ESF - Science Meeting - Final Report

Theory, Simulation and Modelling of SiGe Nanostructures: from Nanoelectronics to Renewable Energy

June 3, 2013 to June 6, 2013
CECAM-HQ-EPFL, Lausanne, Switzerland

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Summary

The study of SiGe nanostructures is one of the most rapidly developing area in materials science, but his future will depend on how some fundamental issues will be really investigated and explained. Our aim was to create a high-level interdisciplinary space, by bringing together a diversified community of researchers coming from Academia and Research Centers all over the world.
We sought to examine limits and perspectives of SiGe nanostructures in order to address a large and general discussion about real applications in current technology, in nanoelectronics, renewable energy, and quantum computing. The workshop served as a space to develop and share ideas, drawing upon personal and academic experiences.

SiGe nanostructures are particularly fascinating, as by bringing together two similar elements –Si and Ge, neighbors in the periodic table–, a rich variety of new chemical and physical properties can emerge, stimulating both fundamental and application-driven research in nanoscience. These materials present unique structural, electronic, optical and transport properties, which are intrinsically associated with their low dimensionality and with the quantum confinement effect.

This points out the main motivation of this workshop: due to the rapid advance of the experimental and devices investigation in this area, we thought as very urgent to assess the state of the art of theoretical/computational understanding and provide the opportunity for theoreticians and experimentalists working in this specific field to discuss latest achievements, progresses, difficulties and open questions.
Indeed we think it is of fundamental importance to develop a precise atomic understanding of these materials because it is clear that its absence is, generally speaking, a barrier to progress in the field, where one of the major goals, today, is to produce SiGe nanostructures with tunable shape, composition, strain and doping which can be easily integrated into devices.

Description of the scientific content of and discussion at the event

Three main hot questions have been considered:

• **Growth and characterization**, to devise simulations and modeling of critical processes during the synthesis of SiGe nanostructures in order to reach a precisely controlled and tunable composition, structure, geometry.
• **Electronic structure and Optical excitations**, to simulate and describe accurately fundamental topics: band offset, impurity activation energy, and optical response.
• **Transport Processes,** to determine the physics governing transport processes including electronic, spin, thermal transport.

The idea has been, for each point, to highlight which is the state-of-the-art and to clarify which are the research efforts done up to now and in which direction they should go in the future.

In summary we can asses that four main scientific advances have been reached:

1. Precise understanding of the relation between structural properties and electron and thermal transport of SiGe nanostructures.
2. Understanding and controlling the atom probe topographic analysis of SiGe nanowires and nanomultilayers.
3. Understanding and controlling the role of doping.
4. Understanding and controlling the role of spin-related properties.

Assessment of the results and impact of the event on the future direction of the field

This workshop has been the first attempt to put together all the scientists both theorists and experimentalists working on SiGe nanostructures.
With 42 participants from very different countries, generally very well qualified, the present workshop has taken benefit from the partnership with CECAM, PSI-K and ESF, whose international reputation has significantly contributed to its success. We plan to organize another workshop on the general subject of SiGe nanostructures, including progress to be identified in the next few years, in 2015.
The workshop has identified four research areas that might be of particular importance for EU community and that could be funded by the EU 2020 program.
More in details, in the documents describing the specific program implementing Horizon 2020 it is explained that the specific plan shall consist of the following parts:

(a) Part I *Excellent science*;
(b) Part II *Industrial leadership*;
(c) Part III *Societal challenges*;
(d) Part IV *Non-nuclear direct actions of the Joint Research Centre (JRC)*.

The output of the workshop are directly linked with “Excellent science”, “Societal challenges” and indirectly with “Industrial leadership”.

PART I Excellent Science employs the following schemes to promote research on enabling technologies: 1. European Research Council 2. Future and Emerging Technologies (FET Open, FET Proactive) 3. Marie Curie actions 4. Research Infrastructures. All these actions must be funded with high priority, in particular the development of major research infrastructures at European Level for High Parallel Computing.

Moreover a clear focus on collaborative research projects entirely based on multiscale and ab-initio calculations is a necessary choice, since it is more and more necessary to understand the properties of new materials at microscopic and atomistic level in order to guide the experimental work towards innovation.

PART II Industrial leadership within Horizon 2020 shall strengthen industrial leadership by pursuing the following specific objectives: (a) boosting Europe's industrial leadership through research, technological development, demonstration and innovation in the following enabling and industrial technologies:
(i) information and communication technologies; (ii) nanotechnologies; (iii) advanced materials; SiGe nanostrutures can play an important role in all these items, in particular regarding advance nanomaterials for application in quantum computing, green energy applications in photovoltaic and thermoelectrics, or nanomedicine.

PART III Societal challenges shall contribute to Horizon 2020 by pursuing research, technological development, demonstration and innovation actions which contribute, among others, to the following specific objectives:
“c) making the transition to a reliable, sustainable and competitive energy system, in view of increasing resource scarcity, increasing energy needs and climate change;”
In particular, regarding priority “3. Secure, clean and efficient energy” we envisage two main

applications for SiGe nanostructures that must be adequately funded:
i) In photovoltaics, on long-term research on various types of photovoltaic cells dealing with several novel concepts, hence directly contributing to reduction of the cost-per-Watt which is the relevant figure of merit for grid parity
ii) In thermoelectric application, where reliable and scalable, devices are presently used in a number of applications for both turning heat into electricity, measuring temperature and using electricity to produce cooling (Peltier cooling and temperature controllers). For the design of practical energy generator devices, not only the efficiency has to be taken into account. Indeed, since the waste heat is abundant (and of course inevitable) in industrial processes, home heating and automotive exhaust, the specific output power, which in the end determines the final utilization of the generated power, turns to be more significant. Thus SiGe based devices assumed a special importance since the have low cost and can be fully integrated.

