

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

**Artikel:** Ab-initio pseudopotential study of Ge<sub>1-x</sub>Sn<sub>x</sub> alloys  
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**DOI:** <https://doi.org/10.5169/seals-116080>

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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 theoretically<sup>1</sup> and experimentally<sup>2</sup> that  $\text{Ge}_{1-x}\text{Sn}_x$  alloys are unstable against phase segregation into Ge and  $\beta$ -Sn. Metastable phases can be grown by non-equilibrium techniques. Our previous work<sup>3</sup> 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<sup>2</sup>. 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 approach<sup>4</sup>.

### 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<sup>4</sup>, adjusted to empirical pseudopotential calculations for Ge and  $\alpha$ -Sn, fitted to experiment at critical points<sup>4</sup>. 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.

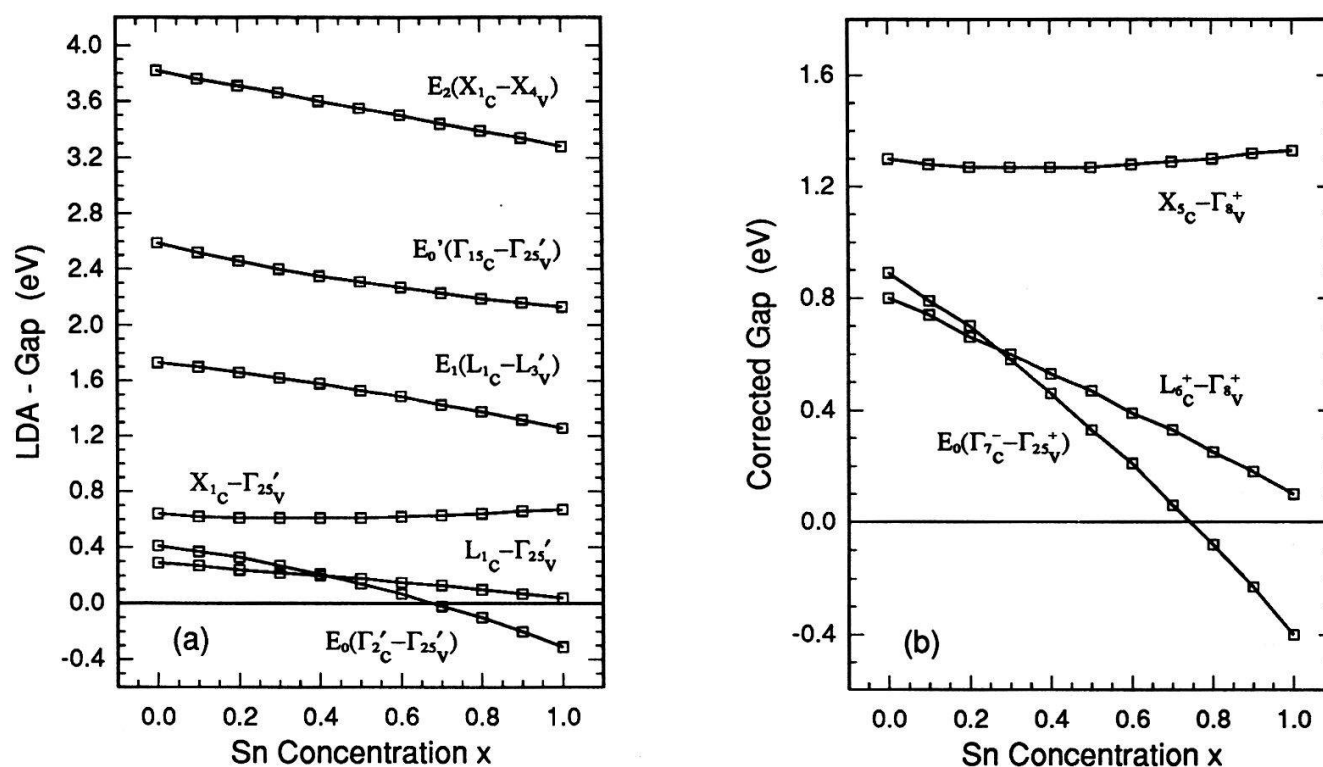


Fig. 1 (a) LDA energy gaps at  $T = 0$  K of  $Ge_{1-x}Sn_x$  vs  $x$ , (b) the three smallest gaps adjusted to the experimental values at the endpoints Ge and Sn, and corrected linearly in between. At  $x = .26$  the alloy has a direct gap of .61 eV which gradually decreases to zero at  $x = .74$ .

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<sup>4</sup>. Deviations of the energy dispersions along certain symmetry lines are already present in the tight binding results with respect to the empirical Ge and  $\alpha$ -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  $\alpha$ -Sn like zero-gap material. Hence potential applications for tunable infrared detectors for wavelengths above  $2 \mu m$  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.

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