First-Principles Investigation of Electronic Properties of $GaAs_xSb_{1-x}$ Ternary Alloys

© A.K. Singh[1], Devesh Chandra[1], Sandhya Kattayat[2], Shalendra Kumar[3], P.A. Alvi[4,¶], Amit Rathi[1]

[1] School of Electrical, Electronics and Communication Engineering, Manipal University Jaipur, Rajasthan, India
[2] Higher Colleges of Technology, Abu Dhabi, UAE
[3] Electronic Materials & Nanomagnetism Lab, Department of Applied Physics, Amity School of Applied Sciences, Amity University Haryana, Gurgaon, 122413, India
[4] Department of Physics, Banasthali Vidyapith, Banasthali-304022, Rajasthan,India

¶ E-mail: drpaalvi@gmail.com

Received Junuary 15, 2019
Revised March 8, 2019
Accepted July 29, 2019

Compositional variations in GaAs based ternary alloys have exhibited wide range alterations in electronic properties. In the present paper, first-principles study of $GaAs_xSb_{1-x}$ ternary alloys have been presented and discussed. Density functional theory (DFT) computation based on the full-potential (linearized) augmented plane-wave (FP-LAPW) method has been utilized to calculate the Density of States (DOS) and the band structure of ternary alloys $GaAs_xSb_{1-x}$ ($x = 0$, 0.25, 0.50, 0.75, 1).The calculations were performed using the exchange-correlation energy functional from Perdew, Burke, and Ernzerhof, a generalized-gradient approximation (GGA-PBE) and Becke-Johnson exchange potential with local-density approximation (BJLDA) available within the framework of WIEN2k code. As compared to PBE, the results obtained from BJLDA are in close agreement with other experimental works. The DOS results show a reduction in bandgap as the Sb fraction is increased in $GaAs_xSb_{1-x}$ ternary alloys. The bandgap obtained by PBE and BJLDA are found to deviate from Vegard's law, i. e., it doesn't vary linearly with composition. However, the bandgap obtained by BJLD is found to closely match Vegard's law when the bowing parameter is considered.

Keywords: GaAsSb, ternary, DOS, LAPW, PBE, Becke-Johnson potential.

Full text of the paper will appear in journal SEMICONDUCTORS.