We plan to organize another workshop on the general subject of SiGe nanostructures, including progresses to be identified in the next few years, in 2015.

Final Program

Day 1 - June, 3 2013

Registration and welcome

- 13:15 to 13:45 - Registration
- 13:45 to 14:00 - Welcome

Thermal -transport i

- 14:00 to 14:40 - **Luciano Colombo**
  Thermal transport in bulk sige nanocomposites
- 14:40 to 15:30 - **Armando Rastelli**
  Thermal transport through ge/si superlattices
- 15:20 to 16:00 - **Antonio Samarelli**
  Thermal and electrical characterization of ge/sige thermoelectric materials
- 16:00 to 16:30 - Coffee Break
- 16:30 to 17:10 - **MING HU**
  generating efficient thermoelectrics with si-nanowires and related nanocomposites
- 17:10 to 17:50 - **Gyeong S Hwang**
  On the origin of thermal conductivity suppression in silicon-germanium alloys
- 17:50 to 18:30 - **Nicola Marzari**
  Engineering thermal transport from first principles

Day 2 - June, 4 2013

Growth

- 9:00 to 9:40 - **Joan Redwing**
  Synthesis and properties of aluminum-catalyzed silicon nanowires
- 9:40 to 10:20 - **Chen Yang**
  Transport modulation in ge/si core/shell nanowires through controlled synthesis of doped si shells
- 10:20 to 10:40 - **Mahmoud Shehadeh**
  Bayesian analysis for robust synthesis of nanostructures
- 10:40 to 11:10 - Coffee Break
- 11:10 to 11:50 - **Hugh Geaney**
  Atomically abrupt silicon–germanium axial heterostructure nanowires synthesized in a solvent vapor growth system
- 11:50 to 12:30 - **Ari Niilo Harjunmaa**
  The path to a porous semiconductor multilayer

- 12:30 to 14:30 - Lunch

Nanocrystals

- 14:30 to 15:10 - **Isabelle Berbezier**
  Sige nanostructures self-organisation

- 15:10 to 15:50 - **Conor Hogan**
  Optical and electronic properties of {105} facets on ge/si quantum dots

- 15:50 to 16:10 - **Margherita Marsili**
  Many-body effects in hydrogenated ge, si and sige nanoparticles

- 16:10 to 16:40 - Coffee Break

- 16:40 to 17:20 - **Silvano De Franceschi**
  Hole-spin control in sige self-assembled quantum dots

- 17:20 to 18:00 - **Friedhelm Bechstedt**
  Influence of material and matrix on nanocrystal properties

Day 3 - June, 5 2013

Optics

- 9:00 to 9:40 - **Moon-Ho Jo**
  Broadband photodetection in si:ge alloy nanocrystals

- 9:40 to 10:20 - **Hans-Christian Weissker**
  Temperature effects on the optical properties of si and ge nanocrystals

- 10:20 to 10:40 - **Nancy Carolina Forero Martinez**
  Temperature effects on the optical and electronic properties of silicon nano-crystals

- 10:40 to 11:10 - Coffee Break

- 11:10 to 11:30 - **Giovanni Pizzi**
  Calculation of near-infrared radiative recombination and optical gain spectra in strained n-type ge

- 11:30 to 11:50 - **Enrique Montes**
  Relation between structural properties and electron transport in si nanowires

- 11:50 to 12:30 - **Giovanni Isella**
  Optical spin injection in sige heterostructures

Thermal -transport ii

- 13:30 to 15:10 - **Chen Jie**
  Thermal transport in core-shell nanowires: the effects of phonon resonance and atomistic coating

- 15:10 to 15:30 - **Claudio Melis**

Thermal transport in sixge1-x alloys

- 15:30 to 15:50 - **Federico Iori**
  Electronic and transport properties of si-ge heterostructure

- 15:50 to 16:20 - Coffee Break

- 16:20 to 17:00 - **Ivana Savic**
  Large scale atomistic simulations of thermal transport properties of sige nanostructured materials

- 17:00 to 17:20 - **Felipe Murphy Armando**
  First principles calculation of the thermoelectric properties of n-type sige

- 20:00 to 23:00 - Social Dinner

Day 4 - June, 6 2013

Defects

- 9:00 to 9:40 - **Naoki Fukata**
  Formation and site selective doping in si/ge and ge/si core-shell nanowires

- 9:40 to 10:20 - **Kee Joo Chang**
  Defects and impurities in ge/si and sige/oxide core-shell nanowires

- 10:20 to 10:50 - Coffee Break

- 10:50 to 11:30 - **Leo Miglio**
  Modeling of dislocations in ge-si heteroepitaxial systems at the nanoscale

- 11:30 to 12:10 - **Lincoln J. Lauhon**
  An intrinsic source of dopant heterogeneity in vls nanowires

- 12:10 to 12:30 - Closing Word

Participant List

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