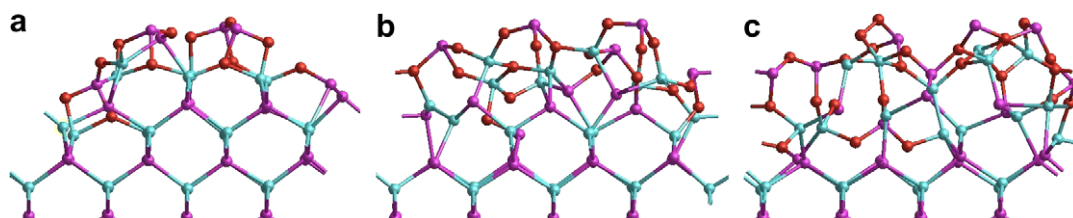


Fig. 1. Illustration of the relaxed atomic structures of the GaAs/oxide interfaces with (a) 1ML, (b) 2ML and (c) 3ML of native oxide. The As, Ga and O atoms are depicted by purple, light blue and red balls, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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