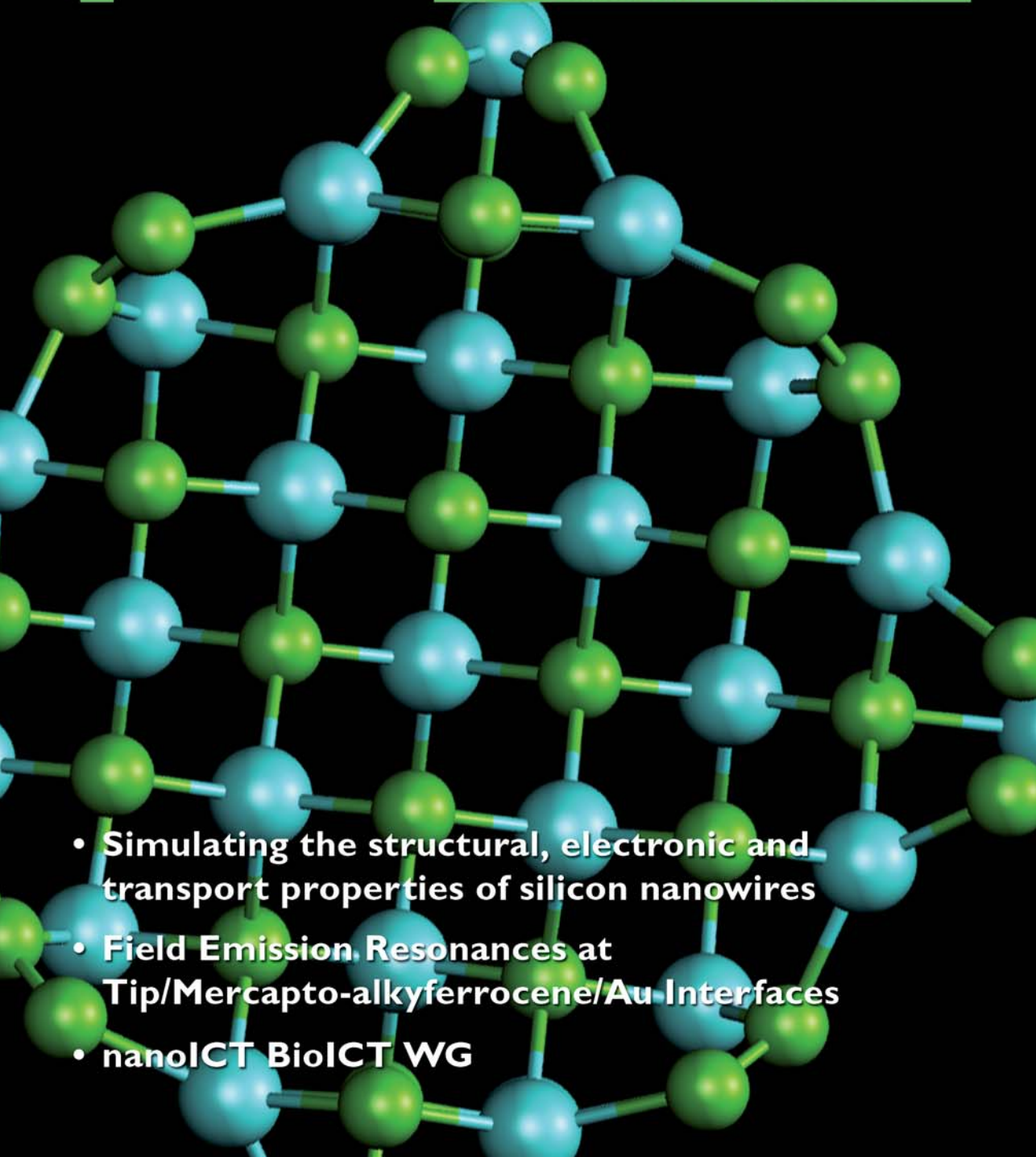


enano newsletter

No. 19 • October 2010 • www.phantomsnet.net

- 
- **Simulating the structural, electronic and transport properties of silicon nanowires**
 - **Field Emission Resonances at Tip/Mercapto-alkylferrocene/Au Interfaces**
 - **nanICT BioICT WG**

CIC nanogune

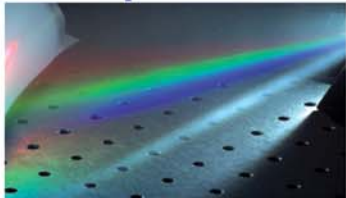
nanoscience COOPERATIVE RESEARCH CENTER



Nanomagnetism



Nanooptics



Self-assembly



Nanodevices



Nanobiotechnology



Nanoscale imaging



www.nanogune.eu
www.nanogune.eu

Dear Readers,

Following the last E-nano Newsletter special double issue dedicated to semiconductor nanowires (NW), this edition contains an article providing new insights in this relevant field for future nanoelectronics applications, i.e. the computational tools used to simulate their structural, electronic and transport properties.

Nanowire-based devices offer unique opportunities in different research areas and represent a possible impact as key add-on technologies to standard semiconductor fabrication.

The BioICT position paper provides an analysis of the current status of the routes to bring bio-inspired nanosystems and nanomaterials in the field of nanotechnology. The bio-inspired method is of particular importance to another central challenge in technology, i.e. constructing multi-scale structures used to organize nanodevices and functional materials.

We would like to thank all the authors who contributed to this issue as well as the European Commission for the financial support (project nanoICT No. 216165).

Dr. Antonio Correia
Editor - Phantoms Foundation

Deadline for manuscript submission

Issue No. 20: December 31, 2010

Issue No. 21: February 28, 2011

Dépósito legal/Legal Deposit:
M-43078-2005

Impresión/Printing:
Madripapel, S.A.

C

Contents

- 5 nanoresearch**
Simulating the structural, electronic and transport properties of silicon nanowires
Xavier Cartoixa et al.
- 19 nanoconferences**
- 20 nanovacancies**
- 24 conference report**
- 28 nanoICT research highlight**
Field Emission Resonances at Tip/Mercaptoalkylferrocene/Au Interfaces.
Lars Müller-Meskamp et al.
- 30 nanoICT BioICT WG**
Jean-Pierre Aimé.

E

Editorial Information

No. 19 October 2010

Published by
Phantoms Foundation
(Spain)



Editor

Dr. Antonio Correia antonio@phantomsnet.net

Assistant Editors

José Luis Roldán, Maite Fernández, Conchi Narros,
Carmen Chacón and Viviana Estêvão

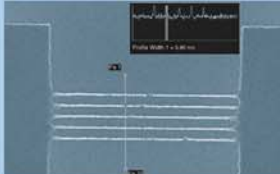
1500 copies of this issue have been printed.

Full color newsletter available at:
www.phantomsnet/Foundation/newsletters.php

For any question please contact the editor at:
antonio@phantomsnet.net

Editorial Board

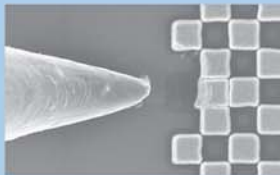
Adriana Gil (Nanotec S.L., Spain), Christian Joachim (CEMES-CNRS, France), Ron Reifengerger (Purdue University, USA), Stephan Roche (ICN-CIN2, Spain), Juan José Saenz (UAM, Spain), Pedro A. Serena (ICMM-CSIC, Spain), Didier Tonneau (CNRS-CINaM Université de la Méditerranée, France) and Rainer Waser (Research Center Jülich, Germany).



Sub 10 nm lithography



E-beam deposition



Nano Sokoban



Photonic crystal with proximity effect correction



X-ray analytics

Ultra high resolution electron beam lithography and nano engineering workstation



eLINE

- ...Nano metrology
- ...Nanoscale imaging
- ...EDX-chemical analysis
- ...Electron beam etching
- ...Electrical and mechanical probing
- ...Electron Beam Induced Deposition (EBID)

Upgrade your SEM / FIB to a nanolithography system

benefiting from a reliable modular attachment concept



ELPHY™ Plus

The advanced lithography system.....



ELPHY™ Quantum

The universal lithography attachment.....



Laser Interferometer Stage

The ultimate positioning tool.....



Simulating the structural, electronic and transport properties of silicon nanowires

Xavier Cartoixà¹ and Riccardo Rurali²

¹Departament d'Enginyeria Electrònica
Universitat Autònoma de Barcelona
08193 Bellaterra, Barcelona, Spain

²Institut de Ciència de Materials de Barcelona ICMAB
(CSIC), 08193 Bellaterra, Barcelona, Spain

1. Introduction

Silicon nanowires (SiNWs) hold great promise to integrate conventional Si devices in future nanoelectronics applications, and their use as bipolar transistors [1], logic gates [2], non-volatile memories [3], solar cells [4], biological sensors [5], energy conversion devices [6, 7] and giant piezoresistance devices [8] has been reported. Semiconducting nanowires (NWs) have also been fabricated with III-V materials, achieving heterojunctions [9], or in II-VIs, where the piezoelectric properties of some of them have attracted a great deal of attention lately [10].

The computational tools used to simulate their properties range from the *ab-initio* based on the density functional theory (DFT) [11] with a number of refinements (hybrid functionals) to extract structural and basic electronic structure information¹, to the GW approximation [12] or time-dependent DFT (TDDFT) [13] for properties involving excited states, to tight-binding for the properties of larger systems [14], etc. Using the tools above, theorists have extracted [15] properties such as Young's modula, Poisson ratios, energy gaps, impurity solubilities, dopant activation energies or conductivities, to name just a few.

Here we will discuss some of the recent developments in the theoretical modeling of the structural, electronic and transport properties of SiNWs, with a special attention on the results that we have obtained at the Computational Nanoelectronics Group (NANOCOMP) at the Universitat Autònoma de Barcelona and at the Theory and Simulation of Materials Department at the Barcelona Materials Science Institute (ICMAB-CSIC) in the last years, showcasing improved ways of passivating SiNWs, bringing up the failure of conventional Si dopants to act as donors or acceptors in thin SiNWs, proposing workarounds for this failure and, finally, studying the effect that some impurities can have in transport within SiNWs. Although specific examples will always be

given for SiNWs, most of the general ideas can be extended to NWs constructed from other materials.

2. Passivation issues

It is widely known that freshly cleaved Si surfaces exposed to vacuum feature highly reactive dangling bonds that, without other species available, produce a rearrangement of the atoms close to the surface in order to share electrons and minimize as much as possible the number of exposed dangling bonds. The specific arrangement of atoms, known as surface reconstruction, will mainly depend on the Miller indices of the exposed plane after cleavage and the surface temperature.

Freshly grown NWs also present surface reconstructions (Fig. 1), which can give rise to surface states and even change the semiconducting character of the NW into a metallic one by means of the formation of delocalized surface states. Such semiconductor-to-metal transition has been predicted theoretically [16], although convincing experimental observation are lacking so far. At the same time, however, the role of surface and interface states has been highlighted by several studies [17].

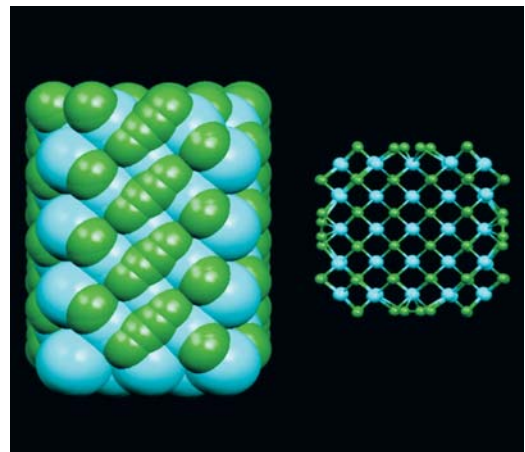


Fig 1. Side and top view of a surface-reconstructed SiC nanowire. This wire features metallic surface states [18].

Thus, in order that the surface properties of the SiNW remain under control, the wire surface is passivated, typically with H atoms. In computational studies, the

¹ It is well known that the DFT underestimates the fundamental gap of semiconductors [11].

choice of hydrogen as a monovalent passivating agent is motivated by its straightforwardness, but also by the fact that it is easy to achieve experimentally through a well-defined protocol where the oxidized wire is attacked with HF. Passivation by oxidation –the most common experimental situation– is more complex. Thermal oxide is amorphous and then difficult to model at the nanoscale, because of the large amount of atoms required to describe the disordered phase. In the study of SiNWs, for most practical effects, hydrogen termination is a reasonable approximation to oxide passivation and this is the strategy adopted in most of the theoretical studies. Despite its simplicity, however, H termination of the Si surface dangling bonds still give rise to a wealth of possible configurations, depending on the orientation of the passivated facet, the surface structure –e.g. previous partial reconstructions [19]– and the type of the Si-H complex that form; mono-, di- and tri-hydrides being possible [20].

It can be shown through a simple particle-in-a-box argument that quantum confinement yields a broadening of the gap, related to squared inverse the nanowire diameter. Clearly, the possibility of tuning the band-gap of a nanowire –and consequently the related optical and electronic properties– is tremendously attractive. However, it is not difficult to imagine how challenging is controlling the wire size with tolerances of the order of a nanometer. A simpler route to band-gap engineering can be found in controlling the surface chemistry of the nanowire. A few studies shows that, if the wire diameter is thin enough so that the eigenstates sense the wire walls, i.e. the wire is in the quantum confinement regime, it is possible to tune the band-gap by controlling the chemical composition and the coverage density of the wire surface [21, 22, 23].

Halogens such as Cl, Br, and I can be used as surface passivation agents instead of H and, while not altering the semiconducting character of the wires, they result in a significant shrinking of band gap. The strongest reduction of the band gap is provided by I, followed by Br and Cl, in the opposite order of the bonding strength of these species and SiNWs. Interestingly, the surface coverage is a further degree of freedom and one can span all the band gap values between a H- and halogen-passivated wire by varying the H:halogen ratio. Similar results have been obtained by Aradi *et al.* [22] with OH, by Ng *et al.* [24] with F and by Nolan *et al.* [23] with NH₂.

Motivated by recent experimental advances [25], we have compared [26] the robustness of methyl passivation (Fig. 2) to the more common surface hydrogenation. We have found that the dissociation energy for the –CH₃ radical is ~5.5 eV, while the dissociation energy for a H atom in the hydrogenated wire is ~3.2 eV, indicating a greater energetic cost to create a dangling bond in the methyl passivated SiNW.

