First-Principle Calculations of Electronic and Dynamical Properties of GeSn

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Abstract. The structural and electronic properties of GeSn in the rocksalt structure have been studied using density functional theory within the local density approximation. Results are given for lattice constant, bulk modulus and its pressure derivative. The calculated structural parameters for this model are given good agreement with previous ab-initio calculations and available experimental results. The electronic band structure is also presented for GeSn. Then, a linear-response approach to the density functional theory is used to calculate the phonon spectrum for GeSn.

Keywords: Electronic Band Structure, LDA, Phonons
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The Ge-Sn alloy system is technologically interesting because of the potential it offers for the development of group IV based optoelectronic devices. It has been predicted from theory and recently shown experimentally that semiconducting $Ge_{1-x}Sn_x$ alloys may have a direct energy band gap for $0.2<x<0.7$ and may be therefore good candidates for fabricating infrared detectors on Si [1,2].

Our calculations were performed using the density functional theory in its local density approximation. We used the Ceperley-Alder[3] electron correlation scheme in the form parameterized by Perdew and Zunger[4]. Ion-electron interactions were treated by using norm-conserving pseudopotentials[5]. Single-particle wave functions were expanded in a plane-wave basis set up to the kinetic energy cut-off 40 Ryd. The number of k points in the irreducible Brillouin zone (BZ) used in the self-consistent calculations was 120. For the vibrational properties of GeSn, we have applied the density functional perturbation theory scheme within pseudo-potential theory[6].

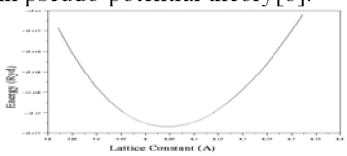

Fig. 1. Calculated total energies as a function of lattice constant for GeSn.

The calculated lattice constant, bulk modulus and its pressure derivative compared to other theoretical results of GeSn .

	$a(\mathring{A})$	B (Mbar)	B'
Present	6.041	0.534	4.66
Other work [7]	5.670	0.740	5.40

The calculated electronic band structure along the various symmetry lines are shown in Fig.2.

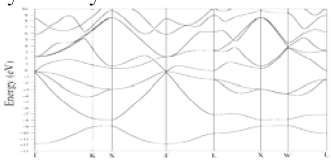

Fig.2. The calculated band structure of GeSn.

The calculated phonon spectrum dispersions of GeSn are plotted in Fig.3.

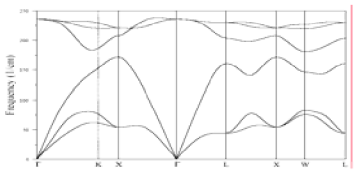

Fig 3. Calculated phonon dispersions for GeSn

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