# An extended Hueckel theory parameterization of Germanium for doped SiGe alloys

D. Dick*‡, F. Fuchs†‡, S. Gemming‡§ and J. Schuster*†‡
*Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany
†Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany
‡Center for Materials, Architectures and Integration of Nanomembranes (MAIN),
Chemnitz University of Technology, Chemnitz, Germany
§Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany
e-mail: daniel.dick@zfm.tu-chemnitz.de

## Introduction

Silicon-germanium (SiGe) heterojunction bipolar transistors (HBTs) have found widespread use in high-frequency applications. Scaling of the HBT base layer thickness to 5 nm and below makes an atomistic treatment indispensable as fluctuations of dopant concentrations play a bigger role. Semi-empirical methods like extended Hueckel theory (EHT) enable us to quickly and efficiently simulate many different permutations of large unit cells with more than a hundred atoms to quantify the influence of atomic-scale fluctuations on the electronic structure and transport properties.

## A new EHT parameterization of Ge

For crystalline structures, Cerda and Soria [1] provide a wide range of parameterized elements in various phases, but lacking a parameterization of Ge. By fitting the EHT parameters to a Ge bandstructure we fill this gap and provide a parameterization capable of describing the band structure of random SiGe alloys of varying Ge concentrations. It is based on a set of s-, p- and d-orbitals and includes spin-orbit interaction to describe split-off bands. Fig. 2 shows the calculated band gap of unstrained SiGe alloy as a function of Ge content, matching the measurements by Braunstein et al. [2]. Straining the alloy biaxially to match the lattic constant of Si reduces the band gap as expected. Simulations were carried out using the QuantumATK simulation software with the unit cell illustrated in fig. 1.

## Unfolding supercell band structures

Interpretion of band structures from supercell calculations is hampered due to bands folding into the smaller Brilouin zone of the sample cell. We unfold bands back into the Brillouin zone of the primitive cell using the approach from Popescu and Zunger [3] as implemented in QuantumATK. Fig. 3 shows the band density calculated this way. From this, singular bands can be extracted and compared, as shown in Fig. 4 for model cells with varying Ge content.

## Conclusion

We extend the existing range of EHT parameterizations by providing a new parameterization capable of describing the band structures of random SiGe alloys with varying Ge content. Unfolding the band structure obtained by supercell calculations allows to observe the change in valence band minimum related to Ge content and atomic structure. Studying the influence of structural fluctuations and investigating the effects of C and B doping on band structure by will be issue of future work.

## References

[1] J. Cerda and F. Soria. *Accurate and transferable extended hueckel-type tight-binding parameters*. Phys. Rev. B, 61:7965-7971, Mar 2000.
[2] R. Braunstein, A. R. Moore, and F. Herman. *Intrinsic Optical Absorption in Germanium-Silicon Alloys*. Phys. Rev. 109, 695: 695-710, Feb 1958.
[3] V. Popescu and A. Zunger. *Effective Band Structure of Random Alloys*, Phys. Rev. Lett. 104, 236403, June 2010

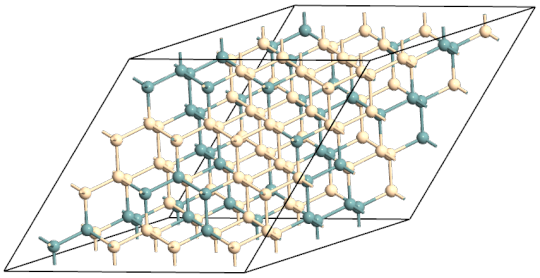

Fig. 1. Example of a SiGe alloy with Ge atoms randomly distributed among the lattice points.

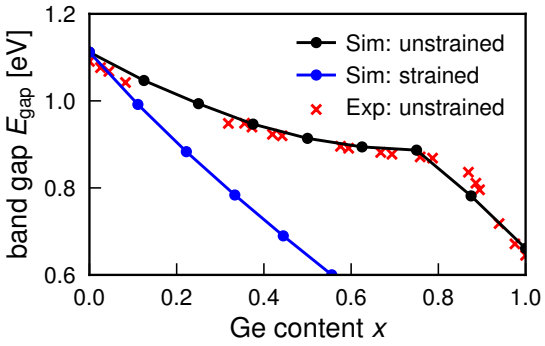


Fig. 2. Comparing the calculated average band gap of unstrained and biaxially strained random SiGe alloys in ralation to Ge content. Red crosses show measurements by Braunstein et al. [2] in good agreement with our simulations.

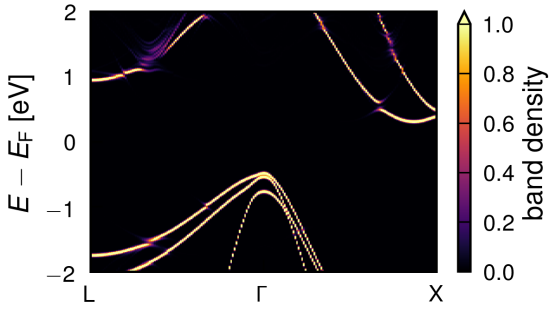


Fig. 3. Unfolded band structure of a random SiGe alloy with 33% Ge content calculated as a band density.

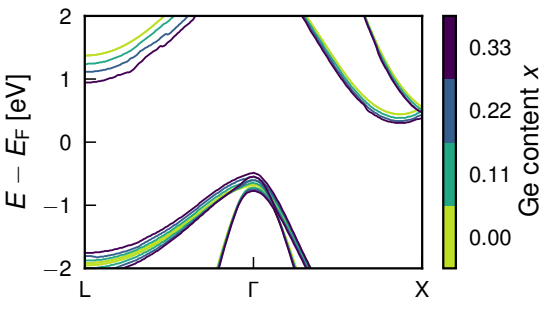


Fig. 4. Extracted band structures of strained SiGe alloy with varying Ge content.