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Theoretical Investigation of the Electronic and Structural Properties of AlN Thin Films

K. K. Abgaryan[a], *, D. I. Bazhanov[b], **, and I. V. Mutigullin[a], ***

[a] *Dorodnicyn Computing Centre, Russian Academy of Sciences, ul. Vavilova 40, Moscow, 119333 Russia*
[b] *Moscow State University, Moscow, 119991 Russia*
**e-mail: kristal83@mail.ru*
***e-mail: dmibaz@sols347-5.phys.msu.ru*
****e-mail: mutigul@ccas.ru*

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Abstract—Studying the electronic and structural properties of AlN thin films is an important problem because such films are widely used as a buffer layer when growing GaN-based semiconductor heterostructures on Si substrates. In this paper, we carry out a theoretical investigation of the properties of an Al-terminated AlN(0001) surface in the framework of the density functional theory. *Ab initio* calculations allow us to analyze the effect of the in-plane lattice strain on the energy of this surface. It is shown that compressive strain causes a decrease in the AlN(0001) surface energy, while tensile strain leads to its increase. Knowing the surface energy values allows us to evaluate the stress of the surface under investigation. In addition, the curvature of the AlN surface is calculated for various AlN film thicknesses in the case of free growth. The obtained values of the surface curvature are in close agreement with the known experimental results.

Keywords: thin films, semiconductor heterostructures, first-principle calculations
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INTRODUCTION

Fabricating multilayer semiconductor nanostructures (MSNSs) [1] with desired parameters and predictable properties is one of the most important directions of modern microelectronics. In recent decades, there has been growing interest in wide-bandgap semiconductors (WBGSs) (for example, AlGaN, GaN, SiC, and diamond) that are regarded as promising materials for electronic and optoelectronic devices. In this class of materials, gallium nitride can be singled out as possessing some unique properties and being widely recognized as a next-generation semiconductor. Presently, gallium nitride is used in the commercial production of blue and green light-emitting diodes.

Technologies for synthesizing WBGS-based structures, which are used for fabricating state-of-the-art microwave devices, are now being developed intensively. As a material for microwave transistors, WBGS-based multilayer structures have a number of substantial advantages that make it possible to radically improve the parameters of both microwave transistors and integrated circuits. The well-established industry for manufacturing GaN-based structures, which provides wide possibilities for modifying the band structure of devices and allows obtaining two-dimensional electron gas (2DEG) of high quality is an important advantage of gallium nitride over other WBGSs.

When growing heterostructures with nano-thick layers, it is fundamentally important to understand, at a microscopic level, the structure of interfaces, as well as the initial stage of growth. In terms of technological usability, Si substrates are most suitable for growing gallium nitride, since silicon is an inexpensive material that is widely used in microelectronics and allows one to form large-diameter wafers. Nonetheless, gallium nitride and silicon considerably differ in their thermal-expansion coefficients, which results in quite a large flexure of the MSNS when cooling it to room temperature and gives rise to strong tensile strains in the GaN layer. These tensile strains cause the GaN layer to crack along the $\{1\bar{1}00\}$ directions. When growing gallium nitride on silicon, to minimize strains between the substrate and the film, as well as to improve the properties of the latter, an AlN buffer layer is generally formed that has its own strains and surface curvature [2]. Thus, to understand the process of MSNS formation at an atomic level, it is important to analyze the electronic and structural properties of AlN buffer films grown on the Si surface.

The purpose of this work is, using the first-principle approach, to investigate the curvature of the AlN film depending on its thickness and on the residual stress arising in the process of epitaxial growth on the Si(111) substrate and to carry out some first-principle calculations of the Al-terminated AlN(0001) surface.

CALCULATION TECHNIQUE

The investigation is carried out in the context of the density functional theory with the use of the plane-wave basis set and PAW potentials [3]. For calculations, the VASP software complex is employed [4]. To describe exchange-correlation interactions, the local-density approximation (LAP) is used, while the conjugate gradient method is used to relax the forces acting on the ions. The atoms are relaxed dynamically until the total energy of the system gets below 0.001 eV. In this case, the residual forces acting on the ions do not exceed 0.1 eV/nm. The plane-wave cutoff energy is set to be 500 eV. The electronic structure is analyzed by integrating in the Brillouin zone on the k grid constructed using the Monkhorst–Pack method [5]. The size of the k grid for interface modeling is $11 \times 11 \times 1$. The values of the parameters presented above are sufficient to provide reliable results.

RESULTS AND DISCUSSION

First, the equilibrium periods of the AlN lattice in the wurtzite structure are found: the obtained values ($a = 0.309$ nm and $c/a = 1.60$) are in close agreement with the experimental values ($a = 0.311$ nm and $c/a = 1.60$) [6]. For comparison, the effective lattice period of the Si(111) surface (on which AlN is generally grown) is $a'_{Si} = 0.382$ nm. Thus, the lattice period calculated for the AlN lattice is 19% lower than the effective period of the Si lattice, which is close to the experimentally found difference between the periods [7]. Such a strong discrepancy between the lattice parameters results in the overstress of the AlN film surface, which is a key factor of film deformation (curvature).

