

Adsorption of group III atoms on silicon (111) substrate surface: Car-Parrinello simulations

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Abstract. The Car–Parrinello molecular dynamics (CPMD) method are performed to investigate the adsorption of aluminum, gallium and indium atoms on silicon surface. The atomic diffusions on silicon (111) substrate surface are investigated. The minimum energy pathways for several diffusion paths along the row of path x sites and path y sites are predicted. The diffusion length in path x is longer than path y for aluminum, gallium and indium ad-atoms on silicon surface. Our calculation results reveal that diffusion barriers of aluminum, gallium and indium atoms on silicon (111) surface are anisotropy.

Keywords: Gallium nitride, Adsorption, Silicon.

1. Introduction

In recent decades, gallium nitride and related group III-nitride compound semiconductors are important compound semiconductor materials [1]. Gallium nitride based materials are receiving much attention due to the current and potential application in light emitting diodes, laser diodes, photo detectors, solar cells, high frequency and high power electronics devices [2, 3]. Silicon substrates afford a lot of advantages for gallium nitride based devices arising from the availability of large diameter wafers. There is significant interest in the growth of gallium nitride films on silicon substrates for many applications owing to its low cost, large size available, and good thermal and electrical conductivities [4]. The growths of gallium nitride based devices on silicon substrate have attracted lots of research attentions. However, the growth of low dislocation density gallium nitride films on silicon substrate is challenging due to the large lattice and thermal expansion mismatches between the two materials. Thick gallium nitride film grown on silicon substrate for device fabrication is hard to achieve without cracks. Gallium nitride based devices on silicon is usually grown on the silicon (111) oriented surface due to the three-fold atomic arrangement of this orientation being compatible to the hexagonal structure of the basal planes of the wurtzite-type crystals. The growth of gallium nitride is also possible on substrates with a silicon (001) surface [5, 6, 7]. However, it is very challenging because of difficulties with different types of surface reconstructions. In order to clarify how strain affects gallium nitride epitaxial growth, a better understanding of the microscopic adsorption mechanisms on gallium nitride surface is demanded. The influence if silicon surface on the chemisorption should be also discussed clearly. In this paper, we investigate the initial growth of group III-nitrides on silicon surfaces by Car–Parrinello molecular dynamics (CPMD) method simulations. Our theoretical approach provides an atomic-scale insight into the regions of the initial growth of group III-nitride on silicon substrates.

2. Computational method

In order to understand the adsorption of group III atoms on silicon (111) surface, the first principle calculations were performed by using the Car-Parrinello molecular dynamics (CPMD) method, which has been successfully used for the study of atom and molecular adsorptions [8]. The CPMD code is an implementation of DFT in the Kohn-Sham (KS) formulation and of the Car-Parrinello

scheme. The valence electrons are included in the calculation with the interactions between valence electrons and atomic cores being described by pseudo potentials. The valence electrons are included in the calculation with the interactions between valence electrons and atomic cores being described by pseudo potentials. In the present work, the interactions of the ion cores with the valence electrons are described by Trouiller-Martins norm-conserving pseudo potentials, and non-local core corrections (NLCC) were included for the gallium and indium species [9, 10]. The electronic wave functions are expanded in a plane wave basis set with an energy cutoff of 80 Ry. The exchange functional given by Becke and correlation energy expression by Lee-Yang-Parr (LYP) are used with the implemented of local density approximation (LDA). Wavefunction optimizations were taken in CPMD to obtain the total energies of the simulation systems. The CPMD code, version 3.11.1, is used.

