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Initial stages of the growth of Al on GaN(0 0 0 1)

Reyes Garcia-Diaz [a], Gregorio H. Cocoletzi [a,b,c,*], Noboru Takeuchi [c]

[a] Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J-48, Puebla 72570, México
[b] Centro de Investigación Científica y de Educación Superior de Ensenada, Km. 107 Carretera Tijuana-Ensenada, Código Postal 22860, Apartado Postal 2732, Ensenada, Baja California, México
[c] Centro de Nanonciencia y Nanotecnología, Universidad Nacional Autónoma de México, Ensenada, Baja California, México

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ABSTRACT

Using the density functional theory, total energy calculations with the inclusion of gradient corrections, we studied the binding and diffusion of Al ad-atoms on GaN(0 0 0 1). It is found that when the Al atom remains on the surface, the most stable configuration corresponds to the adsorption at T4 sites on top of the N atom. Adsorption on the hollow site (H3) results in a slightly higher energy. The transition site corresponds to the bridge position, with an energy barrier of 0.66 eV. However, a configuration with the Al atom replacing a first layer Ga atom and the latter occupying T4 sites is more stable. Surface diffusion of this newly created Ga ad-atom is now more favorable, with an energy barrier as low as 0.43 eV. At full coverage, in the most stable configuration, the Al atoms replace the first Ga layer, with those atoms located almost on top of the Al atoms and forming chains. In this configuration, no dangling bonds are left behind.

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1. Introduction

Gallium nitride (GaN), a wide gap semiconductor (with an experimental gap of 3.4 eV), has been extensively studied because of its technological applications [1]. Different from the case of Si, it has a direct band gap. Therefore it is used in the fabrication of optoelectronic devices that work in an ample range of the electromagnetic spectrum. For example, GaN is the basic compound in the fabrication of blue diodes and lasers [1]. The fabrication of $Al_xGa_{(1-x)}N$ systems has further increased the possible applications of GaN [2]. Due to its ability to form alloys and hetero-structures with AlN, it is possible to fabricate materials with continuously varying band gaps in the 3.4–6.2 eV energy range, with the upper part range being important in the fabrication of optoelectronic devices in the ultraviolet region [2].

In all applications, it is fundamental to have very good quality layers. Therefore, attempts have been made to grow high-quality AlN films under different growth conditions on GaN substrates [3]. In order to improve the quality of the grown material and to ensure the formation of sharp interfaces, good knowledge of the atomic surface structure of the GaN and AlN surfaces and initial stages of the growth of Al on GaN is needed. Progress has been made in the past decades on the understanding of surface structures of GaN [4–6] and AlN (0 0 0 1) [7,8]. A number of reconstructions have been observed depending on stochiometry, and detailed atomic arrangements for these reconstructions have been determined. However, less effort has been dedicated to investigate the interaction of Al with GaN surfaces. In this paper, we have studied initial stages of the growth of Al on GaN(0 0 0 1). Specifically, we have calculated adsorption sites and energy barriers for diffusion of Al ad-atoms on the bulk terminated GaN(0 0 0 1) surface, from a single ad-atom up to a full monolayer.

2. Method

The calculations were performed in the framework of periodic density functional theory as implemented in the PWscf code [9]. We treat the exchange and correlation potential energies according to the generalized gradient approximation (GGA) with the gradient corrected Perdew, Burke and Enzerhoff (PBE) functional [10]. We have used the repeated slab geometry, each slab consisting of 4 GaN double layers and a (2×2) configuration, plus the ad-atom on top of the surface. The bottom surface was saturated by fractional pseudo-hydrogen atoms. Two consecutive slabs were separated by an empty space $\sim$9.0 Å wide. The three topmost GaN bilayers of the slab and the ad-atoms had full freedom to move. The bottom GaN bilayers and the saturating pseudo-H atoms were frozen in order to simulate a bulk-like environment. A $(3\times3\times1)$ Monkhorst–Pack mesh [11] has been used to sample the Brillouin zone. We used Vanderbilt ultra-soft

* Corresponding author at: Instituto de Física, Benemértia Universidad Autónoma de Puebla, Avenida 18 sur y San Claudio, CU, Puebla, CP 72570, Puebla, Mexico.
E-mail address: cocoletz@sirio.ifuap.buap.mx (G.H. Cocoletzi).

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pseudopotentials [12], and the Ga 3d electrons were explicitly treated as valence electrons. We used kinetic energy cutoffs of 25Ry and 200Ry to represent the wave function and charge density, respectively.

3. Results

3.1. Adsorption of a single Al ad-atom

It has been found that under N-rich conditions a (2×2)-H3 N ad-atom model is energetically the most stable, while for Ga-rich conditions a (2×2)-T4 Ga ad-atom structure is favored. In both configurations, the ad-atoms are on a Ga terminated GaN bilayer. In the Ga rich limit, a contracted Ga bilayer model is the most stable configuration [5]. Since we are interested in the non-extreme Ga rich regime, our calculations correspond to Al ad-atoms on a Ga terminated GaN bilayer. Ad-atom kinetics can be studied by calculating the potential energy surface (PES). This is obtained by fixing the ad-atom laterally at a given position $\mathbf{r}_{\text{parallel}}$ and allowing its height and all other atomic coordinates to relax. The minima of the PES give the adsorption sites. Other important information that we can obtain from the PES are diffusion barriers and minimum energy paths. In Fig. 1, we mark some possible adsorption sites, and the dashed line shows the diffusion pathway. A two dimensional cut of the PES along this path is plotted as a solid line in Fig. 2a for the Al ad-atom. We find that the most stable site corresponds to adsorption on top of a second layer N atom (this site is usually called the T4 site). Adsorption on the hollow site (H3) results in a slightly higher energy. The transition state corresponds to the bridge position, with an energy barrier of 0.66 eV. This energy barrier is very similar to the one found for the diffusion of Ga ad-atoms on the same surface [6]. Migration over the on-top position (T1 site) is energetically very unfavorable.