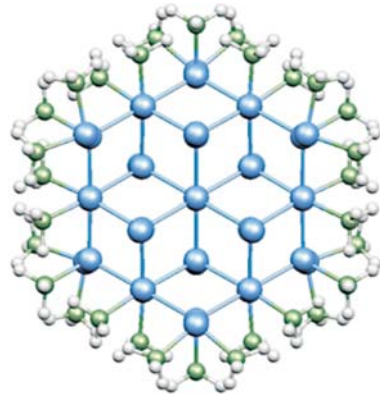


Fig 2. Cross-section view of a structurally relaxed 1.0 nm $\langle 111 \rangle$ SiNW with CH₃ passivation.

The presence of dangling bonds at the wire surface can be detrimental, especially if the NWs are to be doped, since it has been shown [27] that dopants such as B and P have a tendency to segregate to the surface of hydrogen passivated SiNWs where, in presence of dangling bonds, they are rendered electrically inactive. This can be simply understood in terms of electron counting: a P at the surface will provide the dangling bond with the electron it is missing to fill up the orbital. On the other hand, a B atom at the surface position will not have a dangling bond at all. In both cases, the net result will be a filled shell without a free radical, i.e. a lower energy configuration without electrical activity.

3. Doping of SiNWs

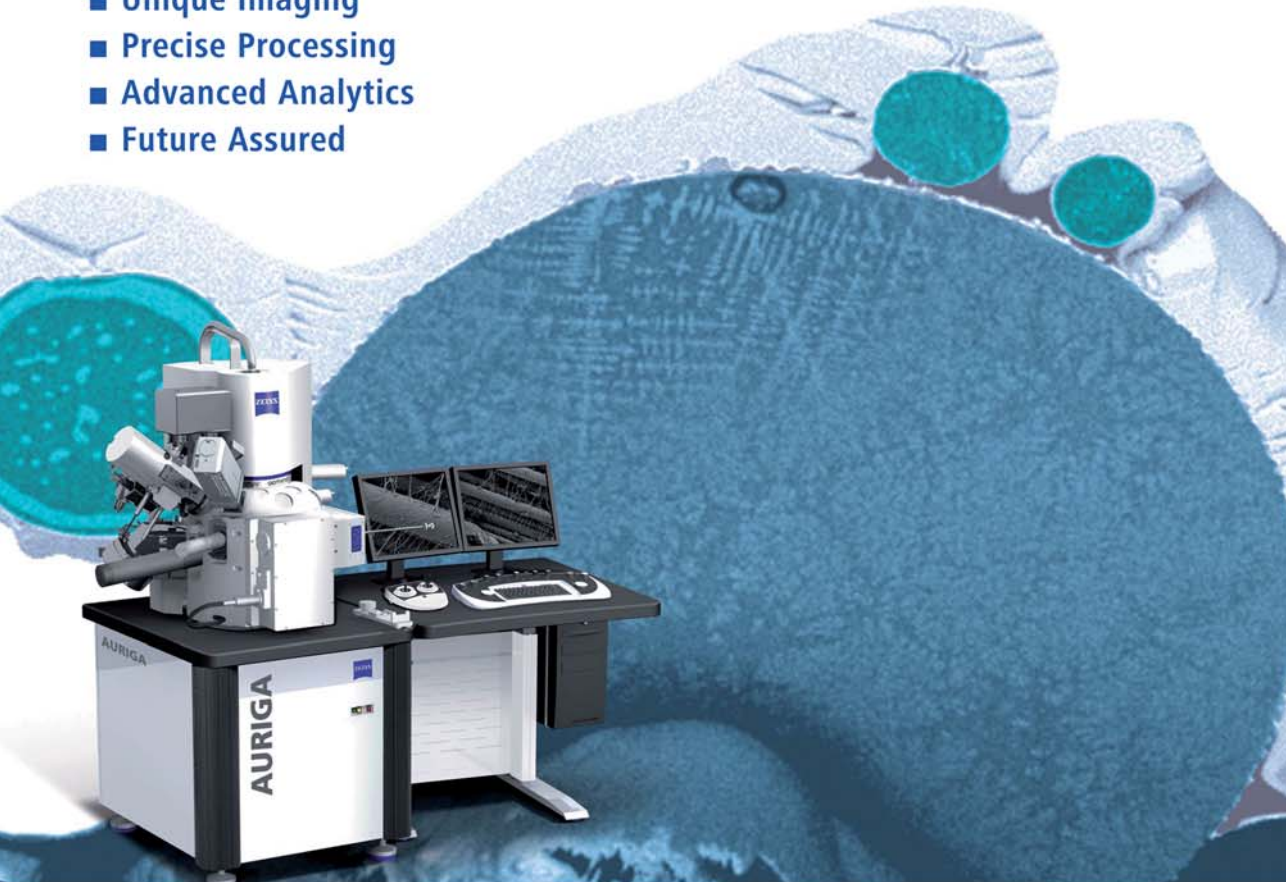
3.1 Introduction

Doping in bulk Si is typically achieved by the introduction of trace amounts of group III (acceptor) or group V (donor) impurities, having a missing or an extra electron in the valence levels, respectively, with regard to the Si atoms they substitute. Because of an acceptor having one less positive charge in its nucleus, it will

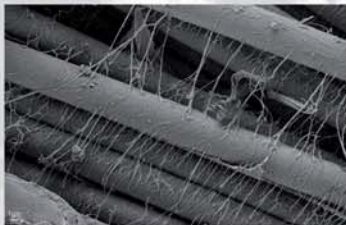
AURIGA™

Information Beyond Resolution

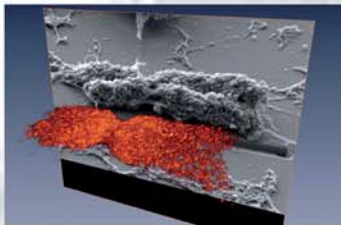
- Unique Imaging
- Precise Processing
- Advanced Analytics
- Future Assured



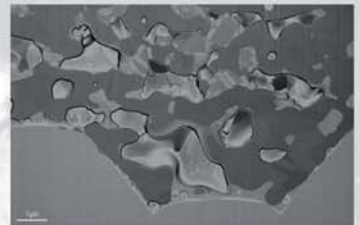
CrossBeam® Workstations (FIB-SEM)



Chamber SE image of an uncoated fibre adhesive (used in modern shipbuilding). Taken with local charge compensation at 5 kV.



3D reconstruction of chromosomes based on real-time movie. Taken with in-lens SE detector at 2 kV. Courtesy of Prof. G. Wannier, Munich, Germany.



Cross section through the front contact of a Si wafer-based solar cell. Taken with in-lens SE detector at 2 kV. Courtesy of Dr. F. Machaleit, erisol Solar Energy AG, Erfurt, Germany.

Carl Zeiss SMT
Nano Technology Systems Division
info-nts@smt.zeiss.com
www.smt.zeiss.com/nts

Enabling the Nano-Age World®



We make it visible.

attract surrounding electrons with less force, and thus its corresponding top of the valence band (TVB) level will lie slightly above the Si TVB levels (see Fig. 3). A similar reasoning for donors, which can attract electrons more strongly than the surrounding Si atoms, shows that the last occupied level in a donor atom will lie slightly below the bottom of the conduction band (BCB) Si levels. The Kohn-Luttinger theory of shallow (hydrogenic) impurities [28] gives a good estimate of the position of these levels, with the only input of the relevant effective mass and the dielectric constant of the host semiconductors.

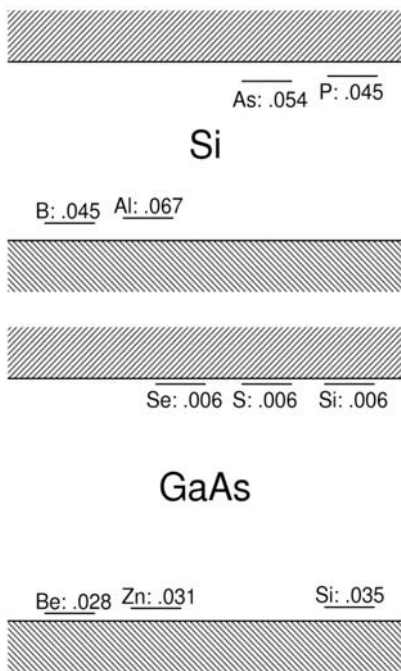


Fig 3. Transition levels for common acceptor and donor impurities in Si and GaAs. The acceptor is neutrally (negatively) charged when the Fermi energy lies below (above) the marked level. The donor is positively (neutrally) charged when the Fermi energy lies below (above) the marked level. Si can behave as a donor or an acceptor in GaAs, depending whether it substitutes a Ga or an As atom, respectively.

Thus, the same strategy is expected to be valid in SiNWs. Indeed, bulk-like doping has been achieved for wires with diameters above ~ 50 nm [29, 30], but as the diameter of the wires is reduced below 20 nm, new effects arise that hinder the effectiveness of the dopants. On one hand consider, for example, the promotion of an electron from a donor-bound state to the SiNW conduction band (CB).

This electron will try to escape the attraction of a positively ionized impurity, but the dielectric mismatch between the wire and the surrounding medium, typically air, induces the build-up of positive polarization charges at the wire surface that will also contribute to the attracting potential. The net effect, termed dielectric confinement, will be an increase of the dopant ionization energy² as the radius of the SiNW decreases and the ratio between the dielectric constants of the wire and the medium increases [31, 32, 33].

On the other hand, as the diameter of the SiNW reaches the Fermi wavelength of the carriers, quantum confinement effects will play a role. Apart from the increased level separation (particle-in-a-box), as the wire gets thinner the problem to be solved tends towards a one-dimensional hydrogen atom, which has an infinitely localized ground state [34].

Altogether, the net effect of quantum confinement will be to separate the impurity and band edge levels, thus increasing the ionization energy as well. Since the donor wave function has a Bohr radius of ~ 2.2 nm (thus a 4.4 nm diameter), wires with a diameter $d \leq 9$ nm can limit its spatial extent [35]. For wires with $d \leq 4$ nm, quantum confinement effects can contribute to the ionization energy a similar amount as dielectric confinement.

3.2 First-principles methods

Of course, first-principles methods are perfectly equipped to study the dopant activation problem since, for their very nature, they are based on the many-body Schrödinger equation, which obviously will describe quantum confinement effects, and the *microscopic* Poisson equation, meaning that the local averaging procedure involved in defining a dielectric constant is not made, and thus the consequences of having regions with dissimilar electrostatic properties are taken into account exactly.

These two equations are solved until self-consistency is achieved between the electronic charge obtained from the Schrödinger equation and the electrostatic potential from the Poisson equation. Very basic information

² The terms *ionization energy*, *activation energy* and *binding energy* are used interchangeably in this paper to describe the escape of a charge carrier from an impurity bound state to an extended state within a band. *Ionization energy* might also refer to the energy required to extract an electron from the Fermi level to the vacuum level. If the latter sense is meant, it will be made explicit in the paper.

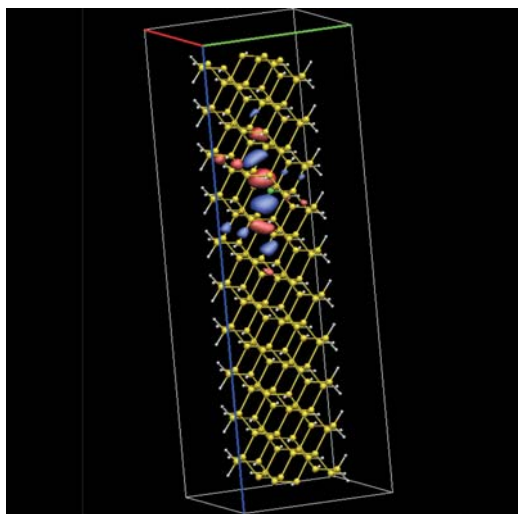


Fig 4. Positive and negative amplitude contours of the LUMO of a hydrogen-passivated SiNW doped with an Al atom (green).

about the system, such as the impurity state wave function shown in Fig. 4, can be extracted with little to none input in form of fitting parameters.

Several criteria can be employed when classifying a particular first-principles scheme, of which a few may be:

- The type of Hamiltonian that is solved: Hartree-Fock (HF), density functional theory (DFT), quantum Monte Carlo, etc.
- The procedure for including many-body effects: configuration interaction, Møller-Plesset perturbation theory, coupled cluster, local density approximation (LDA), generalized gradient approximation (GGA), on-site repulsion, etc.
- The treatment of excited states: hybrid functionals, GW approximation, time-dependent DFT, etc.
- The basis sets used for the expansion of the solution: plane waves, wavelets, localized orbitals (eg. gaus-

Advertisement

The latest member of the physica status solidi journals

physica status solidi RRL – Rapid Research Letters, the fastest peer-reviewed publication medium in solid state physics!



www.pss-rapid.com

2010, Volume 4, 12 issues.
Print ISSN: 1862-6254
Online ISSN: 1862-6270

Focus on Carbon Electronics: Graphene - Nanotubes - Diamond

graphene
Si radiation
SiC
STM
Ab initio calculation

WILEY-VCH

First Impact Factor 2.147

>>> communicates important findings with a high degree of novelty and need for express publication, as well as other results of immediate interest to the solid state physics and materials science community.

>>> offers extremely fast publication times: typically less than 14 days from submission to online publication. This is definitely a world record for Letter journals in solid state physics! Peer review by two independent referees guarantees strict quality standards.

With a brilliant first Impact Factor of 2.147 (2008 Journal Citation Reports®, Thomson Reuters 2009) *pss RRL* is the most highly cited journal publishing exclusively Letter articles in Condensed Matter Physics.



For more information please contact Wiley Customer Service:

■ cs-journals@wiley.com
(Americas, Europe, Middle East and Africa, Asia Pacific)

■ service@wiley-vch.de
(Germany, Austria, Switzerland)

■ cs-japan@wiley.com
(Japan)

sians, Slater type orbitals, atomic, Sankey, grid-centered).

- The description level of core electrons: all electron, pseudopotential, projector-augmented waves.

As the computational power available to theorists has increased, condensed matter physicists and materials scientists have attacked the problem of doping in NWs from their experience dealing with extended systems within a DFT framework, moving from the 3D periodic boundary conditions (PBCs) of bulk materials to the 1D PBCs typical in NWs.

