Electronic structure analysis of $InSb_{1-x}N_x$ alloys by first-principles calculation

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III-V-N alloys have a property called giant bandgap bowing caused by nitrogen incorporation. This is because the electronegativity of N is significantly different from that of group III and V atoms. $InSb_{1-x}N_x$ alloys, which is one of the III-V-N alloys, is expected to close the energy gap by bandgap bowing because InSb is a narrow bandgap semiconductor. So far, there is a report of band calculation of $InSb_{1-x}N_x$ alloys ($x = 0 \sim 0.1$) using the k・p perturbation method [1], but there is no report on the electronic structure with a negative bandgap. In this study, we investigated the electronic structure of $InSb_{1-x}N_x$ alloys ($x = 0 \sim 1$) using first-principles calculations.

Electronic structures of InSb, cubic InN and $InSb_{1-x}N_x$ alloys were calculated using the all-electron density functional program WIEN2k [2]. For the structure of the $InSb_{1-x}N_x$ alloys, a supercell was used in which the basic unit cell of the zincblende structure was doubled in the direction of the basic translational vector, and x = 0.125, 0.375, 0.50, 0.625, 0.75 was varied by replacing 1 to 6 of the 8 Sb atoms with N atoms. We also calculated the electronic structure for various atomic sites in the same N composition. These were not used relaxed structures for all N compositions and atomic sites. We used a modified Becke-Johnson exchange potential [3] and a calculation considering the spin-orbit interaction.

The band structure for $InSb_{1-x}N_x$ alloys (x = 0.375) with N atoms at coordinates (0,0,0), (1,0,0) and (0,0,1) in the vicinity of the Γ point was indicated band inversion the valence band was s-like and the conduction band was p-like. In the band-inverted structure, the energy difference between the p-like and s-like bands at the Γ point was defined as a negative band gap energy (E_g). The value of E_g was -0.454 eV. We also calculated the N composition dependence of the bandgap for all $InSb_{1-x}N_x$ (x = 0, 0.125, 0.375, 0.50, 0.625, 0.75, 1) alloys with different N compositions and atomic sites. As a result, we confirmed band inversion in many N compositions and atomic sites and found that the bandgap does not change linearly with the N composition but deviates greatly to the negative side. We also confirmed that the electronic structure of the same N composition varies significantly depending on the atomic site. From these results, it is concluded that $InSb_{1-x}N_x$ is a peculiar material capable of band reversal in the intermediate N composition region.

References

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