ENERGY-BAND STRUCTURES OF III-NITRIDE SEMICONDUCTOR SUPERLATTICE

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Introduction

Over the last decades, III-nitride and II-oxides semiconductors have been one of most exciting wide-gap materials. The direct electron transition process across the energy-gap between the conduction and valence bands is preferable for short-wavelength light emission [1-4], and high-quality Blue LED (Light Emitting Diodes) and LD (Laser Diodes) are commercially available. More recently, the alloys among these III-nitrides extend the high-availability of the materials. The energy band-gap of these alloys is dependent on the atomic constituent ratio, and the artificial control of the energy band structure is possible. These materials are expected to be very promising in the future wide-gap semiconductor application fields. But the detailed information on these materials has not been clarified and is not always available. We calculated the electronic structures of these alloys. Alloying atomic arrangements in the materials are essentially random. The special quasi-random structure model and the super-cell models are proposed, but large computing resources are more required. The details of these alloy systems are not clear enough.

Recently, microelectronics technology has been greatly developed, and microscopic hetero-structures and superlattices have been fabricated, and new promising devices are expected.

In this paper, we have investigated the energy-band structure and density of states of the III-nitride-related superlattice by using density functional theory.

Calculations

On the basis of density functional theory (DFT) with ultra soft pseudopotentials, we calculated the band structure, density of states and other important properties of III-nitride superlattices ($(AN)_m(BN)_n$ layers), where the of A,B atoms (=Al,Ga,In) and m,n layers were combined[5]. Here, we accepted several models. The first one (1) ZB-$(AN)_1(BN)_1$ was constructed by zinc-blende AN-(nitride) and BN-(nitride) monolayer layers along (001) direction. The second (2) W-$(AN)_1(BN)_1$ was composed of the wurtzite (AN) and (BN) supercells, and the third model (3) W-(ABN) was produced from W-supercell of AlN along c-axis, replacing some A atoms by B atoms.

The generalized gradient approximation (GGA) was accepted. The cut-off energy was 340 eV. After the many cycles of calculating iteration process to minimize the total energy, the self-consistent solutions were obtained to give the optimized structure. The lattice constants and others were calculated in the geometrically optimized structure.

Results and Discussion

Figures 1, 2 and 3 show the band structures in the model (1) of $ZB(AlN)_1(GaN)_1$, $ZB(AlN)_1(InN)_1$, $ZB(GaN)_1(InN)_1$, respectively. The top of the valence band (measured at E=0) and the bottom of the conduction band are located at G point in the Brillouin zone, suggesting the direct electron transition in these materials. Among these systems, the valence band structures are not changed so much. However, the bandgap is varied with including In atoms. Other extreme points of the conduction bands were changed greatly at X point but not at M point. The bandgap can be controlled by adding In layer, and the same behavior was also observed in other models. In Fig. 4, the density of states is shown. Also, the lattice constants, a and c and some elastic constants were calculated. As known well, the band-gap energy is underestimated in the density functional theory. When the energy band-gap energies in each model is corrected to fit the experimental results, a fair agreement is found with the relative changes.

Summary

We studied the energy-band structure, and other fundamental properties of III-nitride superlattices with the density functional method. When the component ratio in each model is changed, the band structure can be controlled artificially. This fact means this material is preferable to fabricate new and high-performance materials for the energy-band engineering in near future. Better properties are expected, compared with the ternary random alloys, to reduce the random alloy scattering and yield high mobility materials.

References

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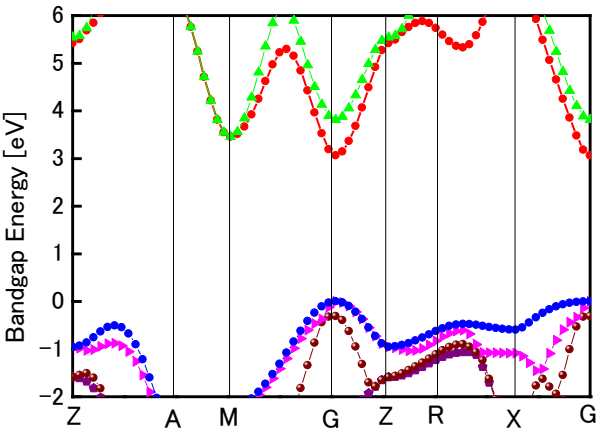

Fig.1 Energy Band Structure of ZB(AlN)(GaN) Superlattice

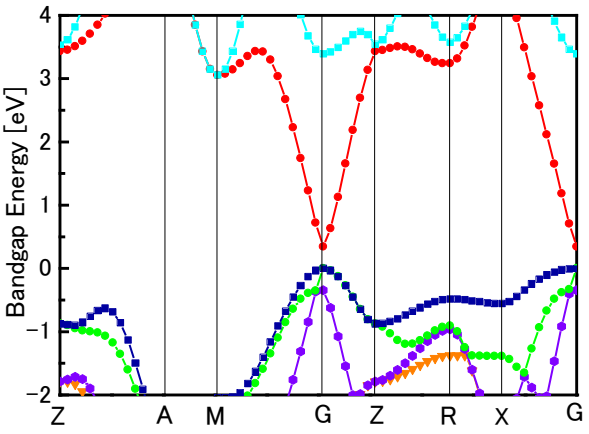

Fig 3 Energy Band Structure of ZB(GaN)(InN) Superlattice

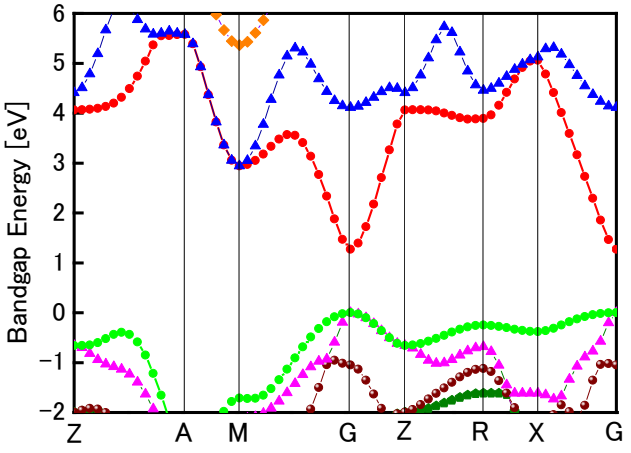

Fig.2 Energy Band Structure of ZB(AlN)(InN) Superlattice

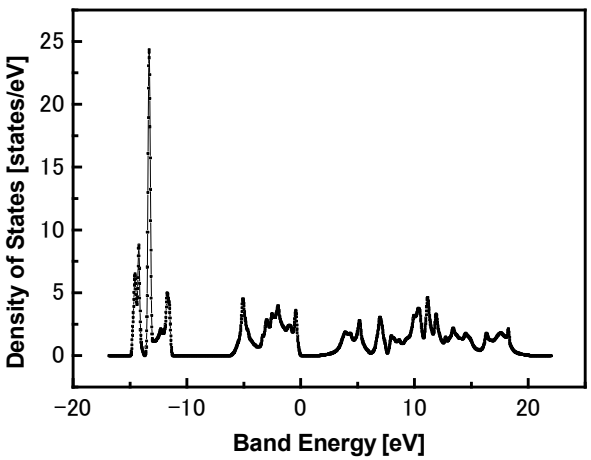

Fig.4 Density of States of ZB(AlN)(GaN) Superlattice