On the other hand, chemists have moved from the study of small molecules with HF and post-HF methods to the bigger unit cells needed for the description of NWs, sometimes adopting the DFT formalism in the process, though with a tendency to keep some of the hybrid formalisms that had proved their merit in molecular studies.

Different aspects of dopant incorporation into SiNWs have recently started to be addressed with DFT studies. We have already mentioned (Sec. II) the tendency of B and P substitutionals to segregate to the surface of ultrathin SiNWs [27], where they are rendered electrically inactive in the presence of dangling bonds, and calculations by other authors [36, 37] have observed similar effects. The same studies [37] do observe, however, that the driving force for surface segregation is rapidly reduced as the diameters grow larger.

Although the promotion of an electron from the VB into an acceptor level or from a donor level into the CB are processes involving excited states, and those are notoriously inaccurate within the DFT-LDA/GGA, it has been argued [38] that the DFT-LDA/GGA is capable of obtaining GW-quality donor binding energies when computing them as a difference of the electron affinities $E_b = A^d(N) - A^p(N)$, where $A^p(N)$ [$A^d(N)$] is the energy released when bringing an electron from the vacuum level to the lowest unoccupied molecular level (LUMO) of the pristine (positively charged) NW.

This would be due to a near cancelation of the unknown exchange-correlation terms for both cases. In any case, dopant binding energies have been calculated both with pure GGA schemes [39, 37] and with GGA plus hybrid functionals [35], which are known to reproduce well the fundamental gap in semiconductors.

3.3 Charged impurity formation energies in SiNWs

A magnitude closely related to the dopant activation energy is the *charged impurity formation energy*, where the dopant does not provide an electron (hole) to the CB (VB) but, rather, the supplied carrier goes to a reservoir with a given electrochemical potential E_F , leaving behind a system with net charge. This is expected [40] to be the magnitude of significance for thin, short or few amounts of semiconducting NWs, which would become totally depleted due to the charge transfer to the growth substrate or to the leads contacting the NW.

In bulk host materials the study of the energetics of the formation of defects is a very well-developed topic, [41, 42, 43] and formation energies are calculated according to the well-established expression due to Zhang and Northrup (ZN) [44, 45], where they are formulated in terms of the chemical potentials of the constituent species and the total energy of the system with the impurities. Additionally, the most stable configuration of an impurity in a semiconductor may have a charge state different from zero, depending on the doping condition of the material. Thus, for example, the formation energy of a vacancy in bulk Si, ΔE^f , would be given by

$$\Delta E^f = E_{tot}^D - E_{tot}^{pure} + \mu_{Si} + q(\varepsilon_v + \mu_e) \quad (1)$$

where E_{tot}^D (E_{tot}^{pure}) is the total energy of the defective (clean) system, μ_{Si} is the chemical potential of Si in bulk phase, ε_v is the energy of the top of the valence band of the clean host and μ_e is the chemical potential for electrons. In a periodic boundary condition (PBC) formalism a finite net charge in the simulation cell would give rise to a divergent Coulomb energy in E_{tot}^D because of the monopole-monopole interaction with its periodic images. While the correct procedure for the removal of this contribution to the total energy is still a matter of debate, recent reports [46] indicate that the uniform background charge [47, 48] and the local-moment counter charge [49] yield similar results for bulk materials.

However, the calculation of formation energies in reduced dimensionality systems has been out of the reach of first-principles methods until recently because of the

³ It must be said that the dispersion relations are fairly accurate, and the inaccuracies can be partially solved with a rigid shift of the CB, i.e. a scissors operation.

need to overcome two conceptual problems that prevented straightforward application of the ZN expressions.

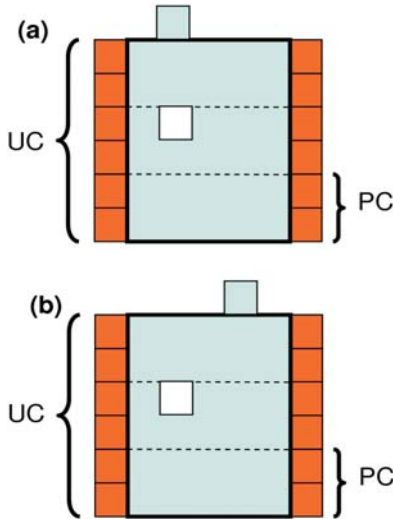


Fig 5. Schematic showing the uncertainty in choosing a final state when considering the formation of a single vacancy.

On one hand, the non-equivalence of the radial atomic positions within the NW renders the definition of a chemical potential impossible. Consider, for example, the formation of a vacancy in a SiNW, an intermediate step for the introduction of a substitutional dopant. When the vacancy is formed, the displaced Si atom must occupy a different lattice position and its contribution to the total energy, ie. its chemical potential, must be computed. In bulk silicon, all positions of the displaced atom are equivalent, and the extraction of the chemical potential is trivial. For the SiNW, there is no *a priori* way of choosing the final occupation site (see Fig. 5). Even if we agreed on one, the dealing of the surface passivation and how to identify the contribution of that specific atom to the total energy with a total energy calculation would pose unsurmountable difficulties.

On the other hand, the procedure for the subtraction of the divergent contribution to the total energy in bulk involves performing an Ewald sum to obtain the Madelung factor, and then dividing by the dielectric constant to account for screening

between the point charges [48]. The Madelung factors are tabulated for the cubic lattices, but, for the orthorhombic cells typical in NW calculations, they have to be computed for each specific case. However, the main difficulty is that, *a priori*, NWs are a highly anisotropic medium, and therefore one must allow for the material permittivity to be a tensor rather than a scalar. Then, of course, it is no longer allowed to divide by the dielectric constant, and it is not straightforward to determine how the dielectric tensor enters the calculation of the Madelung factor.

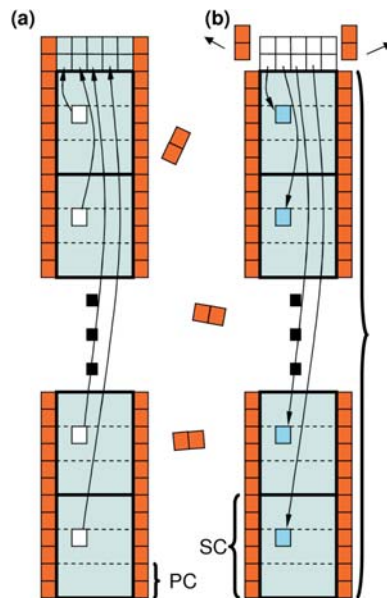


Fig 6. Construction for determining the formation energy of (a) vacancies and substitutionals, and (b) self-interstitials.

We have very recently developed a formalism [40] that solves these two difficulties. The arbitrariness in the definition of the Si chemical potential in a SiNW can be avoided if one considers the formation of many defects instead of one (see Fig. 6). The energy difference between the two different final states (eg. many vacancies vs. pristine system) allows the obtention of the following expression for the vacancy formation energy in a SiNW:

$$\Delta E^f = E_{tot}^D - N E_{NW}^{PC} + \frac{1}{n_{Si}^{PC}} (E_{NW}^{PC} - n_H^{PC} \frac{E_{H_2}}{2}) + q(\epsilon_v + \mu_e) \quad (2)$$

where N is the number of primitive cells used in the clean system calculation, $E_{PC,NW}$ is the energy of the NW clean primitive cell, satisfying $E^{pure,tot} = NE_{PC,NW}$, $n^{PC,H}$ is the number of passivating atoms in a NW primitive cell (taken to be hydrogens) and $E_{H2}/2$ is the corresponding chemical potential. Comparison with Eq. (1) shows that, in the NW case, we have made the substitution $\mu_{Si} \rightarrow (E_{PC,NW} - n^{PC,H}E_{H2}/2) / n^{PC,Si}$. In other words, we have learnt that the correct procedure is to substitute the Si chemical potential for the average energy of the Si atoms in the SiNW primitive cell, after having subtracted the contribution of the passivating agents.

Regarding the computation of the Madelung constant in an anisotropic medium, one can start with the potential due to a point charge in a homogeneous anisotropic medium [50], and following analogously to the standard procedure [51], one can obtain the following expression for the Madelung constant in the general case

$$\frac{\alpha}{L} = \sum_i \frac{\text{erfc}(\gamma R_i)}{R_i} + \sum_i \frac{4\pi \exp(G_i^2 / 4\gamma^2)}{G_i^2} - \frac{2\gamma}{\sqrt{\pi}} - \frac{\pi}{V_c \gamma^2} \quad (3)$$

where the sum over \mathbf{R}_i (\mathbf{G}_i) extends over all vectors of the direct (reciprocal) lattice except for zero, γ is a suitably chosen convergence factor and V_c is the volume of the primitive cell.

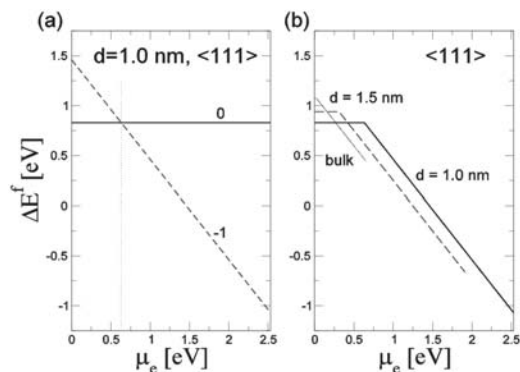


Fig 7. (a) Formation energy of the neutral (0) and the negatively charged (-1) Al substitutional in a $\langle 111 \rangle$ SiNW with a diameter of 1.0 nm, as a function of the electronic chemical potential. The crossing μ_e signals the ionization energy. (b) Formation energy diagram for three different $\langle 111 \rangle$ SiNW diameters. The slope gives the charge state of the Al substitutional for a given electronic chemical potential.

We have used this formalism to compute the ionization energy of the Al substitutional in thin SiNWs [40, 52].

In this case, the ionization energy is found as the value of the electron chemical potential for which the formation energy is the same for the neutral and the charged impurity [see Fig. 7.(a)]. Figure 7.(b) shows that, as expected, the ionization energy increases with decreasing NW diameter. We also observe from those plots that, due to the lower formation energies, growth on negatively charged substrates—that is, under conditions of high μ_e —would induce massive incorporation of Al into the SiNW. This is specially relevant if, for example, an Al nanoparticle is used to catalyze the vapor-solid-solid (VSS) growth of a thin SiNW [53]. Thus, we predict that controlled biasing of the growth substrate can be useful tool to favor or limit the incorporation of impurities during the NW growth.

3.4 Molecular doping of SiNWs

Having seen in the previous subsections that the efficiency of substitutional dopants will be very low as the NWs decrease in diameter, a different route to doping in thin nanowires should be sought. We believe that molecular adsorption onto the SiNW surface can play this role, and we have verified it with electronic structure calculations [54] of a set of different molecules chemisorbed on a 1.5 nm thick $\langle 111 \rangle$ SiNW (Fig. 8).

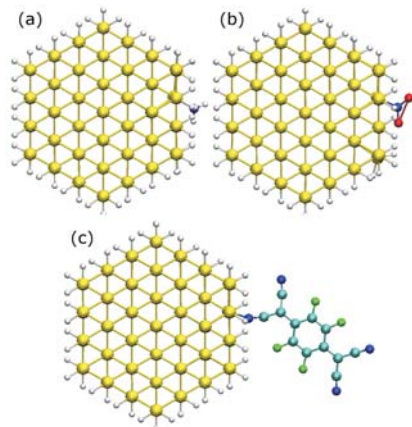


Fig 8. Several candidate molecules for SiNW doping: (a) NH_3 , (b) NO_2 , (c) $\text{C}_{12}\text{N}_4\text{F}_4$.

In particular, we have found that NH_3 constitutes an effective n -type dopant for thin SiNWs (Fig. 9), in agreement with the experimental observations where mesoporous Si augmented its conductivity when

exposed to ammonia [55]. On the other hand, the same experiments observed NO_2 induced p -type doping, while calculations indicate that it passivates a dangling bond. Theory and experiment can reconcile if the NO_2 adsorbs at a site with a subsurface B atom, and the role of NO_2 is to reactivate the B rather than supplying a carrier itself. Other molecules, especially those with low ionization energies or high electron affinities (substitution of H by F in organic compounds increases the electronic affinity), can provide carriers directly into the valence and conduction bands.

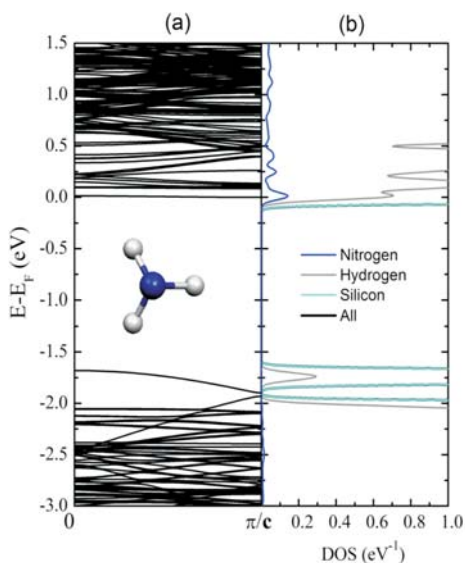


Fig 9. Electronic structure of an NH_3 molecule adsorbed at a dangling bond, resulting in n -type doping. (a) Band structure, with the Fermi level lying at the conduction band minimum, and (b) projected density of states (PDOS) showing strong hybridization of the N levels with the conduction band states.

4. Transport in SiNWs

The study of electron transport is one of the most rapidly growing fields in nanowire research. On one hand carrying out transport measurements is often the most straightforward way to test theoretical predictions [56, 57, 58, 59]; on the other hand, the conductance is intrinsically the most important property of building blocks of future nanoelectronics applications. The behavior can be much different from bulk Si and can be exploited for enhanced performance in applications, whereas other times it can be detrimental.

The most obvious difference of nanowires with their bulk counterpart is their reduced dimensionality. This property, combined with a nanoscale dimension, leads directly to the most significant fingerprint of a nanowire: a very large surface-to-volume ratio. As we have seen previously, this fact accounts for the high sensitivity of nanowires to the surface chemistry or the passivation of surface segregated dopants, among others. For this reason, it is natural to analyze the surface structure in search for causes of the conductance degradation. As a matter of fact, several experimental studies have reported non-smooth surfaces [60, 61].

