Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 6-7

Artikel: Ab-initio pseudopotential study of Ge_1-xSn_x alloys
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DOI: https://doi.org/10.5169/seals-116080

Ab–initio Pseudopotential Study of $Ge_{1-x}Sn_x$ Alloys

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Electronic properties of $Ge_{1-x}Sn_x$ alloys are studied using a self-consistent *ab-initio* pseudopotential scheme in a plane wave basis set. Total energy results prove the instability of the solid solutions against phase segregation. The band structures indicate very interesting properties, such as a direct energy gap range for $0.26 < x < 0.74$. Metastable compounds grown by non-equilibrium techniques could therefore turn out to have promising opto-electronic applications.

1. Introduction

Silicon is technologically still the most important semiconductor for a wide range of microelectronic devices. For opto-electronic applications however, it lacks of efficient light absorption properties due to its indirect energy gap. Novel crystal growth techniques give rise to the hope that direct–gap materials compatible with the silicon technology will be available in the future. In this work we discuss the Ge–Sn system as a candidate for such a material. It has been shown theoretically[1] and experimentally[2] that $Ge_{1-x}Sn_x$ alloys are unstable against phase segregation into Ge and β–Sn. Metastable phases can be grown by non-equilibrium techniques. Our previous work[3] confirms these findings with first-principles total energy results. Single crystals have been grown for $x \leq 0.08$ only, whereas amorphous alloys are available over a wider composition range[2]. It is therefore of interest to study the electronic band structure of metastable $Ge_{1-x}Sn_x$. The first study in this direction was done by Jenkins and Dow, using a tight binding approach[4].

2. Methods

We use *ab-initio* non-local pseudopotentials and solve the LDA Kohn–Sham equations self-consistently in a plane wave basis set, with an energy cutoff of 16 Rydbergs. More details on the methods can be found in ref. 3. The energy gaps are empirically modified a posteriori to correct the underestimation of excitation energies by the local density approximation (LDA), and to include spin-orbit splitting. The alloys are treated in the virtual crystal approximation (VCA).

3. Results

In figure 1 we show the lowest energy gaps as obtained by LDA and after correction. Our results agree qualitatively with the relativistic tight binding band structures of Jenkins and Dow[4], adjusted to empirical pseudopotential calculations for Ge and α–Sn, fitted to experiment at critical points[4]. Our calculations on the other hand are non-relativistic and use the LDA. We estimate the quantitative differences between the two energy gap predictions to lie within the errorbars of the methods.

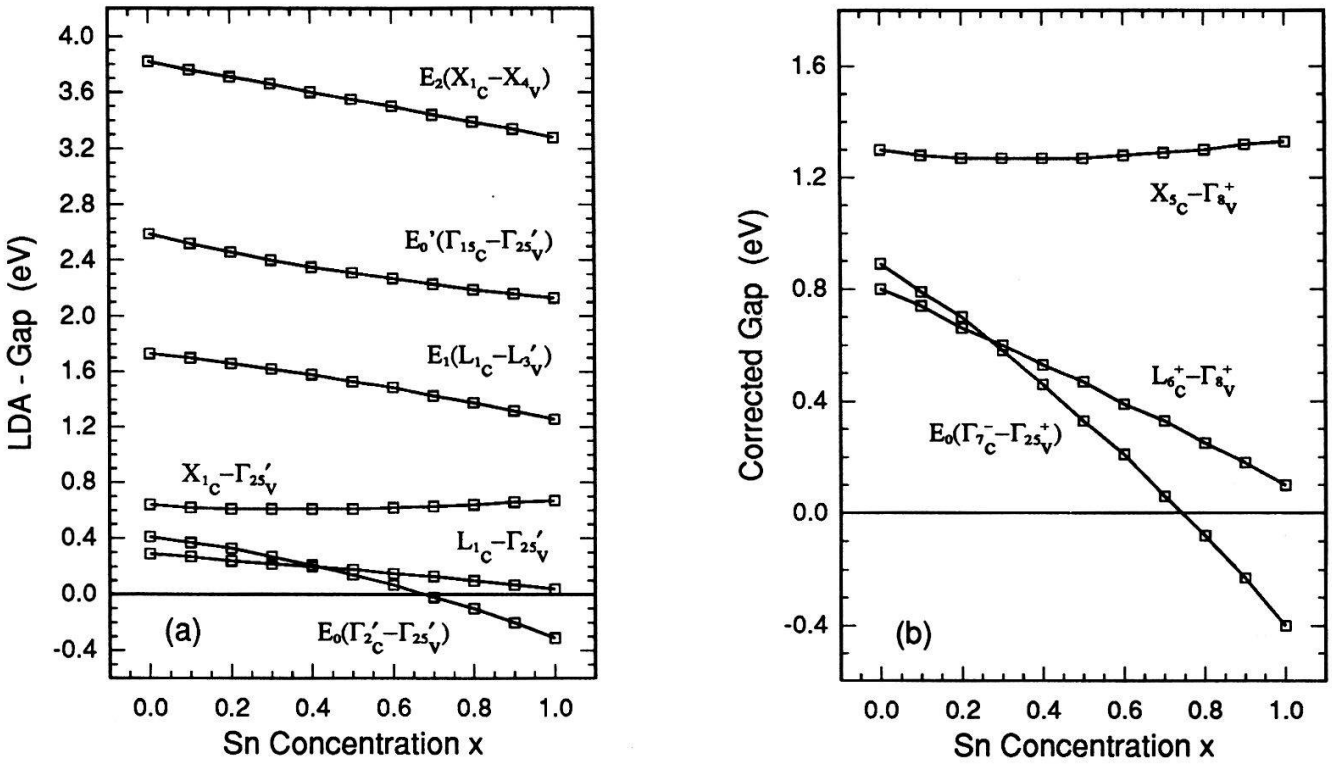

Fig. 1 (a) LDA energy gaps at T = 0 K of $Ge_{1-x}Sn_x$ vs x, (b) the three smallest gaps adjusted to the experimental values at the endpoints Ge and Sn, and corrected linearly in between. At $x = .26$ the alloy has a direct gap of .61 eV which gradually decreases to zero at x = .74.

The small differences in the gap cross-over points are mainly due to an upward bending of the gaps vs x (fig. 1b) whereas the tight binding results show a downward bending[4]. Deviations of the energy dispersions along certain symmetry lines are already present in the tight binding results with respect to the empirical Ge and α–Sn band structures, but do not affect the excitation energies. We obtain that metastable $Ge_{1-x}Sn_x$ has a Ge–like indirect energy-gap for $0 \leq x \leq .26$ (.2 in ref. 4), a direct energy-gap for $.26 \leq x \leq .74$ (.6 in ref. 4), ranging from .61 eV (.76 eV in ref. 4) to zero. For $.74 \leq x \leq 1.0$ $Ge_{1-x}Sn_x$ is a α–Sn like zero-gap material. Hence potential applications for tunable infrared detectors for wavelengths above 2 μm can be anticipated in the direct-gap regime.

The authors would like to acknowledge gratefully financial support through a grant of the Swiss Council of the Federal Institutes of Technology.

4. References

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