TITLE: Theoretical study of electronic and thermoelectric properties of Ge nanowires polytypes

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Scientific Context

A PhD position is available in the COMputationnal electronICS group (http://computational-electronics.ief.u-psud.fr) and is aimed to investigate theoretically the electronic and phononic structures of Ge nanowires polytypes by applying a powerful combination of quantum-mechanical theory and computer simulation. The work will be carried out in strong collaboration with experimentalists.

Nanowires have acquired in the last years a prominent role in several cutting-edge research topics in nanoscience such as electronics, optoelectronics and renewable energy (photovoltaics and thermoelectrics) thanks to their unique electronic and thermal properties and compatibility with the existent microelectronics.

Among various parameters characterizing a nanowire (such as size, composition, geometry, etc.), recently the polytype has emerged as an important aspect of investigation. Polytypism is a one-dimensional variant of the well known phenomena of polymorphism, i.e. the ability of a solid material to exist in more than one form or crystal structure [1]. In our lab, the Heterna group (http://heterna.ief.u-psud.fr/) has recently developed an experimental method to achieve an unexpected martensitic phase transformation in Ge nanowires under external stress. The transformation process results in an unprecedented heterostructure characterized by the presence of hexagonal ordered phases as atomic stacking in cubic domains (homojunctions). Though hexagonal Ge were observed 30 years ago [2], its structure and physical properties remain widely unexplored and a unified description of its main functionalities is still lacking. A deep investigation of the basic physical properties of novel Ge nanowires polytypes is needed to evaluate the actual potential of this novel system for technological applications. Both theoretical and experimental investigations are needed to understand the specific behavior of such particularly appealing structure.

Methodology

A hierarchical multiscale approach will be adopted in order to link together different simulation levels to investigate the electronic band structure and phonon modes of nanowire polytypes:
(i) as a first step, a full first-principles approach for both the electronic and vibrational properties of the system in the framework of Density Functional Theory (DFT) will be employed. This method will be applied to investigate both size and interfacial effects [3], both for pure and polytype nanowires.
(ii) then, in order to simulate systems with size of the order of the experimental one, results of DFT simulations both for electrons and phonons will be linked to semi-empirical methods, i.e. Tight Binding and Force Constant Model. This stage will permit to have an accurate description on the dependence of the electronic structure (band structure, localization of electrons) and photonic structure (force constants and phonon dispersions) on the size of the system in order to give deep insights on quantum confinement effects in these nanostructures.
(iii) finally, a self-consistent solver of non-equilibrium Green's functions (NEGF) and Poisson's equation will be used to describe the quantum transport of particles in Ge/hGe nanowires. Both size and interfacial effects both for pure and polytype nanowires will be investigated.

This work will be developed under the support of the ANR JCJC NOE project 2012-16.

[1] A.R. Verma and P. Krishna, Polymorphism and Polytypism in Crystals, Wiley, New York (1966). [2] R.H. Wentorf and J.S. Kasper, Science 139, 238 (1962) [3] Amato M. et al., Nano Lett., 11,594–598 (2011)

Skills learned during the thesis

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

Candidate's Profile

Successful candidates must have a MSc in Physics, Chemistry, 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 and good knowledge of English are also desirable, but not mandatory.

How to apply

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