Scattering occurring at the surface in presence of surface roughness has been studied by Svizhenko *et al.* [62], Persson *et al.* [63] and Lherbier *et al.* [64]. Uncorrelated surface bumps or random Lorentzian fluctuations are used as modeling approaches. As common for many properties of extremely thin wires, the surface backscattering has shown to strongly depend on the growth orientation, the anisotropy coming from the differences in the underlying band structure. In particular, electrons are less sensitive to surface roughness in $\langle 110 \rangle$ SiNWs, whereas holes are better transmitted in $\langle 111 \rangle$ SiNWs.

The other obvious source of carrier scattering is the presence of impurities or, more in general, lattice defects. The key point here is that with the reduction of the wire size below 10 nm, the impurity cross-sections become of the same order of the wire characteristic dimension and can result in total backscattering. A very special case among defects is represented by dopants, purposely introduced impurities to provide the material with tailor-made electric features. Therefore, while they increase the carrier density at device operation temperature, they might induce a significant scattering which leads to a drop in the conductance.

The study of the resistance associated to a substitutional impurity has first been tackled by Fernández-Serra *et al.* [65]. They focused on the radial dependence of the scattering properties, finding that impurities in the core of the wire have a scattering cross-section much larger than impurities located at the surface or at the subsurface. These results, together with their previous study of surface segregation [27], shed a light on how critical the doping of very thin nanowires can be: dopant impurities either segregate to the surface where they are likely to form an electrically inactive complex or they stay in the wire core where they produce a stronger

HV sources

Senoidal HV source (HV-7030)



10 kV bipolar voltage source (HV-7010)



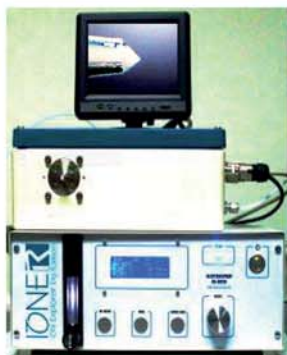
Unipolar 20kV source (HV-7020)

- 0.1V resolution
- Max current 0.3mA
- Ripple: 0.001% pp
- Programmable
- Optional USB/RS485/Zig-
bee output
- Applications: mass
spectrometry, electron and
ion beams, SEM



- Delivers a pure senoidal voltage
- Freq range 50kHz-1MHz
- Amplitude up to 300Vpp
- Auxiliar DC output up to 50V

Electrospray source (ES-3020)



Fluid-electrodynamic device that generates an electrically charged nanoparticles or ions from a dispersion or solution.

- Can be operated downwards, upwards or horizontally
- Easy maintenance
- Separate control module (pressure, voltage and sheath gas flowrate) and spraying head for greater versatility.
- Taylor's cone can be monitored thanks to a video camera installed in the spraying chamber. Capture of images and video is also possible.
- Applications: nanoparticle generation, mass spectrometry, thin films

Corona charger (CC-8020)



- Device for charging aerosols and particles based on corona effect.
- No radioactive source, no cumbersome paperwork.
- Especially effective for ultrafine particles.
- Bipolar
- Includes high DC voltage source
- Current measurement

Electrometers



EL-5010, an all-purpose electrometer:

- Range: +/- 9999.9 fA, Resolution: 0.1 fA
- Noise: < 1 fA (RMS)
- A/D effective resolution: 21 bits
- Selectable digital filter
- Selectable amplifier gain
- Remote control interface: USB, RS485
- Labview control software
- Electronic offset correction
- CE-marked

EL-5020, compact electrometer (16 x 6 x 3 cm), battery-powered (8 working hours) and communicated through wireless protocol Zig-Bee, especially conceived for the measurement of ultra-low current at high voltages. It is PC-controlled, with an option of a console for manual interface.

EL-5030, electrometer for the measurement of ultra-low currents generated by ionized gases and electrically charged aerosols. It includes, besides the electronics for the measurement of the current, a Faraday cup with a HEPA filter inside for the collection of nanoparticles and a flowmeter for the calculation of the concentration of particles or ions.





backscattering. In both cases the current is reduced. These works pioneered the study of impurity scattering in SiNWs. However, they neglected two important issues: (i) in realistic, long nanowires the overall resistance is the result of multiple scattering events, induced by a random distribution of defects along the wire length; (ii) dopants are by definition ionized impurities at device operation temperatures, and the proper charge state must be taken into account. The first of these problems was tackled by Markussen *et al.* [66]. This is a difficult task, because solving the electronic structure from first-principles (often mandatory when dealing with nanoscale systems where reliable parameterizations do not exist) for a long wire is a prohibitive task.

The authors circumvented this problem constructing the Hamiltonian of the long wire with building blocks obtained from the single-impurity calculations (see Ref. [67] and Fig. 10). With this approach the electronic structure problem has not to be solved directly in the long wire, but the conductance can be calculated. The interesting (and surprising) result is that the transport properties of the long wire, e.g. mean free path, resistance vs length, total resistance, can be entirely predicted from single-dopant conductances. What one must do is classically adding the resistances of each individual scatterer according to Ohm's law:

$$\langle R(L, E) \rangle = R_c(E) + \langle R_s(E) \rangle L/l \quad (4)$$

where $\langle R_s(E) \rangle$ is the average resistance estimate based on single-impurity calculations, $R_c(E)$ is the contact resistance, L is the length of the wire and l the average separation between dopants.

As stated in the previous section, modeling charged defect within periodic boundary conditions poses well-known problem related to the spurious interaction of the point charge with its periodic images. In general, the computational cell has to be large enough to make this interaction negligible, but in practice it is a goal difficult to accomplish due to the slowly decaying Coulomb potential. In their work, Rurali *et al.* [68] proposed combining density-functional calculation with more approximate electrostatic calculations based on finite element method.

The underlying idea is very simple. If one approximates a charged impurity with a point charge, its electrostatic potential can be obtained in a very cheap way with a fi-

nite element calculation. Far from the impurity this is a reasonable approximation—a B^- impurity gives rise to essentially the same Coulomb potential of an Al^- impurity—and the agreement with a self-consistent electronic structure calculation is indeed very good. Close to the impurity, on the other hand, quantum electronic structure accounts properly for the different chemical nature of different impurities. In this way the authors could show that the scattering associated to an impurity changes significantly when the charge state is taken into account.

The change is drastic, leading to total backscattering in a large energy window close to the band edges, when minority carriers—electron in a p-doped system or holes in a n-doped system—are concerned. In such cases dopants constitute an effective barrier in the potential landscape. When the energy of the carrier is lower than the barrier height, it must tunnel through the potential, yielding an exponentially suppressed transmission. The suppression of minority carrier conductance can be used in the design of efficient Schottky contacts in nanowire-based field effect transistors.

5. Conclusions

In conclusion, the structural, electronic and transport properties of SiNWs are adequately computed in the DFT formalism, albeit some modifications or less commonly employed techniques must be used to extract dopant- or transport-related magnitudes. From our calculations, we predict that

- CH_3 can act as a possibly improved passivating agent with respect to hydrogen passivation in SiNWs.
- Proper biasing of a substrate can be used to control the amount of impurities incorporated into a NW during its bottom-up growth.
- Molecular adsorption can be a viable alternative to substitutional doping in thin NWs.
- In sufficiently thin NWs, minority carriers can be entirely backscattered by ionized dopants.

Acknowledgements

We acknowledge discussions with A. Miranda and the financial support of the Spanish Ministerio de Ciencia e Innovación under contracts No. TEC2009-06986 and FIS2009-12721-C04-03.

References

- [1] Y. Cui and C. M. Lieber, *Science* 291, 851 (2001).
- [2] Y. Huang, X. Duan, Y. Cui, L. J. Lauhon, K.-H. Kim, and C. M. Lieber, *Science* 294, 1313 (2001).
- [3] X. Duan, Y. Huang, and C. M. Lieber, *Nano Lett.* 2, 487 (2002).
- [4] T. J. Kempa, B. Tian, D. R. Kim, J. Hu, X. Zheng, and C. M. Lieber, *Nano Lett.* 8, 3456 (2008).
- [5] Y. Cui, Q. Wei, H. Park, and C. M. Lieber, *Science* 293, 1289 (2001).
- [6] A. I. Boukai, Y. Bunimovich, J. Tahir-Kheli, J.-K. Yu, W. A. Goddard III, and J. R. Heath, *Nature* 451, 168 (2008).
- [7] A. I. Hochbaum, R. Chen, R. D. Delgado, W. Liang, E. C. Garnett, M. Najarian, A. Majumdar, and P. Yang, *Nature* 451, 163 (2008).
- [8] R. He and P. Yang, *Nat. Nanotechnol.* 1, 42 (2006).
- [9] M. T. Björk, B. J. Ohlsson, C. Thelander, A. I. Persson, K. Deppert, L. R. Wallenberg, and L. Samuelson, *Appl. Phys. Lett.* 81, 4458 (2002).
- [10] Z. L. Wang and J. Song, *Science* 312, 242 (2006).
- [11] R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods* (Cambridge University Press, Cambridge, UK, 2004).
- [12] F. Aryasetiawan and O. Gunnarsson, *Rep. Prog. Phys.* 61, 237 (1998).
- [13] M. A. L. Marques and E. K. U. Gross, *Ann. Rev. Phys. Chem.* 55, 427 (2004).
- [14] D. A. Papaconstantopoulos, M. J. Mehl, and B. Akgim, in *Proceedings of the International Symposium on Novel Materials*, edited by B. K. Rao (1998), pp. 393–403.
- [15] R. Rurali, *Rev. Mod. Phys.* (2010), in press.
- [16] R. Rurali and N. Lorente, *Phys. Rev. Lett.* 94, 026805 (2005).
- [17] S. Zhang, E. R. Hemesath, D. E. Perea, E. Wijaya, J. L. Lensch-Falk, and L. J. Lauhon, *Nano Lett.* 9, 3268 (2009).
- [18] R. Rurali, *Phys. Rev. B* 71, 205405 (2005).
- [19] T. Vo, A. J. Williamson, and G. Galli, *Phys. Rev. B* 74, 045116 (2006).
- [20] R. Q. Zhang, Y. Lifshitz, D. D. D. Ma, Y. L. Zhao, T. Frauenheim, S. T. Lee, and S. Y. Tong, *J. Chem. Phys.* 123, 144703 (2005).
- [21] P. W. Leu, B. Shan, and K. Cho, *Phys. Rev. B* 73, 195320 (2006).
- [22] B. Aradi, L. E. Ramos, P. Deák, T. Köhler, F. Bechstedt, R. Q. Zhang, and T. Frauenheim, *Phys. Rev. B* 76, 035305 (2007).
- [23] M. Nolan, S. O’Callaghan, G. Fagas, J. Greer, and T. Frauenheim, *Nano Lett.* 7, 34 (2007).
- [24] M.-F. Ng, L. Zhou, S.-W. Yang, L. Y. Sim, V. B. C. Tan, and P. Wu, *Phys. Rev. B* 76, 155435 (2007).
- [25] H. Haick, P. T. Hurley, A. I. Hochbaum, P. Yang, and N. S. Lewis, *J. Am. Chem. Soc.* 128, 8990 (2006).
- [26] X. Cartoixà and R. Rurali (2010), in preparation.
- [27] M. V. Fernández-Serra, C. Adessi, and X. Blase, *Phys. Rev. Lett.* 96, 166805 (2006a).
- [28] W. Kohn and J. M. Luttinger, *Phys. Rev.* 98, 915 (1955).
- [29] Y. Li, F. Qian, J. Xiang, and C. M. Lieber, *Materials Today* 9, 18 (2006).



- [30] V. Schmidt, J. V. Wittemann, S. Senz, and U. Gösele, *Adv. Mater.* 21, 2681 (2009).
- [31] L. Bányai, I. Galbraith, C. Ell, and H. Haug, *Phys. Rev. B* 36, 6099 (1987).
- [32] A. F. Slachmuylders, B. Partoens, W. Magnus, and F. M. Peeters, *Phys. Rev. B* 74, 235321 (2006).
- [33] M. Diarra, Y.-M. Niquet, C. Delerue, and G. Allan, *Phys. Rev. B* 75, 045301 (2007).
- [34] R. Loudon, *Am. J. Phys.* 27, 649 (1959).
- [35] R. Rurali, B. Aradi, T. Frauenheim, and A. Gali, *Phys. Rev. B* 79, 115303 (2009).
- [36] H. Peelaers, B. Partoens, and F. Peeters, *Nano Lett.* 6, 2781 (2006).
- [37] C. R. Leão, A. Fazzio, and A. J. R. da Silva, *Nano Lett.* 8, 1866 (2008).
- [38] Y. M. Niquet, L. Genovese, C. Delerue, and T. Deutsch (2009), <http://es.arxiv.org/abs/0907.4853v2>.
- [39] E. Durgun, N. Akman, C. Ataca, and S. Ciraci, *Phys. Rev. B* 76, 245323 (2007).
- [40] R. Rurali and X. Cartoixà, *Nano Lett.* 9, 975 (2009).
- [41] P. M. Fahey, P. B. Griffin, and J. D. Plummer, *Rev. Mod. Phys.* 61, 289 (1989).
- [42] E. G. Seebauer and M. C. Kratzer, *Mater. Sci. Eng. R* 55, 57 (2006).
- [43] M. Cardona, in *Topics in Applied Physics*, edited by D. A. Drabold and S. K. Estreicher (Springer Verlag, Berlin (Germany), 2007), vol. 104.
- [44] S. B. Zhang and J. E. Northrup, *Phys. Rev. Lett.* 67, 2339 (1991).
- [45] J. E. Northrup and S. B. Zhang, *Phys. Rev. B* 47, 6791 (1993).
- [46] A. F. Wright and N. A. Modine, *Phys. Rev. B* 74, 235209 (2006).
- [47] M. Leslie and N. J. Gillan, *J. Phys. C: Solid State Phys.* 18, 973 (1985).
- [48] G. Makov and M. C. Payne, *Phys. Rev. B* 51, 4014 (1995).
- [49] P. A. Schultz, *Phys. Rev. Lett.* 84, 1942 (2000).
- [50] L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon Press, 1984).
- [51] J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, UK, 1972), 2nd ed.
- [52] R. Rurali, M. Palummo, and X. Cartoixà, *Phys. Rev. B* (2010), submitted.
- [53] Y. Wang, V. Schmidt, S. Senz, and U. Gösele, *Nature Nanotech.* 1, 186 (2006).
- [54] A. Miranda-Durán, X. Cartoixà, M. Cruz Irisson, and R. Rurali, *Phys. Rev. B* (2010), submitted.
- [55] E. Garrone, F. Geobaldo, P. Rivolo, G. Amato, L. Boarino, M. Chiesa, E. Giamello, R. Gobetto, P. Ugliengo, and A. Viale, *Adv. Mater.* 17, 528 (2005).
- [56] J.-Y. Yu, S.-W. Chung, and J. R. Heath, *J. Phys. Chem. B* 104, 11864 (2000).
- [57] Y. Cui, X. Duan, J. Hu, and C. Lieber, *J. Phys. Chem. B* 104, 5213 (2000).
- [58] H. Sellier, G. P. Lansbergen, J. Caro, S. Rogge, N. Collaert, I. Ferain, M. Jurczak, and S. Biesemans, *Phys. Rev. Lett.* 97, 206805 (2006).

