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# Non-linear behavior of germanium electronic band structure under high strain

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ABSTRACT

The electronic band structure of Germanium has been studied under high strain (>1%) using a combination of Keating's model and Tight-Binding formalism. The study has been performed for different kinds of strains (uniaxial and biaxial) and considering the three main crystallographic directions of Germanium: ⟨001⟩, ⟨110⟩ and ⟨111⟩. Our results have been compared with the predictions of Deformation Potential Theory, observing an important disagreement for deformations higher than 1% and showing a non-linear dependency on the strain applied. These results are corroborated experimentally, proving the accuracy of the approach.

## 1. Introduction

In the last decades Silicon Photonics has arisen as a promising way to create optical interconnects and devices that would allow us to go beyond Moore's Law. The use of photons instead of electrons to transport and manipulate information, offers many advantages compared to traditional electronic links found in todays computers [1–3]. The main advantage of silicon as a photonic material is the fact that the manufacturing process infrastructure is widely extended (CMOS-technology), allowing a high yield and low cost. Although significant progresses have been made developing silicon devices, such as photo-detectors [4–6] or high-speed modulators [7,8], silicon has an important drawback, it is an inefficient light emitter due to its indirect bandgap. Recently, germanium has caught the attention to obtain gain material compatible with CMOS-technology, opening new possibilities to develop laser sources implementable in the same chip and allowing a miniaturization of future devices.

One of the most interesting approaches to obtain optical gain material based on Ge was proposed by Jifeng Liu and co-workers [9–11]. The approach consists of the combination of doping and strain to achieve a pseudo-direct bandgap in Ge with a direct bandgap emission highly efficient. This approach has given interesting results by different research groups [12–17]. Follow this approach involves having a correct model of Ge electronic band structures under strain to predict the value of Γ and *L*-bandgap to obtain: (i) the correct emission wavelength and (ii) the doping necessary to compensate the energy difference between Γ and *L*-valleys.

Hitherto, all papers that have followed this approach [12–17] have used a perturbation model based on Deformation Potential Theory (DPT) [18–27] to predict the evolution of Ge electronic band structure as a function of the strain applied (Table 1 shows the deformation potential values used in this work [28]). DPT is a theory based on the perturbation of the Hamiltonian of Ge electronic band structure by strain. Due to the perturbative nature of this theory, its predictions may be only valid for deformations not exceeding 1%, being able to provide incorrect values of the strain required to achieve a direct bandgap semiconductor and consequently the incorrect wavelength emitted and doping necessary to obtain a pseudo-direct bandgap. Several experiments using different methods [29–31] have shown evidences about the limitation of DPT to predict correctly the electronic band structure of Ge under strains applied higher than 1% [18–23]. Considering the above said, in the present work we have used a combination of Keating's model (KM) [32–36] and Tight-Binding formalism (TBF) [37,38] to perform a computational study of Ge electronic band structure under high strains (>1%). The study has been performed for different type of deformations (uniaxial and biaxial) and along different crystallographic directions (⟨001⟩, ⟨110⟩ and ⟨111⟩). The results obtained are in full agreement with the experimental results mentioned above [29–31].

The present work is organized as follows. In Section 2 the computational details of the study carried out are given. In Section 3, we compare the calculations performed with the results obtained by DPT. Finally, we present our conclusions.

## 2. Computational details: Keating's model, Tight-Binding formalism and TB-Sim code

The strained crystal lattice of Ge and its electronic band structure have been computed with TB-Sim package [40] (based on TBF [37,38])

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**Table 1**
Deformation potential parameters, Ge elastic constant and Ge bandgap simulated at two different temperature.

| Def. Pot. Parameters | | Elastic constant | Bandgap($T = 0K$) | Bandgap($T = 300K$) |
|---|---|---|---|---|
| $a_c$ (eV) $= -8.24$ | $a_v$ (eV) $= 1.24$ | $C_{11} = 126.0$ | $E_\Gamma = 0.90626$ eV | $E_\Gamma = 0.802$ eV |
| $\Xi_u$ (eV) $= 15.13$ | $b$ (eV) $= -2.9$ | $C_{12} = 44.0$ | $E_L = 0.73717$ eV | $E_L = 0.661$ eV |
| $\Xi_d$ (eV) $= -6.58$ | $d$ (eV) $= -5.3$ | $C_{44} = 67.7$ | | |
| $\Delta_o$ (eV) $= 0.29$ | | | | |

In Ref. [29] there is a summary table for where it is possible see the different values of these potentials depending on the work consulted.

