First-principles calculations of band structures of α-Ga_2O_3/Al_2O_3 superlattices

Takahiro Kawamura[1]*, Toru Akiyama[1], Yoshihiro Kangawa[2].
*lead presenter: tkawamura@mach.mie-u.ac.jp
1 Graduate School of Engineering, Mie University, Japan
2 Research Institute for Applied Mechanics, Kyushu University, Japan

Metastable α-Ga_2O_3 with corundum structure can form an alloy, heterostructure, and superlattice structures combining with α-Al_2O_3. Owing to lattice distortion caused by the difference in the lattice constants of each layer, fabrication of high-quality α-Ga_2O_3/Al_2O_3 superlattices is difficult [1] and their properties are not clearly understood. Therefore, it is necessary to understand the basic properties of α-Ga_2O_3/Al_2O_3 superlattices as well as improve crystal growth technology. In this study, we performed band structure analysis of α-Ga_2O_3/Al_2O_3 superlattices using first-principles calculations and investigated the dependence of bandgaps on lattice strain and thickness of superlattice layers.

The Quantum ESPRESSO (QE) program package [2] was used for all calculations. The pseudopotential self-interaction correction method, implemented in the QE code [3,4], was used to obtain realistic bandgap values. Figure 1 shows a simulation model of the α-Ga_2O_3/Al_2O_3 superlattice consisting of a hexagonal unit cell of α-Ga_2O_3 and α-Al_2O_3 accumulated in the *c*-axis direction. To investigate the influence of lattice strain on bandgaps, the biaxial strain was applied in the *a*- and *b*-axes directions by fixing the lattice constants to the same values as that of α-Ga_2O_3 and α-Al_2O_3.

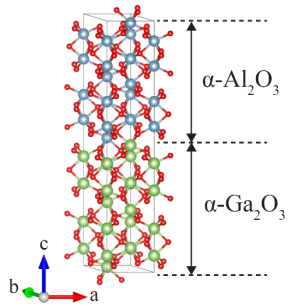

Fig. 1 Simulation models of α-Ga_2O_3/Al_2O_3 superlattice.

Figure 2 shows the change of bandgaps under biaxial strains. The values of bandgap and strain corresponding to bulk α-Ga_2O_3 and α-Al_2O_3 are indicated by arrows. The direct and indirect bandgaps of the strain-free ($\varepsilon = 0$) α-Ga_2O_3/Al_2O_3 superlattice were 5.12 and 5.05 eV, respectively. The bandgap increased under compressive strain ($\varepsilon = -2.5\%$) and decreased with tensile strain ($\varepsilon = 2.5\%$). The same tendency is shown in bulk α-Ga_2O_3 [5]. In addition, because bandgaps also depend on the thickness of superlattice layers and composition, it is expected that precise bandgap tuning will be possible by controlling them simultaneously.

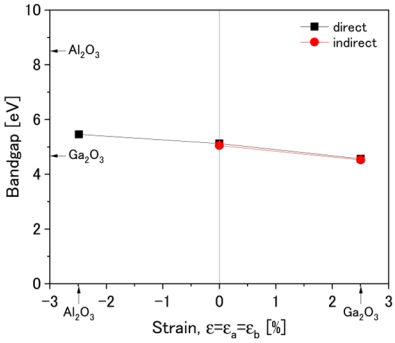

Fig. 2 Bandgaps of α-Ga_2O_3/Al_2O_3 superlattices under biaxial strain.

References

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