- [59] M. T. Björk, H. Schmid, J. Knoch, H. Riel, and W. Riess, *Nature Nanotech.* 4, 103 (2009).
- [60] S. Kodambaka, J. Tersoff, M. C. Reuter, and F. M. Ross, *Phys. Rev. Lett.* 96, 096105 (2006).
- [61] F. M. Ross, J. Tersoff, and M. C. Reuter, *Phys. Rev. Lett.* 95, 146104 (2005).
- [62] A. Svizhenko, P. W. Leu, and K. Cho, *Phys. Rev. B* 75, 125417 (2007).
- [63] M. P. Persson, A. Lherbier, Y.-M. Niquet, F. Triozon, and S. Roche, *Nano Lett.* 8, 4146 (2008).
- [64] A. Lherbier, M. P. Persson, Y.-M. Niquet, F. Triozon, and S. Roche, *Phys. Rev. B* 77, 085301 (2008).
- [65] M.-V. Fernández-Serra, C. Adessi, and X. Blase, *Nano Lett.* 6, 2674 (2006b).
- [66] T. Markussen, R. Rurai, A.-P. Jauho, and M. Brandbyge, *Phys. Rev. Lett.* 99, 076803 (2007).
- [67] T. Markussen, R. Rurai, M. Brandbyge, and A.-P. Jauho, *Phys. Rev. B* 74, 245313 (2006).
- [68] R. Rurai, T. Markussen, J. Suñé, M. Brandbyge, and A.-P. Jauho, *Nano Lett.* 8, 2825 (2008).

Advertisement



e-CLIPSE COLUMN

NANOSOLUTIONS
by
ORSAY PHYSICS

UHV Focused
Electron Beam
For surface analysis

95, Av des Monts Auréliens
ZA Saint Charles
13710 Fuveau FRANCE
Tél. : +33 442 538 090
Fax : +33 442 538 091
Email : nano@orsayphysics.com

www.orsayphysics.com

⊙ **4th Spanish Workshop on Nanolithography (NANOLITHO 2010). November 10-12, 2010. Oviedo (Spain)**

The 4th Spanish Workshop on Nanolithography (NANOLITHO 2010) is a meeting mainly focused in the research on nanolithography methods performed in Spanish-based centres or institutions, although it is also opened to international contributions in this research field.

www.cinn.es/nanolitho2010.html

NanoLithography, NanoImprint

⊙ **NanobioTech2010. November 15-17, 2010. Montreux (Switzerland)**

This is a unique Conference at the frontiers of both Micro- and Nano- technologies, with a special emphasis on Biological, Chemical and Medical applications.

www.nanotech-montreux.com/index.html

NanoBiotechnology, NanoMedicine

⊙ **Nanosafe2010. November 16-18, 2010. Grenoble, (France)**

The objectives of the conference will be to make available the major progresses and future trends in the domain of the safe production and use of nanomaterials:

www.nanosafe.org

Scientific Policy, Nanotechnologies

⊙ **Nano Thailand Symposium 2010 (NTS2010). November 18-20, 2010. Bangkok (Thailand)**

The 2nd biannual NanoThailand Symposium (NTS) will be held during November 18-20, 2010 in Bangkok, Thailand. NTS is conceived as a series of premier international conference and exhibitions on Nanotechnology to bring together world-leading researchers and exhibitors, in several focused areas of science and technology at nanoscale.

www.nano-thailand.com

Energy, NanoSensors & NanoDevices, Nanotechnologies

⊙ **The Future of Reference Materials – Science and Innovation. 23-25, November, 2010. Geel, (Belgium)**

Organised in the frame of the 50th anniversary of the Joint Research Centre's Institute for Reference Materials and Measurements.

<http://irmm.jrc.ec.europa.eu/html/events/events/future-rm.htm>

NanoMaterials, NanoMetrology & Standards

⊙ **NANOSENS 2010. December 2-3, 2010. Vienna (Austria)**

Continuing the success in 2007 and 2008, the 3rd conference NANOSENS 2010 highlights latest developments of nanosensors for industrial applications.

www.nanosens.at/

NanoSensors & NanoDevices

⊙ **7th International Conference on Biomedical Applications of Nanotechnology (NanoMed 2010) . December 2-3, 2010. Berlin, (Germany)**

On December 2 – 3, 2010, experts from all over the world will gather for the NanoMed 2010 – 7th International Conference on Biomedical Applications of Nanotechnology in Berlin to discuss the state of the art in this field of research.

Focus Topic 2010: Nanotechnology-Enabled Diagnosis and Treatment of Cancer

www.nanomed-berlin.de

NanoMedicine

⊙ **ElecMol - 5th International Meeting on Molecular Electronics. December 6-10, 2010. Grenoble (France)**

The 5th edition of ElecMol will focus on recent advances in molecular and organic electronics:

www.elecml.com

Molecular Electronics, NanoTubes, Nanowires

⊙ **International Conference on Nanotechnology and Biosensors - (ICNB 2010). December 28-30, 2010. Hong Kong (China)**

The conference will be held every year to make it an ideal platform for people to share views and experiences in Nanotechnology and Biosensors and related areas.

www.icnb.org/

NanoBiotechnology, NanoSensors & NanoDevices, Nanotechnologies

🔗 PostDoctoral Position (IMDEA, Spain): "Carbon Nanomaterials-Nanocrystals Composites"

Fellowship Description: We offer a post-doctoral position to study hybrid systems composed of carbon nanotubes or carbon fibers and semiconductor and metallic nanoparticles. The work includes synthetic activities and characterization by means of optical spectroscopy, electron and near field microscopy. In the frame of this project collaboration with other laboratories focused on electrical transport measurements are contemplated. We are looking for applicants with a PhD preferably in materials science with experienced in carbon nanotubes or carbon fibers as well as good knowledge of English. We offer a 2 years contract according to standard regulations in Spain at the Madrid Institute for Advanced Studies-IMDEA Nanoscience www.nanoscience.imdea.org/.

The deadline for submitting applications is December 01, 2010

For further information about the position, please contact: **Beatriz H. Juárez**
beatriz.hernandez@imdea.org

🔗 PhD Position (ESRF Grenoble, France): "X-ray micro diffraction study of strain, elemental distribution and defects in semiconductor devices"

With x-rays as a local tool, new possibilities open up in terms of the characterization of device structures, where spatial resolution has to be combined with x-ray diffraction to respect the local inhomogeneities. We propose the use of these recently developed methods of x-ray diffraction microscopy in combination with anomalous diffraction and coherent diffraction imaging in order to analyse the local strain distribution and the eventual presence of defects. Local strain in e.g. Si/SiGe devices as nanowires for thermoelectric applications are objects of choice for these as well as III-V compound heterostructures in combination with silicon substrates for their potential in optoelectronics and photovoltaics. The sample preparation will be done in collaboration with the University of Linz.

The deadline for submitting applications is December 01, 2010

For further information about the position, please contact: **Tobias Schulli**
schulli@esrf.fr

🔗 PhD Studentship Positions (University of Jyväskylä, Finland): "Particle physics, material physics or nuclear and accelerator-based physics"

The Department of Physics is an internationally recognized research and teaching unit. The main research areas in the Department are particle physics, material physics and, nuclear and accelerator-based physics. The research in particle physics is carried out in cosmology, neutrino physics, ultra-relativistic heavy ion collisions, and the Beyond the Standard Model physics.

In condensed matter physics experimental research of nanophysics and nanoelectronics (especially low temperature physics in nano- and microstructures as well as molecular electronics) with their applications are carried out as well as research of porous and disordered materials and crystal defects. Themes of theoretical material physics are atomic clusters and other nanoscale structures, ultracold gases, surfaces, and nonlinear phenomena. In nuclear and accelerator based physics in the Accelerator Laboratory the research focuses on studies of atomic nuclei and nuclear matter under extreme conditions, with many links to material physics and applied research. Furthermore the Department is contributing to the ALICE and ISOLDE experiments in CERN as well as Facility for Antiproton and Ion Research in GSI and FAIR Laboratories. The focus of the research in theoretical nuclear physics is on nuclear models and their applications

The department is currently seeking to recruit PhD students (3-4 positions), starting 1 January 2011, (contract length maximum of four years).

The deadline for submitting applications is December 08, 2010

For further information about the position, please contact: **Jukka Maalampi**
jukka.maalampi@jyu.fi

🔗 PhD Studentship: "Quantum nano studies at Imperial College London"

One PhD studentship is available at Imperial College London for the theoretical investigation of quantum effects in surface plasmon polaritons / metamaterials. This theoretical investigation is supervised by Professor Myungshik Kim and Professor Stefan Maier. The studentship includes European/UK student fees and full stipend with London weighting during the PhD period.



The studentship is available now until it is filled. If the candidate prefers, they can join the Doctoral Training Programme for Controlled Quantum Dynamics at Imperial College.

The deadline for submitting applications is December 18, 2010

For further information about the position, please contact: **Myungshik Kim**
m.kim@imperial.ac.uk

⊗ PhD and M.Sc.A positions (Université Laval, Canada): "Biomedical micro/nanoelectronics"

We seek highly motivated, talented and creative PhD/M.Sc.A candidates to join the Biomedical Microsystems Laboratory of Dr Benoit Gosselin at Université Laval, Quebec City. Our research interests focus on designing novel high-performance, analog / digital / mixed-mode biomedical VLSI circuits to supply the next generation of assistive technologies. Among other activities, our team is working toward the implementation of direct neural interfacing microsystems and ultralow-power wireless sensor interfaces. Successful applicants will be involved in 1) the design, simulation and layout generation of VLSI mixed-mode circuits within the latest nano-CMOS technology available through CMC Microsystems, Canada, 2) the assembly and packaging, 3) bench top testing and 4) validation of microsystems with collaborating medical institutions. Some research projects will be developed in collaboration with the Georgia Tech Bionics Lab (Atlanta, USA) and Polystim Neurotechnologies Lab in Polytechnique (Montreal, Canada). Students can look forward for a research-stimulating environment and access to the state-of-the-art equipment in microsystems design, assembly and packaging. Moreover, full financial support is available.

The deadline for submitting applications is January 01, 2011

For further information about the position, please contact: **Benoit Gosselin**
benoit.gosselin@gel.ulaval.ca

⊗ Two Research Scientists/Engineers positions (Hitachi Chemical Research Center, United States): "Biochemistry, polymer chemistry"

Hitachi Chemical Research Center, Inc. (HCR) is a research and development company directed towards

novel technology platforms and related bio or bio mimetic materials for life sciences. HCR is a subsidiary of Hitachi Chemical Company, Ltd., a chemical manufacturer producing innovative technologies in the areas of Electronic Related Products and Advanced Performance Products.

In this multifaceted role as a researcher you will utilize your technical skills and knowledge to create, develop, and direct your own project in the nanotechnology or nanomaterial fields. The goal, to develop polymer based functional materials/composites to support human health and the environment. With the support of the business development group you will understand the market value of your project and help guide it to commercialization.

The deadline for submitting applications is January 14, 2011

For further information about the position, please contact: **Lisa Osborn**
recruiting@hcrcenter.com

⊗ PostDoctoral Position (CIDETEC, Spain): "Hybrid photovoltaics position"

CIDETEC, which is located in San Sebastián, Basque Country (Spain), is currently looking for a post-doctoral researcher who is interested in working in an inspiring international and interdisciplinary environment in the area of hybrid photovoltaics. The position holder, joining the CIDETEC photovoltaics research group, will systematically evaluate various polymers and organic molecules as hole transporter materials in hybrid solar cells. Additional to the planning and conducting the experimental activities, the suitable candidate will report on the experimental work. The position requires a PhD in Chemistry, Physics, and/or Materials Science. Candidates should have experience in the fabrication and characterization of solar cells, with a preferred expertise in hybrid inorganic/organic devices. Knowledge on the synthesis and/or processing of hole transporter materials will be especially considered. Proficiency in spoken and written English is required.

The deadline for submitting applications is January 26, 2011

For further information about the position, please contact: **Soledad Larrocha Redondo**
slarrocha@cidetec.es

🌀 **PostDoctoral Position (CIDETEC, Spain):** *"CIGS photovoltaics"*

CIDETEC, Center for Electrochemical Technologies, which is located in San Sebastián, Basque Country (Spain), is currently looking for a post-doctoral researcher who is interested in working in an inspiring international and interdisciplinary environment in the areas of electrodeposition and photovoltaics. The position holder, joining the CIDETEC photovoltaics research group, will investigate innovative routes for chalcopyrite (e.g. copper indium gallium selenide, CIGS) electrodeposition as well as its application to solar cells.

Additional to the planning and conducting the experimental activities, the suitable candidate will report on the experimental work. The position requires a PhD in Chemistry, Physics, and/or Materials Science. Candidates should have experience in the electrodeposition processes. Knowledge on the ionic liquid based electrolytes and CIGS will be especially considered. Proficiency in spoken and written English is required.

The deadline for submitting applications is January 26, 2011

For further information about the position, please contact: **Soledad Larrocha Redondo**
slarrocha@cidetec.es

🌀 **Post-doctoral Research Associate Position (CEMES-CNRS, France): "Graphene ribbon nanoelectronics"**

The proposed work will be dedicated to the rapidly evolving field of nanostructured graphene electronics. It will involve nanofabrication, magneto-cryo-transport in graphene nanoribbons and modelization.