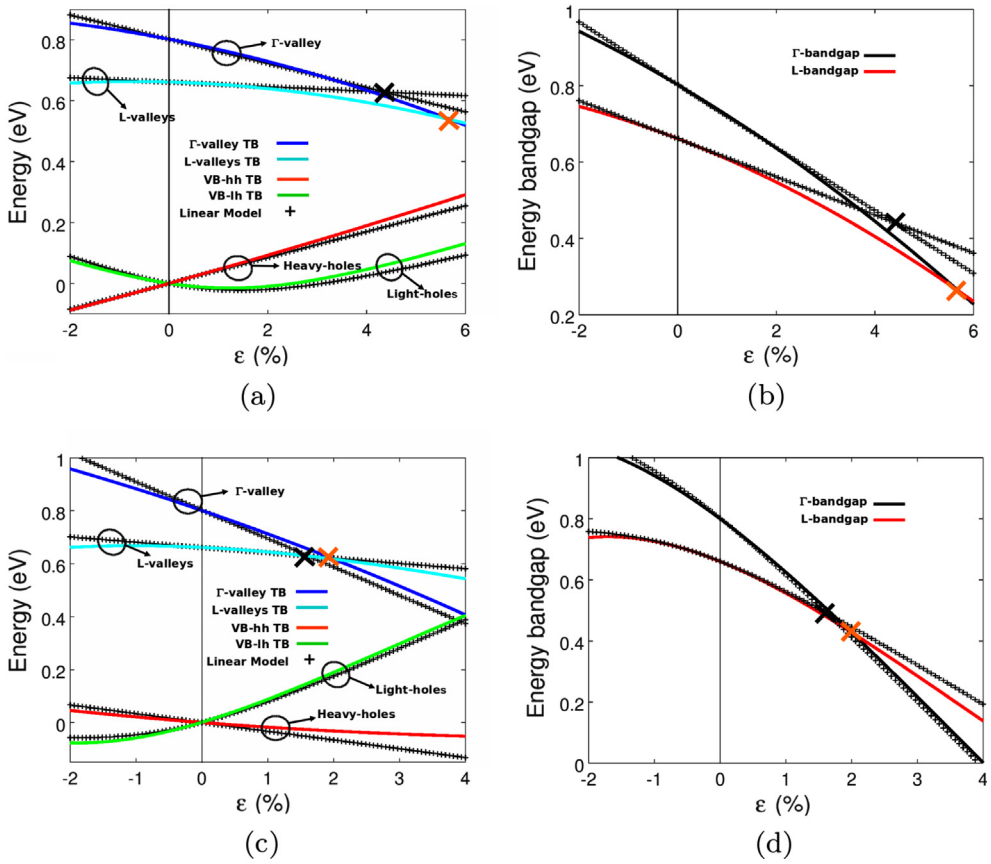


**Fig. 1.** (a) Ge electronic band structure and (b) Ge energy bandgap under uniaxial strain along ⟨001⟩. (c) Ge electronic band structure and (d) energy bandgap under biaxial strain along ⟨001⟩. The black cross points present the results of DPT and color solid lines show the results of KM + TBF. The big black cross and big orange cross indicate the point where Ge becomes a direct bandgap semiconductor given by DPT and KM + TBF.

in combination with Keating's valence force field [32–36] with a parametrization of the electronic structure of Ge based on *ab initio* calculations [39,40]. One of the advantages of this approach (TBF + KM) over DPT [18–27] is that it remains accurate at high strains, while DPT fails as the experimental results have shown [29–31].

KM allows us to know the position of atoms inside unit cell under deformation. This model describes the forces induced on neighborliness atoms when one atom is moved in a crystal lattice [36]. These forces are just considered to be applied on nearest neighboring atoms. Such movement induces attractive and repulsive forces which produces displacements in an atom/ion or a set of them from their equilibrium positions, modifying the unit cell. The model is the result of a general method proposed to ensure that the elastic strain energy satisfies the requirement that it is invariant under a simple rotation of the crystal, without deformation. Initially, KM was applicable just for small atomic displacements in the crystal lattices [33,35]. Later the model was extended to include anharmonic effects (third-order elastic constants) [33] to observe how the unit cell and therefore the crystal lattice are modified under a wide range of strain (>1%).

Knowing how the crystal structure has been deformed, TBF is applied to calculate the electronic band structure of the strained crystal lattice, which works quite well for semiconductors [39,41]. The idea of this formalism is based on the fact that the electronic wave functions for atoms located in a crystal lattice can be describe with a restricted Hilbert space spanned by atomic orbitals of an isolated atom. The method is closely related to the **linear combination of atomic orbitals** (LCAO) [37,38], method used in chemistry.

Initially, the simulations were been performed at $T = 0$ K (see Table 1). The values of Γ and *L*-bandgaps at room temperature, $T = 300$ K (see Table 1), have been obtained using Varshni's coefficients [42] to calculate the bandgap narrowing induced by temperature. The variation of Varshni's coefficients with the strains applied is unknown, so we assumed that they do not depend on the applied deformation. This assumption has been confirmed experimentally [29–31].

## 3. Computational results

In this section we present the results obtained using KM + TBF and compared with DPT results. Figs. 1–3 show the dependency on strain of