Short Visit Grant ☒ or Exchange Visit Grant ☐

(please tick the relevant box)

Scientific Report

The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event. It will be published on the ESF website.

Proposal Title: Si-SiC core-shell nanowires: ab initio modelling of electronic structure

Application Reference N°: 7196

1) Purpose of the visit

The main objective of this activity consisted in using the state-of-the-art ab initio electronic structure simulations - in the framework of Density Functional Theory as implemented in the SIESTA code- to investigate the electronic structure of Si-SiC core shell NWs in order to assess their viability as efficient biosensors.

2) Description of the work carried out during the visit

The principal activity of this project consisted in ab initio simulations of the structural and electronic properties of Si-SiC core-shell NWs. The project started before the visit of M. amato at ICMAB in order to optimize the proposed work plan. After a careful preliminary work to find the optimal convergence parameters of the studied systems, a systematic investigation of their main electronic and structural features has been performed. The first step was focused on the effect of the Si-C shell on the electronic properties of Si NWs. Full geometry relaxations of Si-SiC core-shell NWs were performed. On the other hand, calculations on pure strained Si NWs were conducted in order to understand the role of the SiC shell on the band structure.
Surprinsingly we found that a SiC shell that is thick enough in comparison with the Si core can drive a semiconductor−metal transition because of the large compressive strain.

This finding offers a very interesting perspective for its use as sensor in biological environments: the Si core maintains its transport properties, with a mobility that is roughly insensitive to the presence of the shell, but benefits from the protection of the biocompatible SiC shell. Moreover, in order to check our results on thicker wires, we performed some calculations based on classical potentials indicating that in all the cases of practical interest a Si−SiC core−shell NW is semiconducting.

3) Description of the main results obtained

We have worked on a novel kind of coaxial structure: Si-SiC core-shell nanowires, which has been synthesized for the first time in 2013 by a group from Grenoble [M. Ollivier, L. Latu-Romain, M. Martin, S. David, A. Mantoux, E. Bano, V. Soulièr, G. Ferro, T. Baron, J. Cryst. Growth, 363, 158– 163 (2013)]. These systems are of great interest for application as biosensors. There is a general consensus on the fact that the chemically inert and hydrophilic surface of SiC makes it a much better biocompatible material than Si. Therefore, one can envisage a biosensor whose backbone is made of Si, thus easily embedded into the existing technology, and where the interface between the electronic and biological world is mediated by the more biocompatible 3C-SiC surface. Our calculations highlight two major points: (i) first, for ultrathin Si−SiC core−shell NWs the presence of a thicker shell (more than one monolayer) has a drastic effect on the electronic structure leading to a semiconductor-metal transition; (ii) this occurrence is fortunately not observed in the case of larger diameter wires, which remain semiconducting also for four monolayer (ML) shells assessing their potential as biocompatible nanostructures.

4) Future collaboration with host institution (if applicable)

This short visit has offered the possibility to assess and consolidate a novel and innovative activity. Of course, this has been only the first step of such ambitious project, which will last in the next months. Once that the main electronic features of such kind of wires have been identified, the next step will be of course the study of the effect of biological and organic molecules on the electronic structure in order to understand the sensing mechanism in these new materials.

5) Projected publications / articles resulting or to result from the grant *(ESF must be acknowledged in publications resulting from the grantee's work in relation with the grant)*

Major outcome of this collaboration is the following publication: Michele Amato and Riccardo Rurali, Shell-Thickness Controlled Semiconductor−Metal Transition in Si−SiC Core−Shell Nanowires, Nano Letters 15(5), 3425–3430 (2015)

6) Other comments (if any)

The continued ESF support for the organization of the visit has been greatly appreciated by all the people involved in this project.