The deadline for submitting applications is February 01, 2011

For further information about the position, please contact: **Erik Dujardin (CEMES, CNRS, France)**
Erik.Dujardin@cemes.fr

🌀 **PostDoctoral Position (CEMES, CNRS, France): "AFM and Fluorescence Microscopy investigations of plasmonics architectures"**

A post-doctoral position for an experimental optical physicist is available in the NanoSciences Group

(CEMES, CNRS) as part of collaborative French national project supported by the Agence Nationale de la Recherche. The proposed work will be dedicated to the implementation of a Total Internal Reflectance Fluorescence set-up to be combined with an AFM (TIRF-AFM) and to the exploration of the evolution of emission properties of molecular and colloidal chromophores in the vicinity of plasmonic nanostructures.

The deadline for submitting applications is February 01, 2011

For further information about the position, please contact: **Erik Dujardin**
Erik.Dujardin@cemes.fr

🌀 **PostDoctoral Position (University of Tor Vergata, Italy): "Electronics for Microsystems and Nanosystems"**

The successful candidate will join a large cross-disciplinary research effort for increasing the efficiency of piezoelectric nanogenerators [1-4] by improving modeling, nano-fabrication, devices, and electronics. Available facilities include SEM, AFM, furnaces, standard instrumentation for electronics, workstations for electronic circuit design and FEM simulations, three deposition systems (conventional PLD and two Laser-MBE), X-ray diffraction, microprobe analysis; resistivity measurements in applied magnetic field, up to 1T, down to 15K; I-V and Hall effect measurements, sputtering, PECVD, ECR-PECVD, optical lithography, electron beam lithography, ion lithography, micromachining, I-V and C-V characterization of semiconductor devices, SEM, AFM, and laser annealing.

The deadline for submitting applications is February 05, 2011

For further information about the position, please contact: **Christian Falconi**
falconi@eln.uniroma2.it

science • industry • society

IMAGINENANO

Bringing together
Nanoscience and Nanotechnology

April 11-14, 2011 - Bilbao Exhibition Centre (Spain)

www.imagenenano.com

ImagineNano will comprise 6 parallel international conferences,
a huge industrial exhibition and a social event where everyone
can meet and greet Nanotechnology side by side



- Graphene 2011
- nanoBio&Med 2011
- NanoSpain 2011 - NanoSudoe (Spain, Portugal & France)
- TNA Energy 2011 Trends in NanoApplications
- PPM 2011 Photonics/Plasmonics/Magneto-Optics
- HPC-NN2011 High-Performance-Computing



ONE Place: 6 Conferences, 1 Industrial Exhibition and Societal Activities.

conference report

OMNT Workshop Which interactions between Synthetic Biology and Micro&Nanotechnologies ? March 30th, 2010, MINATEC Grenoble

The Workshop “**Which interactions between Synthetic Biology and Micro&Nanotechnologies?**” organised by the OMNT on March 30th 2010 in MINATEC (Grenoble) was aimed at gathering scientists from various areas including biologists, researchers in microtechnologies and microfluidics as well as computer scientists, to enlighten them on Synthetic Biology (SB), to sensitize them to novel bio-engineering approaches and to highlight recent developments in nanotechnology which might have potential interest for SB advancement.

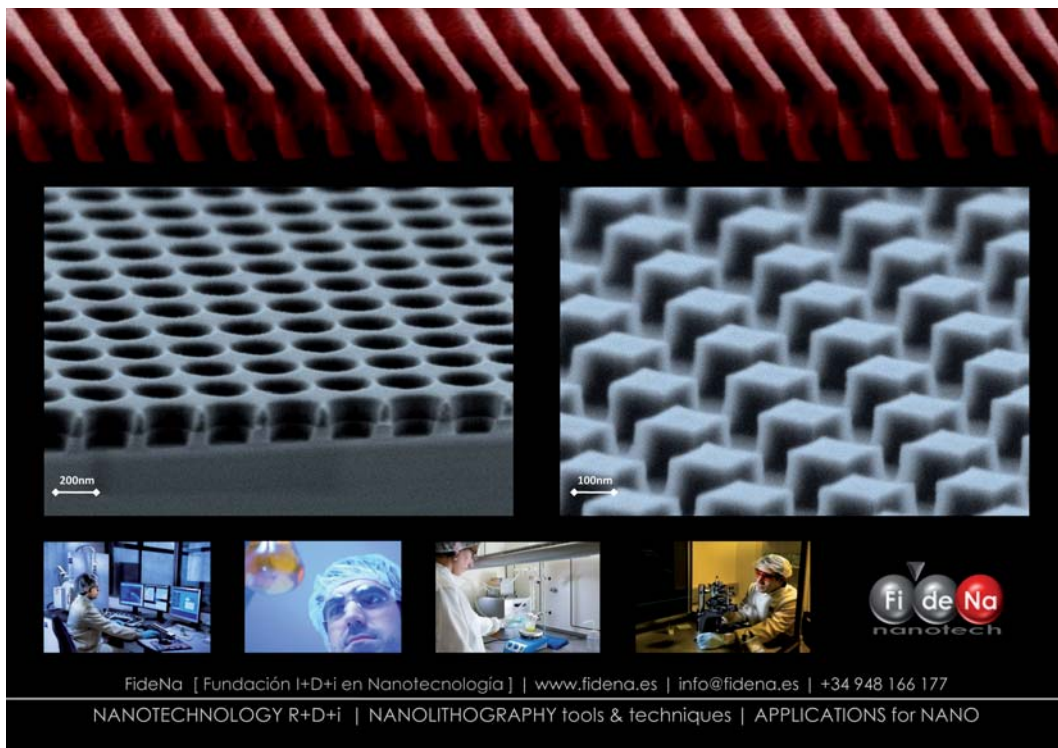
This workshop provided scientists from traditionally disconnected fields, the unique opportunity to develop mutual interest, to discuss challenges and explore opportunities for interdisciplinary collaborations.

The workshop brought more than **150 participants**, including 95 academic researchers, 30 students, 10 industrial actors and 16 other people (including institutional, incubator and government employee).

A number of talks were delivered by several national keys experts in SB and Micro&Nanotechnologies. During the morning session, invited speakers offered an **introduction to SB** for non-specialists while the second part of the day was dedicated to the presentation of **Micro&Nanotechnology applications** potentially useful for SB development. **Ethical issues** associated with SB and Micro&Nanotechnologies were also addressed.

The workshop was concluded by a **Round Table** were invited speakers and the audience discussed the challenges and the opportunities of SB as well as the potential collaborations to set up between the SB and Micro&Nanotechnology research communities.

Advertisement



The advertisement features a large background image of a red, ribbed microstructure. Below this, there are two SEM images: one showing a grid of circular holes with a 200nm scale bar, and another showing a grid of hexagonal pillars with a 100nm scale bar. At the bottom, there are four small photos: a person at a computer workstation, a person in a lab coat and mask, a person in a lab coat working at a bench, and a person in a lab coat working at a bench. The FideNa nanotech logo is in the bottom right corner.

FideNa [Fundación I+D+i en Nanotecnología] | www.fidena.es | info@fidena.es | +34 948 166 177

NANOTECHNOLOGY R+D+i | NANOLITHOGRAPHY tools & techniques | APPLICATIONS for NANO

Morning session: Definition of Synthetic Biology – chaired by Hans Geiselmann (UJF, Grenoble)

Franz Bruckert (INP, Grenoble) presented the “*Basic principles of the cell (organisation and functioning) & the tools for genomic modifications*”. In a first part introducing the organisation of the living, **FB** described the main constitutive elements of the cell and exposed the general principles for gene expression regulation. In a second part, **FB** developed the various methodologies developed for studying cells at the molecular level.

In “*A general definition of Synthetic Biology*”, **Alfonso Jaramillo (CNRS – Ecole Polytechnique)** introduced the audience to the concept of SB. **AJ** underlined the main objectives of the discipline (to engineer new biological systems and to allow the mechanistic comprehension of different modules operating independently in a system). **AJ** outlined the design principle of SB (decoupling the complexity/abstraction/standardization of components) and finally discussed the developments of “Genetic circuits and Microfluidics”.

Jean-Louis Giavitto (CNRS-Ibisc, Univ. d’Evry & Genopole) introduced the “*Bio-inspired calculation models for Biology*” which consist in mathematical simulations of biological processes. He first introduced the principles for mathematical modelling applied to dynamic biological systems; **J-LG** then outlined the various rewriting processes applied to SB and provided various examples of application.

Philippe Marlière (Isthmus, SARL) presented the “*Minimalist approaches in SB*”. **PM** introduced the audience to the “top-down” and “bottom-up” approaches and illustrated these concepts with several experimental examples.

In his presentation entitled “*Cell engineering and considerations on SB applications*”, **David Bikart (Institut Pasteur)** outlined the potential applications of SB. Based on the various life properties (energy conversion, catalysis, information processing, reproduction, etc...), SB applications might have useful impacts in many different sectors (energy production and recycling, health & medicine, security, etc...). **DB** detailed several examples of SB achievements (including progress in genomic synthesis and genomic transplantation) and underlined the remaining difficulties related to the design and the

predictability of “in silico system” (bottom-up/biobrick based systems, whole cell models and combinatorial approaches).

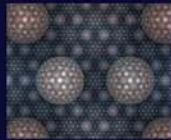
Ethical and societal issues associated with SB and nanotechnologies have been discussed by **Alexei Grinbaum (SPEC/LARSIM-CEA)** in his talk entitled “*Ethical issues of synthetic biology; comparison with nanotechnologies*”. **AG** highlighted the initiatives developed in the US and in Europe to open the ethical debate on SB, the emergence of this problematic in France and the increasing awareness of organisations and in the general public on societal and ethical issues associated with SB. **AG** mentioned that many governing issues are not specific to SB and are relevant for most new technologies. Nanotechnologies and SB also shared several structural similarities in terms of fundamental questions (definition, novelty, scope, industrial impacts...). **AG** underlined that SB however holds specific issues (lack of transparency of the objectives, blurring/transgression of religious or moral frontiers...) and further cultural references as compared to nanotechnologies.

Afternoon session: Micro&Nanotechnology toolbox potentially useful for Synthetic Biology - chaired by David Peyrade (CNRS – LTM)

Jean-Louis Viovy (Institut Curie) presented “*Microfluidic: a valuable tool for high throughput screening*”, **J-LV** outlined the principle, the progresses and benefits of the technique, highlighting the screening possibilities offered by small sample volumes, automation, multi-channeling and compartmentalization of the microfluidic devices. **J-LV** illustrated his talk with several examples of application.

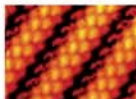
In his presentation entitled “*Nanoparticles of semi-conductors for in vivo imaging*”, **Benoît Dubertret (ESPCI)** exposed the properties and the technical advantages of quantum dots used as fluorescent probes for biological imaging.

Philippe Andreucci (Leti-CEA) presented the “*MEMS & NEMS for potential applications in Biology*”. **PA** introduced the properties and functionalities of MEMS & NEMS and mentioned their main fields of applications, describing examples of the different types of detection (gas detection, mass spectroscopy and biological detection). **PA** also outlined the possibilities to combine



RESEARCH PROGRAMMES

Molecular Nanoscience

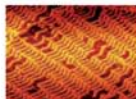


Organic nanotubes



Self-organized donor and acceptor molecules

Scanning probe microscopies and surfaces



Array of PCBM molecules on Au(111)



Monolayer of graphene / Ru (0001) periodically rippled

Nanomagnetism



Magnetic dots



Magnetic nanoparticles inside lamellar cells

Nanobiosystems: biomachines and manipulation of macromolecules



AFM image of a two dimensional crystal of the bacteriophage F29 connector

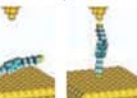


Diagram of the study of a molecular motor operating on DNA

Nanoelectronics and superconductivity

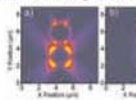


Single molecule conductivity



C60 nanoparticles

Semiconducting nanostructures and nanophotonics



Resonance for a photonic molecule



C60 nanoparticles

Nanofabrication and advanced instrumentation



Molecular smile assembled with the STM tip



STM microscope

IMDEA-Nanociencia is a private Foundation created by joint initiative of the Comunidad de Madrid and the Ministry of Education of the Government of Spain in February 2007 to manage a new research Institute in Nanoscience and Nanotechnology (IMDEA-Nanociencia). The Institute is located at the campus of the Universidad Autónoma de Madrid in Cantoblanco.

The Institute aims at performing research of excellence in selected areas and offers attractive opportunities to develop a career in science at various levels from Ph.D. students to senior staff positions.

The Madrid Institute for advanced studies in Nanoscience also develops an important program of technology transfer and creation of spin-offs companies.

E-mail

contacto.nanociencia@imdea.org

Phone 34 91 497 68 49 / 68 51

Fax 34 91 497 68 55



[Nanociencia y Nanotecnología: lo pequeño es diferente
Nanoscience and Nanotechnology: small is different]

NEMS with microfluidic in order to improve the development of technical approaches compatible with living systems (in fluid medium).

Round-Table – chaired by **Robert Baptist (CEA)**

Participants: **Bernard Limon (Biomérieux), Franz Bruckert (INP, Grenoble), Alfonso Jaramillo (CNRS-Ecole Polytechnique), Philippe Marlière (Isthmus, SARL), David Bikart (Institut Pasteur), Alexei Grinbaum (SPEC / LARSIM-CEA), Jean-Louis Viovy (Institut Curie), Philippe Andreucci (Leti-CEA)**

All participants to the Round table were invited to discuss and answer the following questions in opened interaction with the audience:

- 1- What are the scientific and technical obstacles encountered by scientists in SB?
- 2- What are the potential technological solutions and the expected difficulties?
- 3- Which short- to middle-term actions can be anticipated to promote the connection of both research communities?

Bernard Limon (Biomérieux) indicated that the main challenges for new technologies to be transferable to the industry are:

- to provide a high-speed analysis system
- to provide a non-toxic system
- to provide a highly reliable (controlled) system

According to BL, the main difficulty for industrialists interested in SB-based technology for diagnosis and biomedical applications, is to produce “predictable” systems. PM added that many molecular phenomenons are not yet fully understood by scientists but simulation is still possible (using black-boxes). Predictability of these synthetic systems is however a very hard challenge.

