Theoretical exploration of widegap materials with the corundum structure for heteroepitaxy on α−Ga_2O_3

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Social demands for improving energy utilization efficiency are increasing to realize a low-carbon society. Therefore, next-generation semiconductors that can reduce conduction and switching losses as low-loss power devices are required. In particular, α-Ga_2O_3 has a wider band gap (ΔE_g = 5.3 eV) than SiC (ΔE_g = 3.3 eV) and GaN (ΔE_g = 3.4 eV) is expected to find applications in new fields, including high-voltage power devices. However, these wide-gap materials show n-type conductivity, making p-type conversion difficult. Usually, p-type conduction is achieved by adding a high concentration of acceptors to the n-type materials. On the other hand, our research group is investigating the fabrication of p-n junctions by the hetero-epitaxy of native p-type wide-gap materials on the n-type material: α-Ga_2O_3. In this study, we explored p-type wide-gap materials that can be grown on α-Ga_2O_3 by first-principles calculations. Assuming heteroepitaxy on the α-Ga_2O_3, first-principles calculations were performed for X_2O_3 (X = Al, In, etc.) with corundum structure using the Vienna Ab-initio Simulation Package (VASP) code [1,2]. It is known that the local density approximation (LDA) and generalized gradient approximation (GGA), which are commonly used in density functional theory (DFT), underestimate the band gap energy. In this study, we used a hybrid functional that improves the reproducibility of the electronic structure by mixing Hartree-Fock exchange terms. Calculations using the PBE0-type hybrid functional showed the band gap energies in Table 1. The difference between the experimental and calculated values for α-X_2O_3 (X = Al, Ga and In) is about 5%, so the calculation method seems reliable. The band gap energies estimated by the same method for materials for which no experimental values have been reported are shown in the same table. In other words, the band gap of unknown materials with corundum structure was revealed by this calculation. We are currently continuing our exploration of p-type wide-gap materials with ΔE_g > 5.0 eV.

TABLE 1. The calculated band gap of corundum materials, X_2O_3. Lattice constants (a and c), the ΔE_g^{calc} are those obtained by ab initio calculations, and the ΔE_g^{expt} are those obtained by experiments [3]. "*" shows narrow or metallic.

X	Al	Co	Ga	Nb	Mo	Ru	In	W	Os	Ir
a (Å)	4.753	4.800	5.075	5.000	4.692	5.270	5.527	4.641	5.413	5.271
c (Å)	12.97	13.01	13.65	16.27	16.85	13.28	14.64	17.32	13.12	14.10
ΔE_g^{calc}(eV)	8.894	4.464	5.517	*	*	*	3.405	*	*	3.568
ΔE_g^{expt}(eV)	8.75	-	5.6	-	-	-	3.7	-	-	3.0

References

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