To model the properties of the AlN film grown on the Si(111) substrate, the formation of the Al(0001) surface is observed experimentally [7]. To find the surface energy, the Al(0001) surface is modeled as a 1×1 supercell in the XY plane that consists of nine atomic layers: five Al layers and four N layers. The thickness of the vacuum layer is chosen so that the two surfaces formed by the slab do not interact with one another under periodic boundary conditions. The energy of the Al-terminated AlN(0001) surface is calculated. Since the supercell includes different numbers of the Al and N atoms, the surface energy is calculated by the formula for nonstoichiometric slabs [8]:

$$\varepsilon = \frac{E^{N}_{slab} - N_{Al}\mu^{bulk}_{AlN} + (N_{Al} - N_{N})\mu_{N}}{2S}, \qquad (1)$$

where E^{N}_{slab} is the total energy of the supercell; N_{Al} and N_{N} denote the number of Al and N atoms in the supercell, respectively; μ^{bulk}_{AlN} is the chemical potential of the AlN structure for a pair of Al—N atoms; μ_{N} is the chemical potential of nitrogen in the structure of a N_2 molecule for one atom; and S is the area of the surface lattice cell.

For the equilibrium period of the AlN lattice, the calculated energy of the AlN(0001)—Al surface is 5.70 J/m^2, which is quite close to the first-principle calculation result (5.68 J/m^2) obtained in [9]. Lattice deformation is modeled by varying the lattice period of the AlN unit cell: −2%, −1%, 0, +1%, +2%. Below is the result of calculating the surface energy.

Lattice parameter variation, %	Surface energy S, J/m^2
−2	5.57
−1	5.63
0	5.70
1	5.74
2	5.75

These values allow us to determine surface stress by using the formula

$$g = \varepsilon + \frac{d\varepsilon}{de}, \qquad (2)$$

where e stands for surface deformation. The calculated value of the derivative $d\varepsilon/de$ is 5.59 J/m^2. Thus, by formula (2), the surface stress is 11.29 J/m^2.

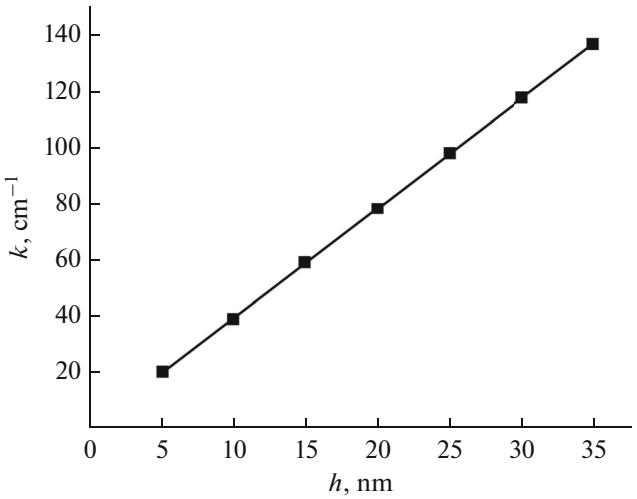
Having found the surface stress, we can analyze, in the context of the classical theory (3), the curvature of the AlN film depending on its thickness and on the residual stress arising in the process of epitaxial growth on the Si(111) substrate.

To evaluate the curvature of the AlN film depending on its thickness and on the residual stress, we use the following relation from the theory of elasticity:

$$g^{f} = \frac{E_s h_s^2 k}{6h_f(1-\nu)}, \qquad (3)$$

where the subscripts f and s denote the parameters of the film and substrate, respectively; g^f is the residual stress in the film; h_f and h_s are the thicknesses of the film and substrate, respectively; E_s and ν are Young's modulus and Poisson's ratio of the substrate; and k is the film curvature.

In this case, it is assumed that the film thickness is lower than the substrate thickness ($h_f \ll h_s$) and that the film is free from any bulk defects (g-const). The figure shows the dependence of the AlN film curvature k on the film thickness h_f for the free AlN growth on the AlN/Si substrate. According to the experimental data, this dependence is constructed using the following AlN parameters: $h_s = 200$ nm, $E = 308$ GPa ($T = 300$ K), and $\nu = 0.287$. The calculated values of the AlN film curvature are close to the experimental values obtained for thin AlN films grown on the Si substrate [10].



AlN film curvature as a function of film thickness for free AlN growth.

CONCLUSIONS

The surface-strain dependence of the AlN(0001)—Al surface energy has been analyzed using the first-principle approach. It has been shown that the compressive strain of the surface cells reduces the AlN(0001)—Al surface energy, while the tensile strain leads to its increase. The obtained values of the surface energy have allowed us to determine the surface stress of the thin AlN film in the case of free growth. In the context of the theory of elasticity, the curvature of the AlN film on the Si substrate has been evaluated depending on the film thickness in the case of free growth.

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