J-LV commented that compared to the classical pharmacological “drug-discovery” approach, production of predictable synthetic systems for biomedical applications is an “inverse process”. However, screening tests for synthetic systems is still required and total predictability is therefore difficult.

FB suggested that decoupling the systems is an essential step in the construction of synthetic applications. For this purpose, exploitation of mathematical tools (modelling, algorithms) is extremely useful. DB added that to meet the challenge of predictability, nanotechnology tools allowing high throughput screening can potentially provide a very efficient support to SB. BL underlined that chemistry specialists are also greatly needed for BS and nanotechnology developments.

AG stressed the importance of education and promotion of ethical and societal debates on SB with stakeholders, NGOs, consumer associations, etc... This would greatly help to avoid misunderstanding on the rational motives and the objectives SB developments between the scientific community and the general public.

Finally, PM mentioned that, as already instituted by US stakeholders of SB, France should promote federative projects involving partners from all scientific communities, including specialists of molecular biology, bio-engineering, computing technologies and Micro& Nanotechnologies in order to stimulate progression of SB.

Organizers:

R. Baptist, Minatec, CEA Grenoble
 Hidde de-Jong, INRIA, Grenoble
 Stéphane Fontanell, OMNT
 Hans Geiselmann, Université Joseph Fourier, Grenoble
 David Peyrade, CNRS - LTM, Grenoble
 Marie-Claire Toufektsian, OMNT
 Anne-Marie Villard, OMNT

Sponsors:



Field Emission Resonances at Tip/Mercaptoalkylferrocene/Au Interfaces

Lars Müller-Meskamp¹, Silvia Karthäuser¹, Harold J. W. Zandvliet^{1,2}, Melanie Homberger³, Ulrich Simon³ and Rainer Waser^{1,4}

¹ IFF-6: Electronic Materials

² Mesa+ Institute for Nanotechnology, University of Twente

³ Institute of Inorganic Chemistry (IAC), RWTH Aachen University

⁴ Institute of Electronic Materials II, RWTH Aachen University

The electrical properties of α,ω -mercaptoalkyl ferrocenes with different alkyl chain lengths, FcC n with $n = 3, 5, 11$, embedded in a self-assembled host matrix of alkanethiols on Au(111) are studied by scanning-tunneling microscopy (STM) and spectroscopy (STS). Based on current-distance spectroscopy (I - s), as well as on the evaluation of Fowler-Nordheim tunneling current oscillations, the apparent barrier height of ferrocene is determined independently by two methods. The electronic coupling of the ferrocene moiety to the Au(111)-substrate depends also on the length of the alkane spacer chain like shown in [1].

The ability to access and to use electronic properties of individual molecules together with the inherent capability of self-organization promises new possibilities for future nanoelectronic devices. Especially interesting are molecules with reliable redox behavior, which have the potential to be used as switches or storage elements. In this study the electrical properties of chemisorbed, standing-up α,ω -mercaptoalkyl-ferrocenes are studied by UHV-STs. To minimize the configurational freedom of the chemisorbed molecules the matrix isolation approach is chosen. The mercaptoalkyl-ferrocene molecules are embedded into self-assembled monolayers of alkanethiols, which serve as well defined host matrices with known electrical and structural properties.

Performing voltage-dependent imaging, shown in Figure 1, the step height between ordered surface domains of mercaptopropyl-ferrocene, FcC3, and the surrounding octanethiol, C8, monolayer is measured in constant-current mode for bias voltages ranging from -0.8 V to -1.8 V using UHV-STM. It is obvious from the selected images that the apparent height of the ferrocene derivatives depends strongly on the bias voltage. This behaviour has not been observed so far for other

molecules inserted in an alkanethiol matrix. For lower bias voltages only slightly elevated features are visible, whereas for higher negative bias bright, well-defined features appear. It is concluded that the apparent step height changes of FcC3 with respect to C8 as a function of U_b are mainly electronic in origin [1].

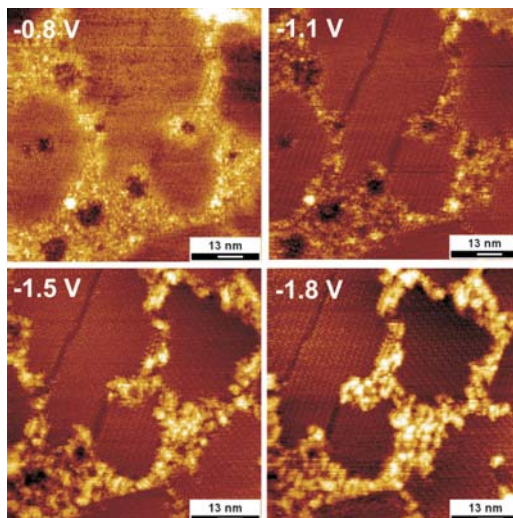


Fig 1. Voltage-dependent imaging: the step height between ordered surface domains of FcC3 and the surrounding C8 monolayer is measured in constant-current mode for bias voltages ranging from -0.8 V to -1.8 V using UHV-STM.

The electrical transport through FcC11 molecules embedded in a C12 SAM matrix was characterized by current-distance spectroscopy, a well accepted method to characterize the chemical specificity of the sample surface and the local electronic charge. The spectra recorded on extended patches of FcC11 inserted into C12 are shown in Figure 2. I - s spectroscopy on mercaptoalkyl-ferrocenes in our measurement setup clearly proves that the decay constant is not constant over the entire length of the system, but depends strongly on the nature of the respective material.

Three different parts of the I - s curve with different decay constants can be identified: the tunneling gap between the STM tip and the molecule (β_{vac}), the ferrocene moiety (β_{Fc}), and the alkane chain (β_{CH}). It was found [1] that in the case of mercaptopropyl-ferrocene a bias voltage of ± 1 V is high enough to be remarkably larger than the apparent barrier height, e.g. the tunneling barrier shape changes to a triangular barrier resulting in

Fowler-Nordheim tunneling or field emission [2]. For this case the experimentally determined $\beta_{Fc} = 2.8 \text{ nm}^{-1}$ corresponds to an apparent tunneling barrier height of 0.62 eV for the ferrocene moiety.

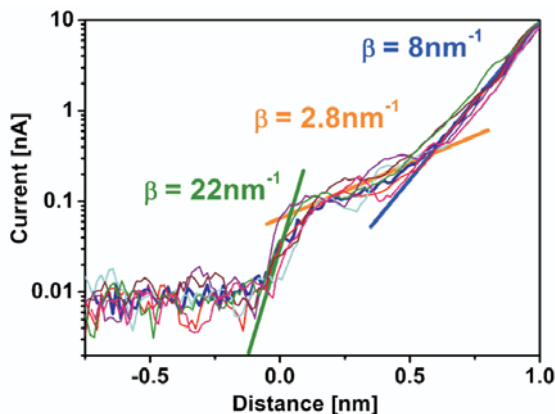


Fig 2. Current-distance (I-s) spectroscopy on mercaptoundecyl-ferrocene. The slopes in the semi-logarithmic I-s plot reflect the decay-constants.

In addition I-U spectroscopy of mercaptoalkyl-ferrocenes with different chain length, FcCn with $n = 3, 5, 11$, inserted into the corresponding alkanethiol host matrices has been performed.

Most interestingly a characteristic increase in current is observed, when the applied bias voltage exceeds the apparent tunneling barrier height of ferrocene due to the onset of Fowler-Nordheim tunneling (Fig 3).

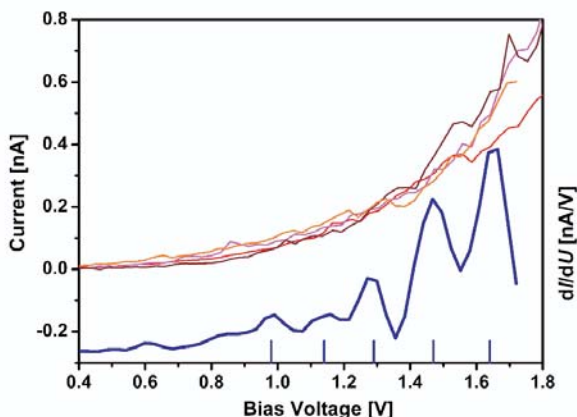


Fig 3. Current-voltage curves of FcC3 (reddish) and differential conductance (bluish) showing Fowler-Nordheim tunnelling with superimposed Gundlach oscillations.

This conduction threshold is found at higher voltages for mercaptoalkyl ferrocenes with longer alkane chains [1].

In the regime of high bias voltages, according to Gundlach [3], the tunneling current exhibits additional oscillations resulting from electron standing waves in the vacuum gap between emitter (e.g. tip) and collector (e.g. ferrocene moiety).

Thus the conductance versus U_b curve shows maxima at well-defined voltages, from which the apparent tunneling barrier height of ferrocene can be calculated. The thus obtained value of 0.60 eV is in excellent agreement with the value of 0.62 eV obtained by current-distance spectroscopy.

In conclusion two UHV-SPS methods, e.g. current-distance spectroscopy and current-voltage spectroscopy, were applied successfully on ordered domains of mercaptoalkyl-ferrocenes embedded into alkanethiols. The results are in excellent agreement and reveal that the main conduction mechanism of ferrocene is Fowler-Nordheim tunneling.

Furthermore Gundlach-oscillations are clearly observed in the current-voltage spectra. The onset of the Fowler-Nordheim tunneling can be additionally modulated by the attached alkane spacer chains. Thus, ferrocene moieties are attractive candidates to tailor the electron transport properties in future nanoelectronic devices.

References

- [1] L. Müller-Meskamp, S. Karthäuser, H. Zandvliet, M. Homberger, U. Simon, and R. Waser, *Small* 5, 496-502 (2009).
- [2] W. Wang, T. Lee, M. A. Reed, in *Nano and Molecular Electronics Handbook*, (Ed: S. E. Lyshevski), CRC Press, Boca Raton, 2007, Ch. 1.
- [3] K. H. Gundlach, *Solid-State Electron.* 9, 949 (1966).

BioInspired Nanomaterials¹

Jean-Pierre Aimé, C'nano GSO (France)

1. Introduction

Over the last decades, biology has made significant advances in providing a rational understanding of the molecular mechanisms governing life's processes. New materials have emerged from life systems, which physicists and chemists have then promptly fabricated, manipulated and addressed at the molecular scale. The emblematic example is DNA technology, which affords the elaboration of programmable chemical synthesis routes to build complex architectures and functions with molecular precision, and sheds light on a new generation of robust tools. During this same period, the semiconductor industry's development has led to impressive performance in miniaturisation. Its current challenge though, is to develop lithographic technology for feature sizes below 20 nm and explore new classes of electronic devices based on carbon nanotubes and nanowires. A central challenge in technology is constructing multi-scale structures used to organize nanodevices and functional materials.

2. Bio-Inspired based information system

Nature possesses an extraordinary capacity to assemble complex nanostructures that have active and specialised functions. Our ability to precisely position distinct components providing rich functions on the nanometre scale is still limited but remains a key goal in nanotechnology and materials science.

To name but a few: DNA is emerging as an attractive tool for nanoscience and nanotechnology; Watson-Crick base pairing can be translated into binary sequences (0, 1) to organise nanomaterials in a programmable way. DNA can be used to dictate the precise positioning and connection of materials and molecules in any deliberately designed structure. Phage and cell display can be used to design new peptide sequences with dedicated functionality, binding organic to inorganic materials. Viruses are self-assembled nanomaterials providing biological materials of well-defined size and shape. Moreover, capsids have surface properties that are well defined

down to the atomic scale and viral materials are amenable to genetic engineering. Nature uses two types of information: the genome's digital information, and environmental information such as cell-surface signals from other cells or chemical gradients.

Treatment of the information at such a complex level requires multi-scale structures with appropriate integration steps. It is a formidable task to understand and copy such multi-scale systems; we face the challenges of determining the different levels of integration and engineering the interfaces from the molecular scale up to several micrometres. These challenges are well known in the fields of nanoscience and nanotechnology.

For instance, the ability to precisely position distinct functional components at the nanometre scale is still limited and this is a key goal at the interface between nanoscience and materials.

3. State of the art

Bio-inspired fabrication methods allow the unprecedented capability to use algorithms to build elaborate, complex, architectures and functions. The bio-inspired strategy also shows capability to organise inorganic materials through biomimetic processes that can readily design biosensors, plasmonic and nanoelectronic networks or electroactive materials. Bio-inspired materials provide new routes to build interface properties using genetic engineering, biological combinatorial methods or targeted chemical synthesis, thus increasing the efficiency of inorganic nano objects. Another important route that should lead to significant improvement in the design of new materials and functions is the development of a new class of bio-inspired micro nanosystems that lead to new conceptions of logical functions and dynamic patterning with error corrections.

A number of European groups are involved in the use of DNA and virus technology. Since the seminal work of N.E. Seeman (<http://seemanlab4.chem.nyu.edu/nanotech.html>), DNA as a material for nanotechnology has been widely used to connect or functionalize different nanostructures, through which versatile 2D and 3D shapes are obtained. Using DNA scaffolding to build DNA origami has further boosted the development of DNA nanotechnology (P.W.K. Rothemund (Nature, V 440, March 2006). Available 3D structures prove new

¹ In April 2010 a new nanoICT Working Group, dedicated to BioICT issues was launched. This is the first version of the BioICT position paper, dealing mainly with the BioInspired Nanomaterials topic. An updated and more extended version will be published (beginning 2011).

INL - CREATING VALUE AT NANOSCALE



Over the next months, the International Iberian Nanotechnology Laboratory (INL) will start installing various scientific equipment which shall enhance and expedite the studies of the scientific community working in the region

INL Building in Braga, Portugal

Over the next months, the International Iberian Nanotechnology Laboratory (INL) will start installing central scientific equipment reinforcing the infrastructure that will become available for the scientific community working in the region.

The new research facility, located in Braga (North of Portugal) occupies more than 47,000 square meters, with 20,000 of them exclusively dedicated to science. The Laboratory launched in 2005 by Spain and Portugal is set to be a global centre of excellence in applied nanotechnology research attracting the world's best scientists and engineers.

