First Principles Calculations of Defect Levels in III-V Semiconductor Alloys

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Abstract

The electronic structure in III-V semiconductor alloys containing an anion vacancy is calculated using first-principles density functional theory. The anion vacancy is modeled by subtracting an anion atom from a supercell of 512 atoms. The results are compared to those of preliminary calculations based on a 64-atoms supercell. New levels appear by introducing the anion vacancy in both the preliminary and present calculations. The bottom edge of conduction band is, however, less heavily affected by the anion vacancy in the present calculations.

Keywords: vacancy, defect level, Advance/PHASE

Deep defect levels in semiconductors are usually undesirable, because they interfere with the properties of electronic and opto-electronic devices. Since some defects are thermodynamically inevitable, it is important to predict whether their levels are deep or not. Therefore, the tight-binding theory was developed for and successfully applied to vacancies[1, 2] and substitutional defects[2-4] of semiconductors, especially of III-V semiconductor alloys.

The defect levels will, however, vary with the local environment, i.e., atoms surrounding the defects. For such a detailed study of the defects, a first-principles method is a more powerful tool. Thus preliminary calculations were performed using the pseudopotential formalism[5] based on the Kohn-Sham density functional theory[6] within the generalized gradient approximation[7] as implemented in the Advance/PHASE code[8]. We chose a semiconductor alloy containing In, As, and some other elements and an anion vacancy as a representative of the III-V semiconductor alloys and defects, respectively. The anion vacancy was modeled by subtracting an anion atom from a supercell of 64 atoms. A calculated band-gap was 0.18 eV without the anion vacancy. New levels appeared in a different way with the amount of surrounding In atoms. A bottom edge of conduction band was, however, so heavily modulated by introducing the anion vacancy that it was difficult to tell the defect

levels from host band levels.

This problem led us to performing the present calculations on the Earth Simulator. Fortunately, the Advance/PHASE code is so suitable for vector-parallel systems that for example, Ohno *et al*. achieved a half of theoretical peak performance of the Earth Simulator using the Advance/PHASE code in the course of electronic structure calculations on doped Si represented by a supercell over 10000 atoms.[9] The anion vacancy was modeled by subtracting the anion atom from a supercell of 512 atoms, instead of 64 atoms. We employed 69 nodes, or equivalently 552 processing units. The most significant improvement in the present calculations was that the bottom edge of the conduction band was less heavily modulated by introducing the anion vacancy. Specifically, the increase in the calculated band gap of about 0.4 eV in the case of the preliminary calculations was reduced to 0.07 eV. Though this reduction is still insufficient, we achieved a milestone toward further large-scale calculations for quantitative studies.

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