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Fundamental properties of zinc-blende AlSb, BSb and their $Al_{1-x}B_xSb$ ternary alloys

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ABSTRACT

The structural and electronic properties of the AlSb and BSb compounds and of the $Al_{1-x}B_xSb$ ternary alloys are investigated using the full potential-linearized augmented plane wave method (FP-LAPW) based on density functional theory (DFT). The lattice constant of the $Al_{1-x}B_xSb$ alloys exhibits a marginal deviation from Vegard's law and a small deviation of the bulk modulus from linear concentration dependence (LCD) is found. The composition dependence of the energy band gap is non-linear. The approach of Zunge and co-workers is used to explain the microscopic origins of the gap bowing. In order to investigate the thermodynamic stability of the alloys, the excess enthalpy of mixing ΔH_m is calculated as a function of the concentration x and the phase diagram is deduced. The quasi-harmonic Debye model is applied to determine the thermal properties of the alloys up to 500 K.

1. Introduction

The antimony compounds were spotlighted due to the growing interest of researchers for their use as wide gap semiconductors. This is due to their physical properties, such as low electronic density, high thermal conductivity, wide band-gap and large resistivity [1]. Boron compounds also have special physical properties, such as low ionicity [2–5], short bond lengths [6], hardness [5], high melting points [7], and wide band gaps [8].

The different band gap bowings in antimony based III-V ternary alloys were calculated by Azzi et al. [9]. To the best of our knowledge there have been no experimental or theoretical studies of the $Al_{1-x}B_xSb$ ternary alloys. In this work, the structural and electronic properties for AlSb, BSb and their ternary alloys have been studied using the full potential linearized augmented plane wave (FP-LAPW) method.

The physical origin of the gap bowing has been studied [10] using the Zunger approach. The thermodynamic stability of the $Al_{1-x}B_xSb$ alloys was investigated by calculating the excess enthalpy of mixing ΔH_m; the calculated phase diagram showed a broad miscibility gap with a high critical temperature. The thermal properties are calculated via the quasi-harmonic Debye model.

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