The first equipment to be installed comprises cleanroom processing equipment (E-beam and laser lithography tools, a mask aligner, resist and developer tracks, three multitarget physical vapour deposition tools, a chemical vapour deposition system, reactive ion etch and ion mill tools). These tools are single wafer tools with capability of handling up to 200mm diameter wafers. In a second phase, planned for the end of 2010 and beginning 2011, characterization equipment including a CD SEM, a ultra high resolution SEM, a dual FIB, a 200kV analytical TEM, a X-ray Photoelectron Spectroscopy (XPS) system, two Scanning Probe Microscopy systems, and two X-ray systems for thin film and nanoparticle analysis will be installed. A set of NMR tools for solids (600MHz) and

liquids (450 kHz) is under consideration. In a third phase, a set of corrected atomic microscopes is being considered. The atomic imaging tools will be installed in the high accuracy labs at the basement of INL. This set of central labs is completed by a central biochemistry laboratory, a packaging laboratory, a magnetometry laboratory, and an electrical characterization laboratory.

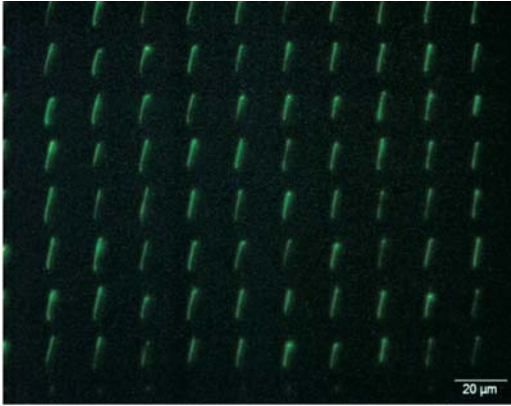
The INL is an international institution created to foster interdisciplinary research in nanotechnology and nanoscience. As a private, non profit organisation, the Laboratory will provide a state-of-the-art research environment and favour an interdisciplinary effort in addressing major challenges in nanomedicine, nanotechnology applied to environmental & food control, nanoelectronics and, nanomachines and molecular manipulation at nanoscale. Last February INL and the Comissão de Coordenação e Desenvolvimento Regional Norte signed the contract that allows INL to benefit from an additional 17MC assistance, under the Portuguese North Regional Operational Program "ON.2 - O Novo Norte", also financed by the European Union through the European Regional Development Fund (ERDF). INL aims to become a vital part of Europe's scientific area setting an example in new types of research collaboration between EU Member States. Its facilities will be open to

future members from European and non-European states, and foster international co-operation with other regions like North America, Latin America, Asia.

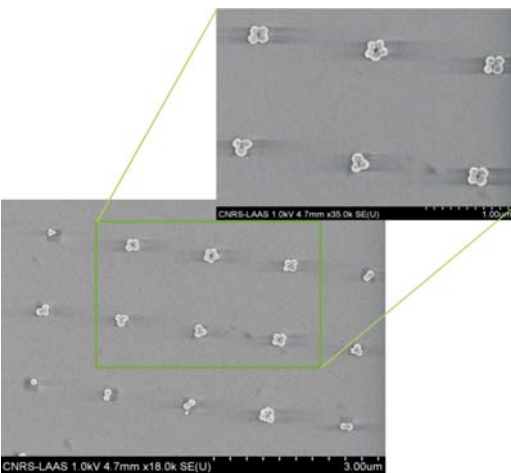
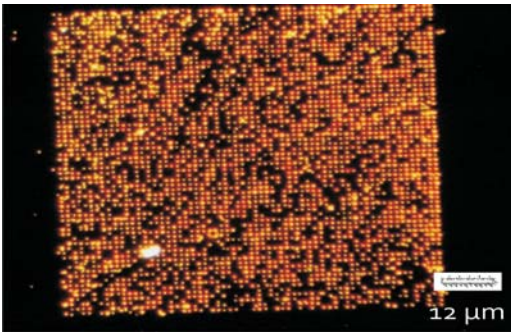
The construction of the INL is also co-financed by 30MC from the ERDF (European Regional Development Fund), within the Cross-border Cooperation Programme Spain Portugal. The INL project falls under Priority 1 of the Programme Cooperation and joint management for the improvement of competitiveness and the promotion of employment.

The INL challenge is not only to assure research excellence, but also to shift its output into economic and social development. INL aims to be at the cutting edge of Public-Private Partnership (PPP's) models and Technology Transfer activities facilitating and accelerating innovative technology transfer from basic research to industry, working closely with industrial partners in the INL research areas to develop new diagnostics, drugs, machines, devices and therapies.

After this project's completion, Portugal and Spain will benefit from a competitive technological infrastructure, increasing the international competitiveness of Iberian and regional businesses, universities and technological centers. The local environment for spin-offs and technological centres will be greatly improved.



Stretched DNA molecules transfer-printed on a surface after directed assembly on a microstructured PDMS stamp (Courtesy Phd thesis A. Cerf, LAAS-Toulouse)



Dark field and SEM images of 100 nm gold nanoparticles transfer-printed on silicon after directed assembly on a nanopatterned PDMS stamp (Courtesy Phd thesis A. Cerf, LAAS-Toulouse) and A. Cerf Colloids and surfaces (2009)

routes of basic units with enough capability to already provide complex properties at their output.

DNA origami can also be used as an information-bearing seed for nucleating algorithm. Self-assembly of defined-structure geometry may introduce errors that can be reduced by controlling the competition between nucleation and growth process. Origami, as a self-supporting information seed, controls a computed structure's growth and prevents competition from the nucleation process. The key point is the encoding of the molecular or macromolecular units so that an appropriate design of short sequences can be reduced to information bits 0, 1.

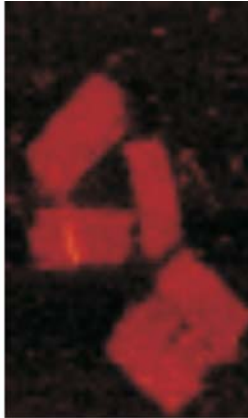
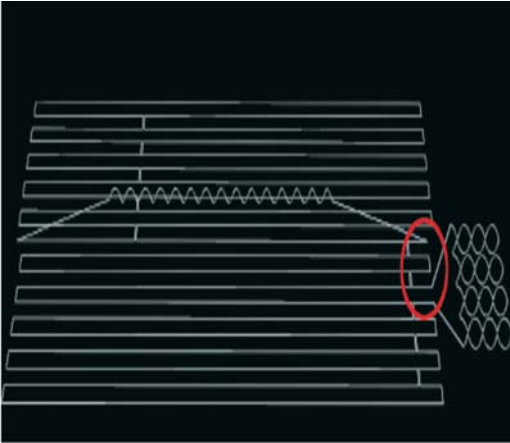
The marriage of the top-down and bottom-up fabrication methods paves the way to arrange complex molecular nano units, to electronically address and integrate them into a functional device.

Viruses are self-assembled materials with controlled arrangement at the molecular scale. Through genetic engineering, viruses provide functionalized arrangements of systems and devices. A known result is the genetically engineered M13 virus, which serves as a model system and is used as a programmable molecular building block to template inorganic materials' growth. Combined top-down, in particular using microcontact printing technology, and bio-inspired bottom-up fabrication methods have been used to assemble nanowires, fabricate microbattery electrodes with viruses (A. Belcher) or microreactor design arrays to investigate bio-molecular motor activity.

4. Synergie between Bio-Inspired methods and information

This fast-growing field and its mature bottom-up fabrication methods provide an almost infinite variety of bio-inspired materials and functions. Within this framework, there is a pressing need to face the challenges to design multi-scale structures with well-defined integration levels and to engineer interface properties from the molecular scale up to several micrometres.

Challenging complexity and providing concrete outcomes are at the heart of the bio-inspired fabrication method. Conception and fabrication of complex arrangements of functional materials and nanodevices is thought to be a key step towards overcoming Moore's Law.



Assembly of bridged DNA origamis, a DNA single strand is kept unpaired to curve and bridge DNA origamis. Above scheme of the calculated structure. (courtesy JM Arbona, J. Elezgaray, JP Aimé.

In biological systems, the same starting material has the potential to form an infinite variety of structures with dedicated functions. Beyond achieving powerful 2D-3D bio-inspired structures, a key aim is to assemble and organise functional materials and systems at increasing levels of complexity. Designing multi-scale structures to create hierarchical order requires the cooperative development of new experimental tools that record information at different scales. The following key challenges are:

- identifying different integration levels used to process information in multi-scale structures
- theoretical modelling of equilibrium and non-equilibrium interaction in different contexts, from molecular recognition to controlling the growth process
- a rationalized route for efficient strategies to engineer interface properties from the molecular scale up to several micrometres
- a rationalized route for instrumentation to record data at different scales

5. EU and outside

Definitely the Bio-inspired method is a fast growing research topic emerging principally in USA, Japan and Israel. Especially, in USA there is a wealth of creative and innovative results. Numerous functionalities emerge; dynamic patterning, elaborate 3D structures with controlled shape, precise positioning of inorganic materials and devices, control of nanoparticles arrangements... At the same time, there is an increasing efficiency in designing and fabricating short sequences with specific functions.

Several European groups are already involved in this research topic, see for instance the Danish group with the noticeable results: Dolphin and DNA Box, Oxford, Munich, etc. Numerous European laboratories have developed high-throughput protocols for biomolecule selection, e.g., aptamers fabricated with the SELEX process or peptide sequences using phage and cell display methods, optimised for chemical or biological applications. Nucleic acid ligands and aptamers are characterized by high affinity and specificity for their target, a versatile combinatorial selection process and small physical size, which collectively make them attractive molecules for targeting diseases or as therapeutics.

Aptamers were first conceived as a medical tool. The other important field concerns nanostructure and nanodevice. Here again, the main interest lies in that the high affinity and specificity as well as their small size, make aptamer tools good candidates for handling interface properties. These properties will enable aptamers to facilitate innovative new nanotechnologies.

The recently EU funded COST Action "BioInspired nanotechnologies: from concepts to applications" aims to bring bio-inspired nanosystems and nanomaterials in the field of nanotechnology and to combine bio-inspired bottom up and top down fabrication methods by bridging multidisciplinary scientific fields and centres on DNA (DeoxyriboNucleic Acid) technology, affording the elaboration of programmable chemical synthesis routes to build complex architectures and functions with molecular precision, and shedding light on a new generation of robust tools.

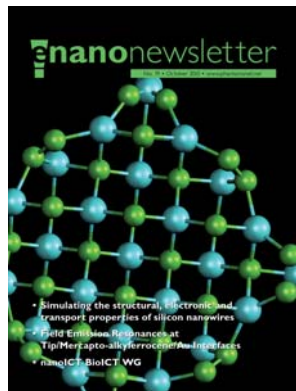
Key challenges addressed are identifying different integration levels used to process information in multi-scale structures, theoretical modelling of equilibrium and non-equilibrium interaction in different contexts, from molecular recognition to controlling the growth process, a rationalized route for efficient strategies to engineer interface properties from the molecular scale up to several micrometres and a rationalized route for instrumentation to record data at different scales.

BioICT Working Group

Contact details:

Jean-Pierre Aimé, C'nano GSO (France)

jp.aimé@cpmoh.u-bordeaux1.fr



Cover Image:
Surface-reconstructed
SiC nanowire

Xavier Cartoixa
Universitat Autònoma
de Barcelona
Spain

Advertisement

Malvern Zetasizer
systems



Light scattering

more than just
size measurement

- Colloids
- Nanoparticles
- Biomolecules
- Proteins

Zetasizer Nano

- Versatile system
- Colloid and biomolecule size
- Dispersion stability
- Zeta potential
- Molecular weight

Zetasizer APS

- Automated using microplates
- Protein size and purity
- Formulation studies
- Crystallization conditions
- Denaturing conditions
- Solubility

Zetasizer μ V

- Protein size and Molecular weight
- 2 μ L sample volume

Feb. 16 Wed. ~ 18 Fri., 2011

Tokyo Big Sight, JAPAN

East Exhibition Hall 3,4,5,6 & Conference Tower

Japan

Green
NANOTECHNOLOGY

Sustainability
with every nanometer

The World's Largest Nanotechnology Show



nano tech

International Nanotechnology
Exhibition & Conference

nano tech 2011

www.nanotechexpo.jp

Concurrent Exhibition

Reserve
Your Booth
Now!!

International Water Solution Exhibition

InterAqua 2011

www.interaqua.jp

Nano & Bio Interdisciplinary Business

Nano Bio Expo 2011

www.nanobioexpo.jp

Advanced Surface Technology Exhibition & Conference

ASTEC 2011

www.astecexpo.jp

The 40th Surface Finishing Exhibition

METEC 2011

www.metecexpo.jp

Integration of Electronics and Printing Technology

Printable Electronics 2011

www.printable-electronics.com

Cutting-edge Converting Technologies

Convertech JAPAN 2011

www.convertechjapan.com

Functional Materials with High Added Value

neo functional material 2011

www.kinousei.com

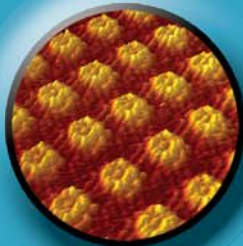
Technologies for Solar Cells, Fuel Cells and Secondary Batteries

Eco cell-Battery Expo 2011

www.ecocell-battery.jp

NEW!

SURFACE ANALYSIS



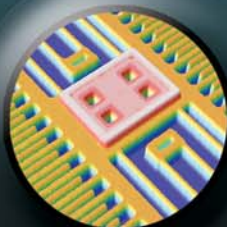
AFM / STM

Materials, polymers, biology, electrochemistry...



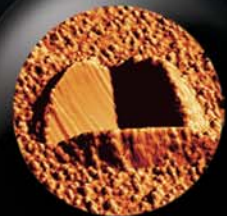
SNOM Microscopy

*Reflection, transmission, Apertureless...
SECM, Deep Trench, nanopipette probes...*



3D Optical Profilometry

*New confocal technology...
Interferometry (PSI/VSI)...*



And also...

Mechanical profilometry, nano-indentation...



Scientec FRANCE

17 Av. des Andes - Batiment le Cèdre
91940 LES ULIS
Tel : + 33 (0)1 64 53 27 00

www.scientec.fr

Scientec IBERICA

C/Buenavista 4, Bajos
28250 Madrid - ESPAÑA
Tel : + 34 918 429 467

info@scientec.fr