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Computer Simulation and Experimental Investigation of the Crystal Structure and Electronic Properties of InN/Si and GaN/Si Thin Films

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Abstract—A modified method for the magnetron deposition of heterostructures on single-crystal substrates that combines a high degree of efficiency and a high production rate is developed. Grown structures are simulated within the density functional theory to determine the most stable atomic positions in the InN/Si and GaN/Si interfaces.

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INTRODUCTION

Predictive computer simulation on a supercomputer now makes it possible to perform detailed calculations of complex phenomena and processes without natural experiments. This factor significantly reduces the cost and time of the development of modern technologies for new nanomaterials. In addition, it becomes easier to gain insight into many complex physical processes.

Much interest has recently been shown in wide-gap materials (AlGaN, GaN, SiC, diamond, etc.), which are considered to be promising semiconductor materials for new electronic and optoelectronic devices. Among these, GaN has unique properties and is universally recognized as a next-generation semiconductor. Multilayers based on wide-gap semiconductors have a number of fundamental advantages when used in microwave transistors. In particular, they allow us to vary the band structure of devices in wide limits and obtain two-dimensional electron gas (2DEG) with good parameters.

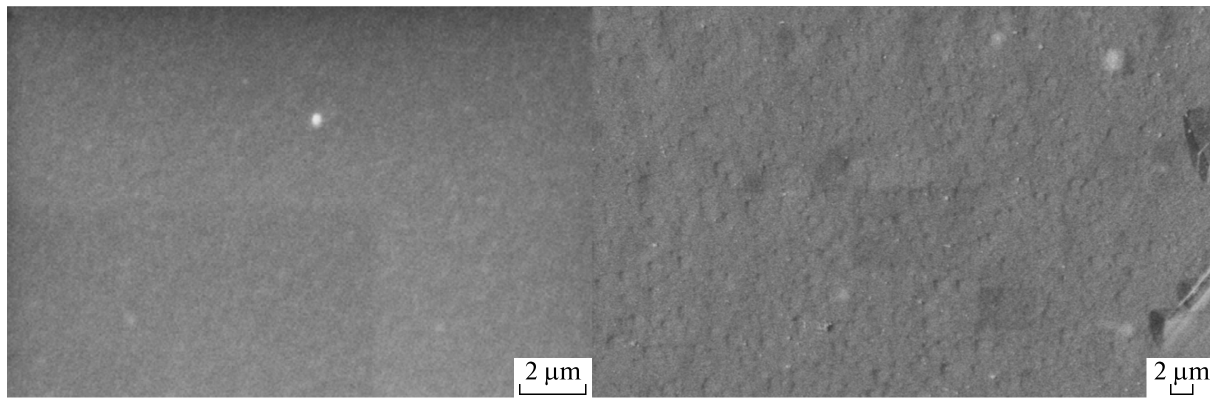
When growing heterostructures with nanolayers, it is very important to understand the structure of interfaces and the initial growth stage at the macroscopic level. For technological applications, the most convenient substrate for growing GaN is silicon: it is inexpensive, widely applied in microelectronics, and can be prepared in the form of large wafers. It is well known that silicon substrates can be nitridized in the initial stage of nitride film deposition. This process is accompanied by the formation of silicon nitride or oxynitride, which, in turn, can degrade the structural quality of nitride films and cause leakage currents [1]. It was nevertheless experimentally demonstrated that, if nitrogen diffusion into the substrate is controlled, we can grow single-crystal GaN films on silicon substrates without forming silicon nitride [2]. This was done by molecular-beam epitaxy (with the [0002] GaN axis oriented along the [111] substrate axis). Another method for growing high-quality semiconductor films on silicon substrates is magnetron deposition. A single-crystal InN(0001) film on Si(111) substrate was formed by magnetron deposition in [3].

In this study, we experimentally grow GaN and InN films on silicon substrates by modified magnetron deposition and theoretically investigate the film–substrate adhesion energy.

EXPERIMENTAL

We designed, fabricated, and tested the main devices for depositing InN and GaN heterostructures on single-crystal substrates using a VUP-4 vacuum system. These devices were a liquid-nitrogen-cooled unbalanced magnetron, a substrate heater with automatic temperature maintainance to 800°C with an error of ±2°C, a unit for plasma etching the films deposited on a dielectric substrate (closed electron drift microaccelerator), a unit for cleaning the substrate surface before depositing heterostructures, and a system for inlet high-purity Ar, N_2, and H_2 gases and their mixtures in different proportions. An advantage of our method is that all of the basic operations necessary for growing heterostructures (particularly heating and cleaning the substrate, the magnetron deposition of semiconductor films, and etching the deposited film) can be performed without extracting the sample from the vacuum chamber.

Using this technique, GaN and InN films were deposited on a single-crystal silicon wafer 20 × 20 mm



Scanning electron microscopy images of surface areas of AlN and GaN films.

in size. The substrate was located at a distance of 40 mm above the magnetron and heated to a temperature of 300°C. The magnetron cathode was coated with gallium or indium layer 1 mm thick and was cooled by liquid nitrogen during the working cycle. The deposition time was 45 min. The working gas was an $N_2 + H_2$ mixture of equal proportions. The film samples obtained were investigated on an EVO-40 scanning electron microscope (ZEISS) with magnification of up to ×50 000. After studying the film surface topography, an energy-dispersive analysis of the surface composition was performed using an INCA attachment (Oxford Instuments).

