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Theoretical prediction of the structural, electronic, and thermal properties of $Al_{1-x}B_xAs$ ternary alloys

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ABSTRACT

First-principles calculations are performed to study the structural, electronic, and thermal properties of the AlAs and BAs bulk materials and $Al_{1-x}B_xAs$ ternary alloys using the full potential-linearized augmented plane wave method within the density functional theory. The structural properties are investigated using the Wu–Cohen generalized gradient approximation that is based on the optimization of total energy. For band structure calculations, both Wu–Cohen generalized gradient approximation and modified Becke-Johnson of the exchange-correlation energy and potential, respectively, are used. The dependence of the lattice constant, bulk modulus, and band gap on the composition x was analyzed. The lattice constant for $Al_{1-x}B_xAs$ alloys exhibits a marginal deviation from the Vegard's law. A small deviation of the bulk modulus from linear concentration dependence was observed for these alloys. The composition dependence of the energy band gap was found to be highly nonlinear. Using the approach of Zunger and coworkers, the microscopic origins of the gap bowing were detailed and explained. The quasi-harmonic Debye model was used to determine the thermal properties of alloys up to 500 K.

1. Introduction

Over the past few years, much attention has been devoted to boron compounds and their alloys, which have a wide range of technological applications, due to their excellent physical properties that include low ionicities [1–4], short bond lengths [5], hardness [5], high melting points [6], and wide band gaps [7]. Investigation of dilute BGaAs and BAlAs has been made on films grown via both molecular beam epitaxy and metal organic chemical vapor deposition. It is expected that the incorporation of boron into III–V semiconductors, will induce a strong perturbation in the electronic and structural properties of these alloys, because boron has highly different properties than the other III and V elements of the periodic table. However, only few theoretical calculations have been addressed to study the structural and electronic properties of III–V boron alloys. The band gap bowing in boron based III–V ternary alloys has been calculated by Azzi et al. [8]. Very recently, Murphy et al. [9] reported on the deviation from Vegard' law in six ternary $M_xN_{1-x}As$ (M and N are B, Al, Ga, and In) random alloys using the CASTEP (Cambridge Serial Total Energy Package) program (Castep Developers Group (CDG), UK). The structural and electronic properties of BNP, BNAs, BPAs, BNSb, BPSb, and BAsSb were studied by El Haj Hassan et al. [10,11]. To the best of our knowledge no experimental or theoretical investigations of $Al_{1-x}B_xAs$ alloy have appeared in the literature. Therefore, the purpose of this paper is to study the structural and electronic properties as well as to investigate the disorder effects in these boron alloys using the full potential linearized augmented plane wave (FP-LAPW) method. The physical origins of gap bowing are investigated by following the approach of Zunger et al. [12]. Finally, the quasi-harmonic Debye model was successfully used to

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