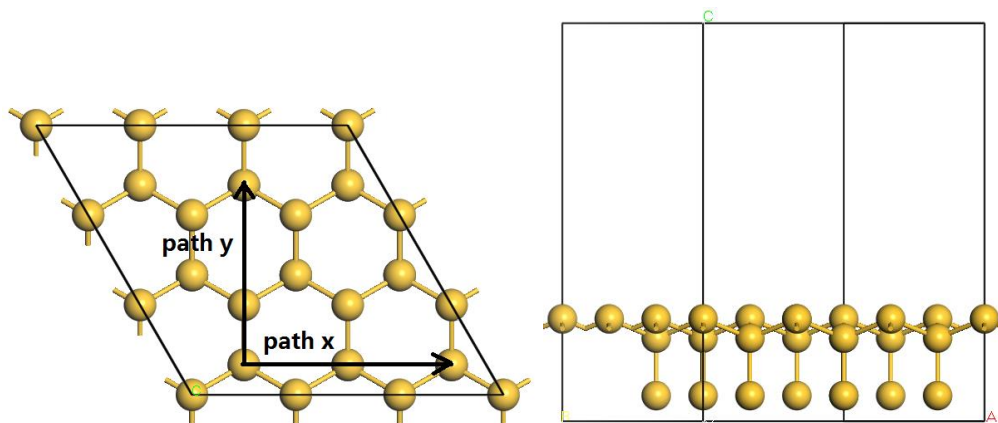


Fig. 1 Silicon (111) surface

To model silicon substrate surface, 27-atom systems are applied. Periodic boundary conditions are applied along the crystallographic axial directions. The Monkhorst-Pack scheme with uniform mesh points is applied in this calculation. Group III adsorbed atoms were placed on the surface with a 20 angstrom vacuum region above the adsorption surface. Two possible diffusion paths for initial surfaces have been considered. The schematic model of III atoms diffusion path is shown in Fig.1. In each adsorption site, the adsorption distance of ad-atoms above the silicon surface plane was considered with 1.5 angstrom. The adsorption distances are defined as the nearest distance between the ad-atoms and silicon surface plane.

The adsorption energy of magnesium ad-atom on gallium nitride surface is defined as follows:

$$E_{\text{adsorb}} = E_{\text{adatom+Si}} - E_{\text{adatom}} - E_{\text{Si}} \quad (1)$$

Where $E_{\text{adatom+Si}}$ is the total energy of the silicon surface with the adsorbed atom, E_{Si} stand for the total energy of the pristine silicon (111) surface without the ad-atom, and E_{adatom} is the total energy of aluminum, gallium and indium atoms.

3. Results and Discussions

The minimum energy pathways for several diffusion paths along the row of path x sites and path y sites are predicted by CPMD calculations. The adsorb energy diagram of ad-atom hopping process for aluminum, gallium and indium are shown in Fig 2, Fig 3 and Fig 4, respectively.

First principle calculations predict that aluminum ad-atom diffuse along path x direction need to overcome a barrier of 2.25 eV from a stable state to a meta-stable state. For path y case, the barrier is 10 eV, which is much larger than path x. These results suggest that aluminum ad-atom tend to diffusion along path x direction.

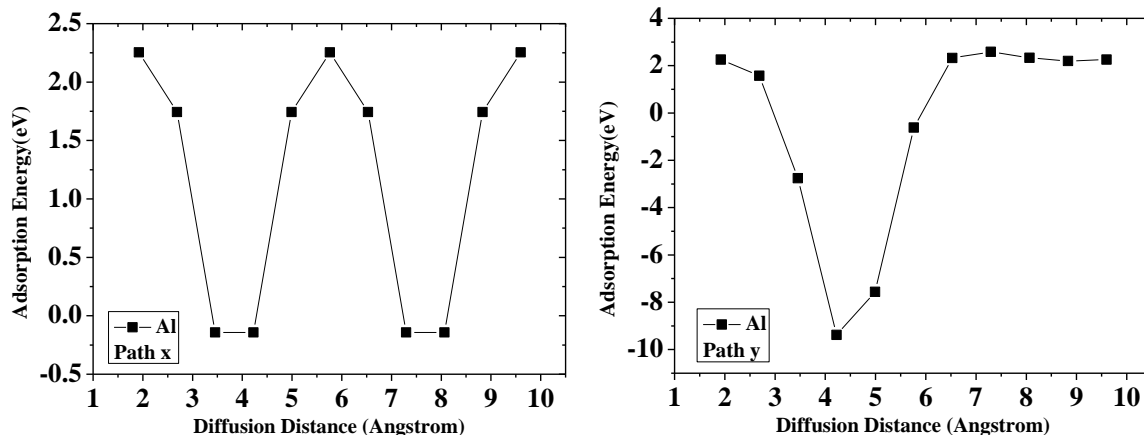


Fig. 2 The diffusion distance of aluminum ad-atom

Gallium ad-atom diffusion along path x and path y directions need to overcome a barrier of 0.8 eV and 5.5 eV, respectively. The diffusion length in path x is longer than path y.