Our theoretical investigation was carried out within the electron density functional theory, using a basis of plane waves and PAW potentials [4]. The VASP program package was applied in our calculations [5]. The local density approximation was chosen to describe the exchange-correlation interaction. The conjugate-gradient method was used for relaxation of the forces exerted on ions. Dynamic atomic relaxation was performed until the change in the total energy of the system became less than 0.001 eV; in this case, the residual forces exerted on ions were less than 0.01 eV/Å. The cutoff energy of the plane-wave basis was chosen to be 500 eV. The electronic structure was calculated by integrating over the Brillouin zone using a *k*net, constructed according to the Monkhorst–Pack method [6]. The dimension of the *k* net for simulating interfaces was chosen to be 11 × 11 × 1. These values of the aforementioned parameters of the design model were sufficient to provide reliable results.

The structures of the InN/Si and GaN/Si interfaces were simulated using periodic supercells within the approximation of periodic crystalline plates. To this end, we used 1 × 1 supercells, composed of 10 silicon atomic layers and 11 InN or GaN atomic layers (6 metal layers and 5 nitrogen layers). The vacuum-layer thickness was chosen such as to make the two surfaces formed by the plate not to interact with each other because of the periodic boundary conditions.

All calculations were performed on supercomputers at the Joint Supercomputer Center of the Russian Academy of Sciences.

RESULTS AND DISCUSSION

As a result of our experiments, we obtained stable films on silicon substrates with good adhesion. Typical images of sample surface areas are shown in Fig. 1. As can be seen, the deposited film had a fairly flat surface and consisted of ~100-nm polycrystals.

Analysis of the film composition and the magnetron cathode surface indicates that gallium nitride was formed both in the deposited film and on the cathode surface. However, the InN and GaN films both contained excess nitrogen. To obtain a single-crystal film of the desired composition (GaN or InN), a series of experiments must be performed with variation of the working gas composition, magnetron operating mode, and substrate temperature.

To theoretically simulate the adhesion of GaN and InN films on the silicon surface, we performed a series of calculations of the total energies of coherent interfaces formed by N-polar nitride on silicon: (InN(0001)/Si(111) and GaN(0001)/Si(111)). The calculations differed in the type of the nitride surface plane (nitrogen or metallic) adjacent to the silicon substrate and the mutual arrangement of the atoms interrupting the surfaces of the Si(111) substrate and the InN(0001) or GaN(0001) film. The adhesion energies calculated for the different cases considered above are listed in the table. The GaN and InN structures both exhibited the strongest substrate–film bond (–2.55 and –2.58 J m^{-2}, respectively) when the film surface contained nitrogen atoms situated directly above surface silicon atoms. Here, the nitrogen–silicon bond length was 1.81 for InN/Si and 1.80 Å for GaN/Si.

Since the grown structures contained impurities in considerable amounts, theoretical study of the effect of impurity atoms on the film adhesion to the substrate was of particular importance. Oxygen was considered

Calculated adhesion energies for different versions of InN(0001)/Si(111) and GaN(0001)/Si(111) interface geometries (the silicon atoms of the surface and subsurface substrate layers have coordinates of (0; 0) and (2/3; 1/3), respectively)

Type of surface interruption	Coordinate of interrupting atom	Adhesion energy, $J \cdot m^{-2}$	
		InN	GaN
N	(1/2; 0)	−0.95	−1.16
N	(0; 0)	−2.55	−2.58
N	(1/3; 2/3)	−1.01	−1.02
N	(2/3; 1/3)	−0.59	−2.49
In	(1/2; 0)	−1.69	−2.38
In	(0; 0)	−1.61	−2.18
In	(1/3; 2/3)	−1.67	−2.23
In	(2/3; 1/3)	−1.57	

as a typical impurity that is always present in experimental structures. A larger (3 × 3) supercell was used to assess the effect of a single oxygen atom on the InN/Si interface adhesion. Earlier ab initio calculations demonstrated that oxygen occupies the substitution position in the InN structure [7]; therefore, one oxygen atom replaced a nitrogen atom at the interface in our calculations. The corresponding adhesion energy was found to be -2.20 J m^{-2}. The presence of oxygen in the InN structure thus degrades the bond between the grown film and the silicon substrate.

CONCLUSIONS

A modified technique was developed for the magnetron deposition of semiconductor heterostructures that combines a high degree of efficiency and a high production rate. Stable GaN and InN structures on silicon were grown using this technique. Ab initio calculations made it possible to determine the energetically optimal mutual position of the atoms forming the surfaces of the silicon substrate and the GaN or InN film and to estimate the adhesion energy characteristic of these structures. In addition, the effect of an oxygen impurity atom in the InN structure on the adhesion energy between the InN film and silicon surface was assessed.

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