Impedance spectroscopy of GeSn/Ge heterostructures by a numerical method

Bruno Baert[a], Osamu Nakatsuka[b], Shigeaki Zaima[b],
Ngoc Duy Nguyen[a]

[a]Solid State Physics - Interfaces and Nanostructures,
University of Liege, B-4000 Liege, Belgium
[b]Department of Crystalline Materials Science, Graduate
School of Engineering, Nagoya University, Japan

Silicon germanium tin, a group-IV semiconductor alloy, is currently receiving an increasing attention as an attractive material for the fabrication of strain-engineered logic components with boosted device performances. Such a growing interest is due to the recent advances in epitaxial growth techniques delivering epilayers with good crystalline quality [1-3]. Nevertheless, despite their recognition as suitable materials for a wide range of applications [3-5], the electrical properties of thin film structures based on these tin-containing compounds need to be investigated in a detailed and systematic manner.

The objective of this work is to carry out a theoretical study of the electrical characteristics of heterostructures based on GeSn. We focused on the response of such material systems under small-signal alternating current regime, which is the framework of impedance spectroscopy measurements. Our approach is based on the numerical solution of the basic semiconductor equations applied to various GeSn/Ge junction configurations. Using a finite-difference method and Scharfetter-Gummel discretization scheme, we obtained, as results of the simulations, impedance (admittance) characteristics for various sets of physical parameters such as dopant concentrations and carrier mobilities. A typical structure in our study comprises a 200 nm thick p-doped $Ge_{1-x}Sn_x$ layer ($x \approx 0.05$) on a 100 µm p- or n-Ge substrate. The interface with a top metal contact was included, as well as a Shockley-Read-Hall trap state with discrete energy level in the bandgap in order to take into account the impact of possible defects.

The computation of the electrostatic potential and of the quasi Fermi levels for free electrons, holes and trapped electrons, as primary functions of the spatial coordinate, allowed us to obtain the band diagram and the carrier concentrations under steady-state conditions. In Fig. 1, we show the depletion width on the GeSn side of a GeSn/Ge p-n junction as function of the p-dopant concentration for various trap densities at zero applied bias. This information is related to the minimal thickness of the epitaxial GeSn layer required for sheet resistance measurements using a four-point probe and can be useful for growth process tuning. The variation of the depletion width with the doping level can be associated to the impedance spectra as shown in Fig. 2 : the low-frequency resistance increases with the dopant concentration, and the capacitance deduced from the peak in the reactance curve corresponds to the width of the depletion region. This peak, located at 2 kHz for $N_A = 2\times10^{17}$ cm^{-3}, results from the electrical behavior of a RC parallel network which the GeSn/Ge heterojunction can be assimilated to. The properties of the interface region were also probed by a capacitance vs. voltage analysis at low-frequency, as shown in Fig. 3 in the case of two different values of the p-type dopant concentration in GeSn.

We also discussed the application to a metal-oxide-semiconductor stack and assessed the impact of partially-occupied trap states on the ac response. These results show that our method provides an access to both microscopic and macroscopic properties, and thereon, to a physical interpretation of the electrical characteristics of GeSn-based structures by linking measurable quantities to micro-scale variations in the structures.

REFERENCES

[1] J. Kouvetakis et al., Annu. Rev. Mater. Res. **36**, 497 (2006) [2] S. Takeuchi et al., Appl. Phys. Lett. **92**, 231916 (2008) [3] B. Vincent et al., Appl. Phys. Lett. **99**, 152103 (2011) [4] R. Roucka et al., Appl. Phys. Lett. **86**, 191912 (2005) [5] J. Werner et al., Appl. Phys. Lett. **98**, 061108 (2011)

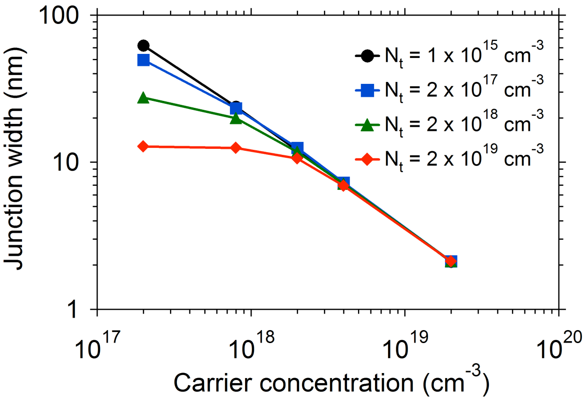

Fig. 1 Depletion width on the side of a p-type GeSn layer deposited on a n-type Ge substrate as function of the carrier concentration in GeSn and for various trap concentrations N_t.

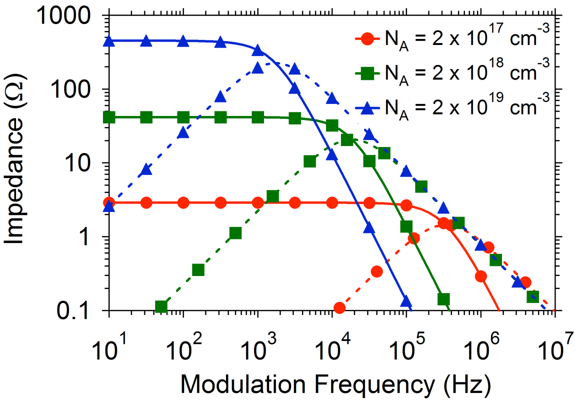

Fig. 2 Resistance (full lines) and reactance (dashed lines) as parts of impedance as function of the modulation frequency for various p-type dopant concentrations N_A.

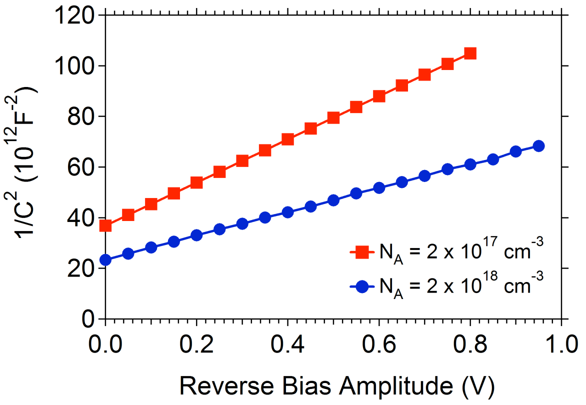

Fig. 3 Inverse low-frequency capacitance squared as function of the reverse bias for a p-GeSn/n-Ge junction with two different p-dopant concentrations in GeSn.