First-Principles Study of Electronic Structures of AlN/GaN Superlattices

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1. Introduction
Aluminum nitride (AlN) has attracted a great deal of attention as basic materials for deep-ultraviolet (UV) light-emitting devices, since it is a direct-band gap semiconductor with a band gap energy of 6.0 eV. Semiconductor light-emitting devices such as light-emitting diodes (LEDs) for the deep-UV light sources are now expected to be an alternative source to the conventional gas light sources because of the possibility of developing more safer, reliable, and portable light sources. Recently, successful fabrication of a deep-UV AlN LED has been reported with the emission efficiency of 10⁻⁴% [1, 2]. However, the emission efficiency of the deep-UV AlN LED is still much lower than that of the near-UV GaN LED. This is ascribed to the fact that AlN has an anisotropic emission pattern where light is emitted barely from the C-plane, but preferentially from the A-plane. This directional light emission properties arises from a different valence band structure from GaN; the wavefunction of the valence band top of GaN is characterized by N p atomic orbitals parallel to the C-plane, while the valence band top of AlN has a character of N p orbitals perpendicular to the C-plane. For the design of the AlN active layer structures for deep-UV LEDs with high emission efficiency, it is thus inevitable to study the electronic structure of AlN/GaN superlattices in details. In this study, we investigate systematically the electronic structure of the AlN/GaN superlattices using first-principles calculations.

2. Methods
The structural model we used in this work is a [0001]-oriented AlN/GaN superlattice in the wurtzite phase (Fig.1). The period of the superlattice along the [0001] direction (c-axis) is fixed to be 20 monolayers. The model thus includes the (AlN)ₓ(GaN)ₙ where N is the number of monolayer (N = 1, 2, and 5). We imposed a pseudomorphic growth of GaN on an AlN substrate, where the lattice parameter in the (0001) planes (parameter a) was set to be a=3.13 Å that was optimized for bulk AlN. For the c-axis, we used the optimized value of 5.01 Å for double layers for bulk AlN.

All calculations were performed using density functional theory. We used the generalized gradient approximation (GGA) for the exchange-correlation interactions among the electrons and pseudopotentials for the interactions between the ions and electrons. The valence wavefunctions were expanded in terms of a plane wave basis set with a cutoff energy of 49 Ry. We used 64 k-points for the Brillouin zone integration. During the geometry optimizations, all atoms were relaxed until the residual forces were less than 0.05 eV/Å. The momentum matrix element was calculated by the method proposed by Kageshima and Shiraishi [3]. Note that spin-orbit effects were neglected in the present calculations. The calculations were performed using the TOKYO AB INITIO PROGRAM PACKAGE [4].

3. Results and Discussion
Table I shows the interband momentum matrix element and energy gap of (AlN)ₓ(GaN)ₙ superlattice (N = 1, 2, and 5). The calculated values for AlN and GaN bulk are also listed in the table. The momentum matrix element was calculated at the Γ point between the highest valence band and the lowest conduction band of the AlN/GaN superlattice. We found that N = 1 and 2 leads to a significant increase of the C-plane components of the matrix element as compared with AlN bulk. In addition to the improvement of the surface emission from the C-plane, the energy gap of these superlattice structures is in the deep-UV region, i.e., ~5 eV (~250 nm). These results indicate that the AlN/GaN superlattice with one and two GaN-monolayers is an efficient structure of the C-plane surface emission of the deep-UV LED.

To fully understand the behavior of the AlN/GaN superlattice with thin GaN-monolayers, we investigated the band structures near the energy gap for these AlN/GaN superlattices. For a wurtzite crystal structure, the valence band at the Γ point is generally split into three bands by spin-orbit splitting energy ΔSO and crystal-field splitting energy ΔCF. In GaN, the order of the valence bands from the low-hole-energy side is heavy hole (HH) band, light hole (LH) band, and crystal-field split off hole (CH) band, since GaN has a positive ΔCF. On the other hand, AlN has a negative ΔCF, and, as a result, the order of the valence bands from the low-hole-energy side becomes CH, HH, and LH bands. Thus, the topmost valence band is the CH band in AlN.

In the AlN/GaN superlattice with one and two GaN-monolayers, these bulk electronic properties were found to be changed. The calculated band structures clearly showed that the valence band at the Γ point is the degenerated two bands, HH and LH bands. On the other hand, the CH band is located below ~0.18 and ~0.35 eV in the cases
of one and two GaN monolayers, respectively, relative to the valence band top. The degeneracy of the HH and LH bands is ascribed to neglect of spin-orbit effects. In addition to the change in the order of the valence band, we also found in the band structure that there is no band dispersion in both of the HH and LH bands and the lowermost conduction band along the G-A direction, while the CH band has a non-zero dispersion along the same direction. This indicates that confinement effects are larger for the former three bands than the latter. These results suggest that the difference in confinement effects on the valence and conduction bands of the AlN/GaN superlattice with one and two GaN-monolayers contributes to both of reversing the $\Delta_{cr}$ sign and spreading the energy gap in the AlN/GaN superlattice (Fig. 2).

Fig. 1  Structural model of the AlN/GaN superlattices with one GaN-monolayer.

Fig. 2  Schematic representation of the effects of using the AlN/GaN superlattices with one and two GaN-monolayers.

Table I  Calculated momentum matrix elements and band gap of (AlN)$_{20}$/GaN$_N$ superlattices. The scissors correction has been applied.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Absolute values of C-plane component of momentum matrix elements (a.u.)</th>
<th>Band gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlN bulk</td>
<td>0.00</td>
<td>6.00</td>
</tr>
<tr>
<td>1</td>
<td>0.33</td>
<td>5.54</td>
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<tr>
<td>2</td>
<td>0.32</td>
<td>5.03</td>
</tr>
<tr>
<td>5</td>
<td>0.17</td>
<td>4.14</td>
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<tr>
<td>GaN bulk</td>
<td>0.44</td>
<td>3.79</td>
</tr>
</tbody>
</table>

4. Conclusions

We have investigated the detailed electronic structure of the AlN/GaN superlattices using total-energy electronic structure calculations based on density functional theory. Our calculations show that in the AlN/GaN superlattices with one and two GaN monolayers, the C-plane component of the momentum matrix elements is significantly increased and the energy gap is kept in the deep-UV region.

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References