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Ab-initio Pseudopotential Study of $\text{Ge}_{1-x}\text{Sn}_x$ Alloys

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Electronic properties of $\text{Ge}_{1-x}\text{Sn}_x$ 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 theoretically¹ and experimentally² that $\text{Ge}_{1-x}\text{Sn}_x$ alloys are unstable against phase segregation into Ge and β -Sn. Metastable phases can be grown by non-equilibrium techniques. Our previous work³ 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 range². It is therefore of interest to study the electronic band structure of metastable $\text{Ge}_{1-x}\text{Sn}_x$. The first study in this direction was done by Jenkins and Dow, using a tight binding approach⁴.

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 Dow⁴, adjusted to empirical pseudopotential calculations for Ge and α -Sn, fitted to experiment at critical points⁴. 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.

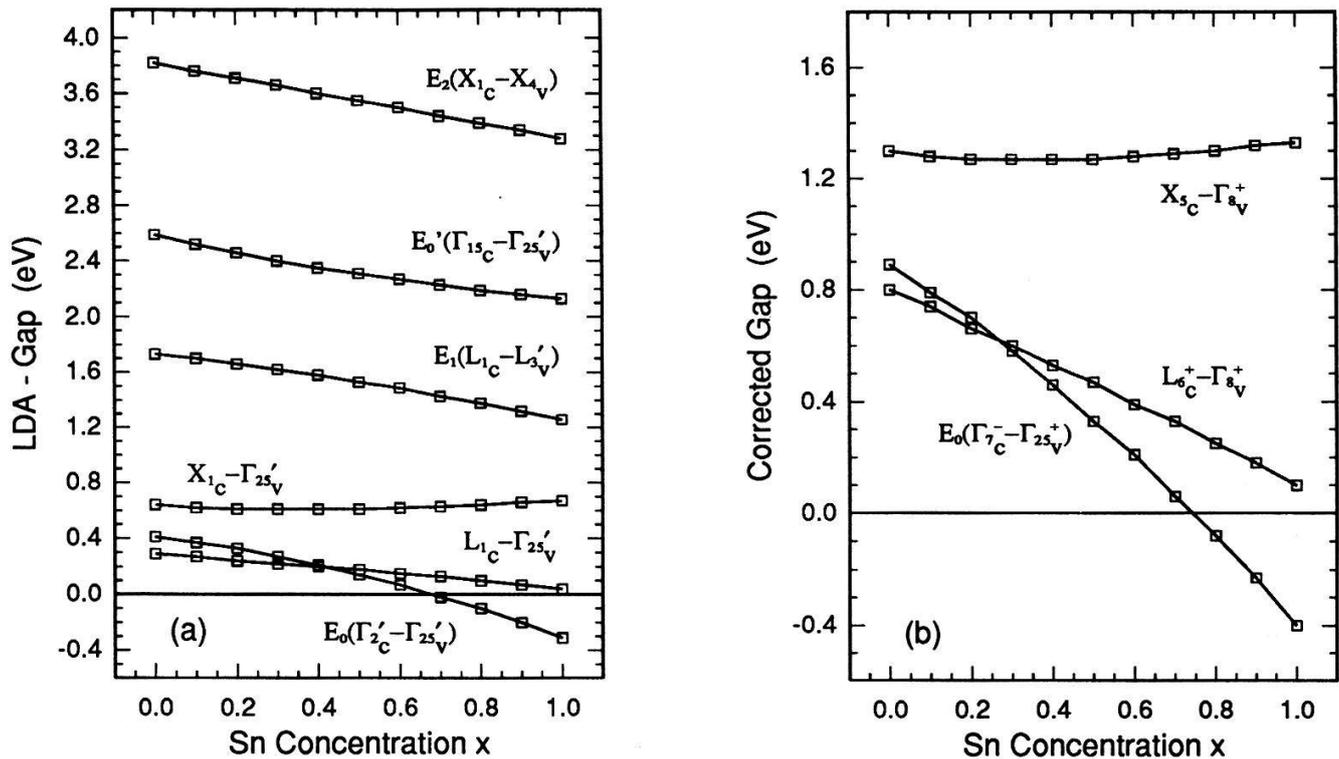


Fig. 1 (a) LDA energy gaps at $T = 0$ K of $\text{Ge}_{1-x}\text{Sn}_x$ vs x , (b) the three smallest gaps adjusted to the experimental values at the endpoints Ge and Sn, and corrected linearly in between. At $x = .26$ the alloy has a direct gap of .61 eV which gradually decreases to zero at $x = .74$.

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 bending⁴. 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 $\text{Ge}_{1-x}\text{Sn}_x$ 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 $.74 \leq x \leq 1.0$ $\text{Ge}_{1-x}\text{Sn}_x$ is a α -Sn like zero-gap material. Hence potential applications for tunable infrared detectors for wavelengths above $2 \mu\text{m}$ can be anticipated in the direct-gap regime.

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4. References

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