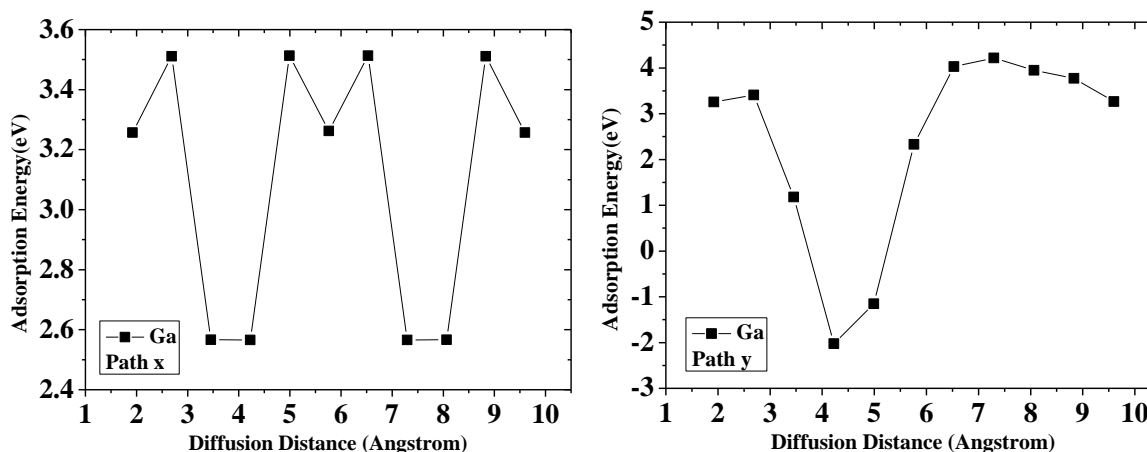


Fig. 3 The diffusion distance of gallium ad-atom

For indium ad-atom case, the diffusion barriers for path x is 3.5 eV. And the max diffusion barrier in path y is 16eV. These results suggest that diffusion barriers of ad-atom on silicon (111) surface are anisotropy. Besides, as Fig.4 shows, the maximum adsorption energy of path x and path y are different, which reveal that a different barrier energy pathway between indium ad-atom diffuse along path x and path y.

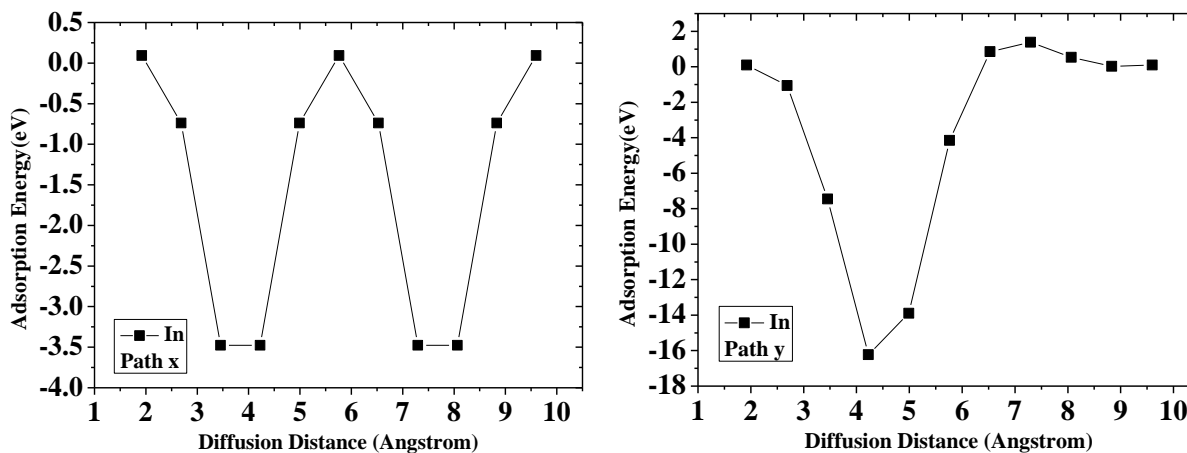


Fig. 4 The diffusion distance of indium ad-atom

4. Conclusion

We have investigated the atomic diffusion on silicon (111) substrate surface. The adsorption energies are taken into account in contrast to CPMD studies. The diffusion length in path x is longer than path y for aluminum, gallium and indium ad-atoms on silicon surface. Our calculation results reveal that diffusion barriers of aluminum, gallium and indium atoms on silicon (111) surface are anisotropy.

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