Research Internship for 2019

Laboratory:
Centre de Nanosciences et Nanotechnologie (C2N),
CNRS/Université Paris-Sud

Address: C2N, Département Nanoélectronique
C2N, Département Nanoélectronique
Avenue de la Vauve, 91120 PALAISEAU
Advisors: Jérôme Saint Martin
Website: http://computational-electronics.ief.u-psud.fr/
E-mail: jerome.saint-martin@u-psud.fr,

Theoretical study of thermal and thermoelectric properties of polytype Ge nanowires by using ab-initio Monte Carlo Simulation

Scientific Context

Nanowires have acquired in the last years a prominent role in several cutting-edge researches and could be used in particular as a material for **renewable energy**. Thanks to their unique electronic and thermal properties and compatibility with the existing microelectronic technology they can find interesting application in photovoltaics and **thermoelectrics**.

A new kind of [1] polytype Ge and Si nanowires (NW) is synthetized in the lab [2] consisting in a sequence of cubic and hexagonal phase (cf. Fig. 1). Though hexagonal Ge were observed 30 years ago [3.], its structure and physical **properties remain widely unexplored** a deep investigation of the transport properties of novel Ge nanowires polytypes is needed to evaluate the actual potential for technological applications.

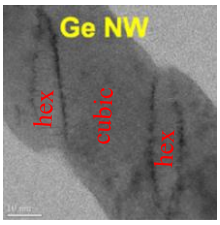

Fig. Ge polytype nanowire [2]

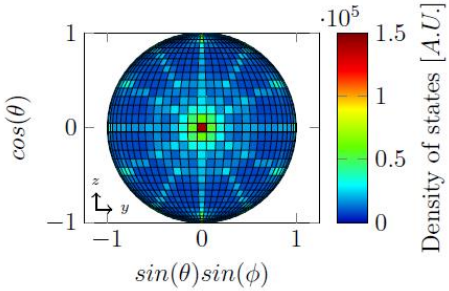

Fig. 2. angular phonon density of states

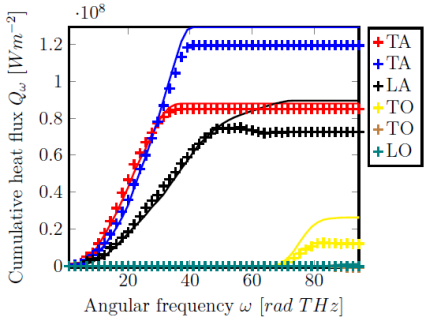

Fig. 3. Spectral distribution of the heat flux

Methodology and objectives

An internship position is available **in the COMputationnal electronICS group** and aims **to investigate theoretically the nanoscale heat transfer in these polytype NWs**.

As the Fourier heat equation does not rigorously describe the thermal transport at the nanoscale, we have developed a unique **home-made Monte Carlo simulator** based on the Boltzmann's transport equation for phonons. Our advanced simulator specifically dedicated to these Polytype Ge Nanowire includes a Full-band description of the material properties (dispersion and scattering rates cf. Fig. 2 and 3) that are parametrized by using ab-initio calculations.

The internship has 3 objectives:

- **(i)** Using the available code to study the thermal transport across the polytype interfaces,
- **(ii)** Making comparison between theoretical and experimental results,
- **(iii)** Developing the coupling between heat and electron transports.

Skills learned during the thesis

The student will acquire a broad range of skills: in solid state physics (band structure, phonon spectrum, electron transport, electron-phonon interaction and phonon-phonon interaction), technology devices, and scientific programming (Fortran and / or C / C + +, Matlab).

Besides, the results that would be obtained during this internship could be easily published in scientific journals. This work could be a relevant preliminary step for a Phd thesis in our group.

Candidate's Profile

Candidates must have a MSc in Physics, Electronics, Materials Science or related disciplines. We are seeking creative and highly motivated individuals well trained and skilled in scientific research, and available to collaborate in an interdisciplinary team. Programming experience is also desirable, but not mandatory.

Please join a CV, a list of courses that you have followed and results of exams in the framework of your master program, and any other information that you judge useful.

References:

[1] A.R. Verma and P. Krishna, Polymorphism and Polytypism in Crystals, Wiley, New York (1966). [2] L. Vincent, et al., Novel Heterostructured Ge Nanowires Based on Polytype Transformation, Nano Lett., 14 (8), pp 4828–4836 (2014) [3] R.H. Wentorf and J.S. Kasper, Science 139, 238 (1962)