3.2. Exchange of the Al ad-atom with a first layer Ga atom

We have also considered the possibility of the Al ad-atom to migrate into the first bilayer by replacing a Ga atom. As seen in Fig. 3, there are now two different T4, H3, bridge, and top sites.

In the first kind, the newly created Ga ad-atom forms bonds with 2 first layer Ga atoms and with the Al atom, while in the second kind, the Ga ad-atom forms bonds with Ga atoms only.

As seen in Table 1 and Figs. 2b and c, replacing a first layer Ga atom by the Al atom is energetically very favorable, since each atomic configuration of a Ga atom above the mixed first layer has a lower energy than that of the adsorption of Al on the T4 site. Among these configurations, those with no Ga–Al bonds are more

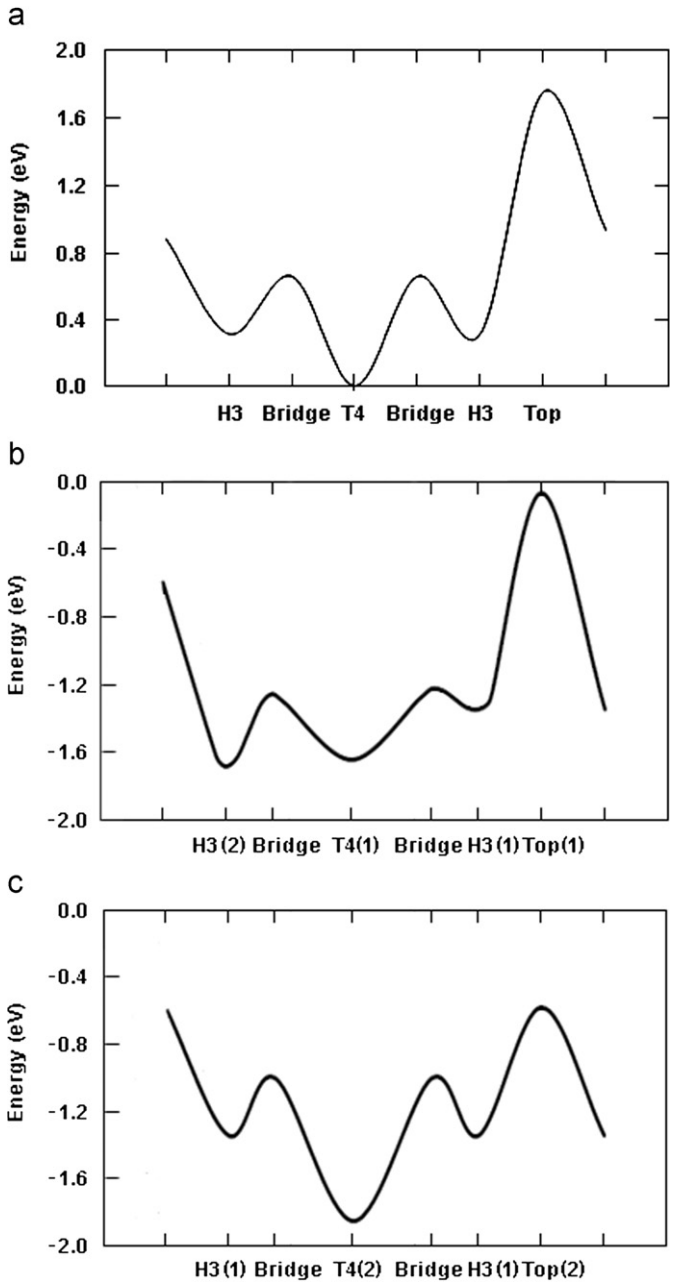

Fig. 2. Relative energies (in eV) for an Al ad-atom at various sites on the GaN bilayer-terminated (0 0 0 1) surface. (a) Al ad-atom over the first layer (b) and (c) Al atom replacing a first layer Ga atom.

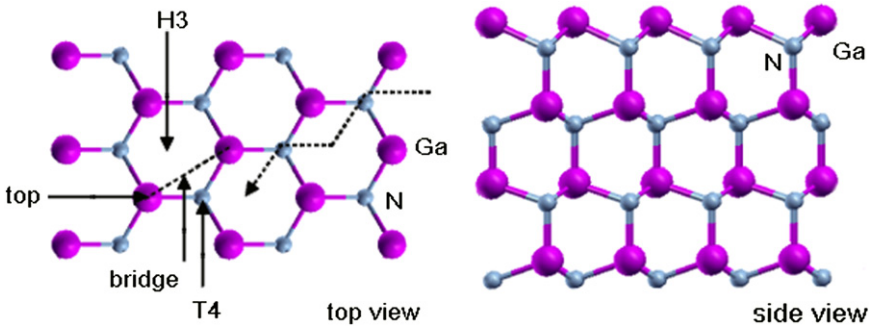

Fig. 1. Schematic atomic structures for the GaN bilayer-terminated GaN(0 0 0 1) surface, showing high symmetry sites. The dashed line in the top view indicates the ad-atom diffusion paths.

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