

Electronic structures of GaNP and InNAs ordered alloys calculated by the pseudopotential method

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GaN_xP_{1-x} alloy is a candidate for blue to ultraviolet optical materials, and InN_xAs_{1-x} alloy is attractive for infrared applications. Photoluminescence and optical absorption of GaN_xP_{1-x} alloy with small x indicate the possibility of large bowing of the band-gap energy dependence on nitrogen content [1]. The simple semi-empirical tight-binding calculations of both alloys [1,2] were performed, and indicated that the band-gap energy bowing is very large. We performed pseudopotential calculations of the electronic structure of the alloys to investigate the band structure and valence charge distribution of these alloys. The calculation shows that the valence charge densities of the alloy are strongly localized around nitrogen and that this localization causes the large bowing of band-gap energy.

The present calculations are based on the local-density-functional theory and the norm-conserving pseudopotential technique. The pseudopotentials are generated using Hamann scheme [3]. We assume zinc blende and simple cubic primitive cells with the lattice constant a . The simple cubic primitive cell contains 8 atoms, and the ordered alloys, GaN_xP_{1-x} and InN_xAs_{1-x} with $x = 0.25, 0.5,$ and 0.75 are constructed by substituting anion atoms (P or As) by N. The alloy lattice constant a is simply assumed to obey the Vegard law. We use 339 plane waves for the zinc blend structure and 515 for the simple cubic structure.

Figure 1 shows the electronic structure of the GaN_{0.75}P_{0.25} ordered alloy. The valence charge contour plot for the alloy in the (1 $\bar{1}$ 0) plane is shown in Figure 2. As expected from other calculations of binary GaN [4], the valence charge densities of the alloy are strongly localized around nitrogen. The bonding character between nitrogen and gallium seems to be ionic, while the bonding character between phosphorus and gallium seems to be covalent. Figures 3 and 4 show the band-gap energy of GaN_xP_{1-x} and InN_xAs_{1-x} ordered alloys as a function of nitrogen content x . The solid and dashed lines are fitting curves. It is apparent from the figures, the bowing of band-gap energy curves is large, except for direct-transition gap of InN_xAs_{1-x}. In particular, indirect-transition ($\Gamma - L, R, A$) gap of GaN_xP_{1-x} is very large, and this large bowing causes indirect transition of the alloy with low nitrogen content. The large band-gap bowing is mainly attributed to the localization of valence charge around nitrogen. The localization is mainly attributed to the large difference in electronegativity between nitrogen and phosphorus (or arsenic).

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- [3] D. R. Hamann: Phys. Rev. B 40 (1989) 2980-2987.
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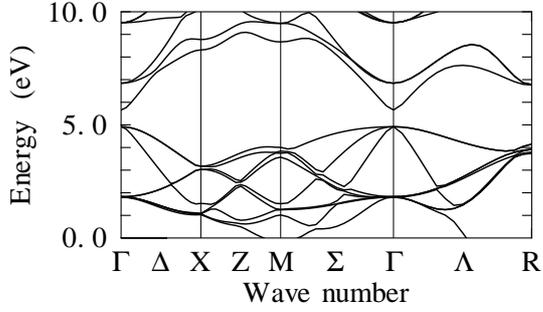


Figure 1: Band structure of GaN_{0.75}P_{0.25}.

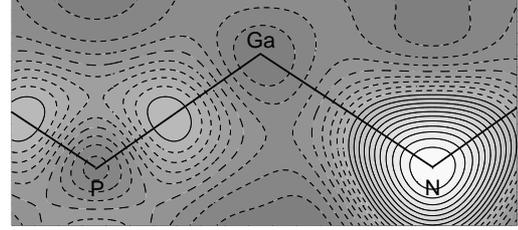


Figure 2: Valence charge contour plot for GaN_{0.75}P_{0.25} in the (110) plane.

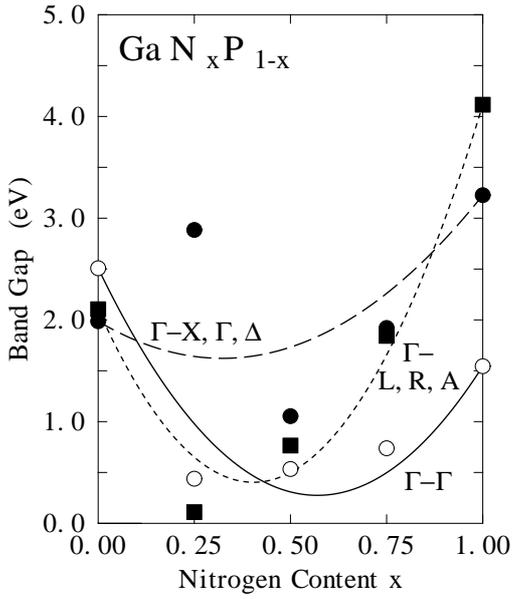


Figure 3: Band-gap energy dependence on nitrogen content x for GaN _{x} P_{1- x} .

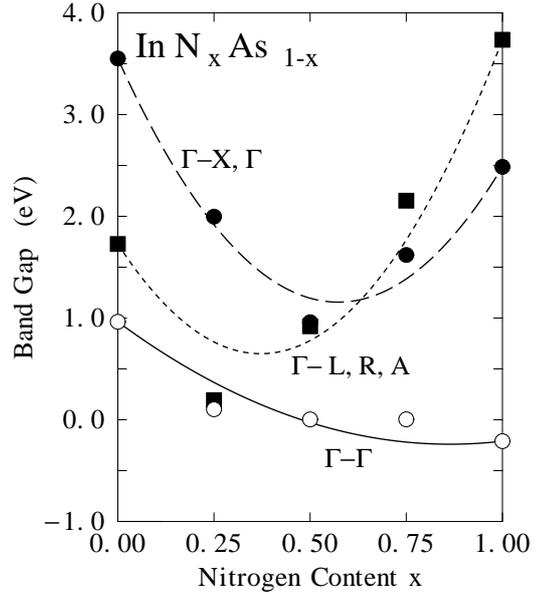


Figure 4: Band-gap energy dependence on nitrogen content x for InN _{x} As_{1- x} .