

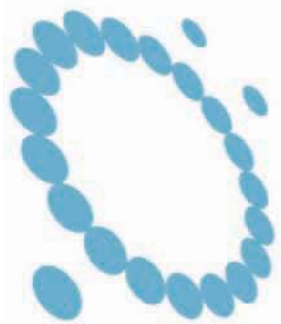


## NanoICT Position Papers

### Nanoelectromechanical Systems (NEMS)

#### Mono-molecular electronics on a surface: challenges and opportunities





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## Dear Readers,

NanoICT position papers aim to be a valid source of guidance for the semiconductor industry (roadmapping), providing the latest developments in the field of emerging nanoelectronic devices that appear promising for future take up by the industry.

This E-Nano newsletter issue contains two new position papers from the EU funded nanoICT Coordination Action Working Group coordinators covering the following areas: Nano Electro Mechanical Systems (NEMS) and Mono-molecular Electronics. In the previous issue (No. 13), carbon nanotubes and modelling at the nanoscale topics were reviewed.

NEMS have unique and useful properties that make them suitable for different applications in various fields, ranging from ICT to bio-chemical detection. The first position paper summarizes NEMS applications and challenges.

The second position paper is dedicated to provide insights in a field devoted to study new approaches and technologies (hybrid molecular electronics) necessary to build computers or telecommunication devices.

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, Ref: ICT-CSA-2007-216165).

2008 has proved to be another successful year of publishing for the E-Nano newsletter. Therefore, we would like to thank you, our readers, for your interest, support and collaboration and finally wish you a healthy and happy New Year 2009!

**Dr. Antonio Correia**

**E-nano newsletter** Editor

Phantoms Foundation

## EDITORIAL INFORMATION

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### Editorial Information

#### Research - NanoICT Position Papers

#### **Nanoelectromechanical Systems (NEMS) 5**

*G. Villanueva, J. Arcamone, G. Abadal, L. Nicu, F. Pérez-Murano, H. Van der Zant, P. Andreucci, C. Hierold and J. Brugger*

1. Introduction	5
1.1. Definition	5
1.2. Interest	5
2. Applications	5
2.1. Sensors	5
2.2. Electronics	6
2.3. Fundamental studies	8
3. Challenges	8
3.1. High Quality factor	8
3.2. Modeling	9
3.3. Transduction in the nanoscale	11
3.4. Fabrication	12
3.5. System Integration	13
4. Conclusions	13
5. References	13

#### **NANO Conferences 18**

#### **NANO Vacancies 21**

#### **NANO News 23**

#### **Mono-molecular electronics on a surface: challenges and opportunities 25**

*C. Joachim, J. Bonvoisin, X. Bouju, E. Dujardin, A. Gourdon, L. Grill, M. Maier, D. Martrou, G. Meyer, J.-P. Poizat, D. Riedel and M. Szymonski*

1. Introduction	25
2. The architecture	25
3. N-Interconnects	25
4. Atom and Molecule Surface science issues	29
5. Packaging	31
6. Conclusions	31
7. References	32

#### **Deadline for manuscript submission:**

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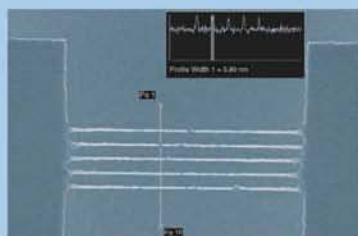


## Ultra high resolution electron beam lithography and nano engineering workstation



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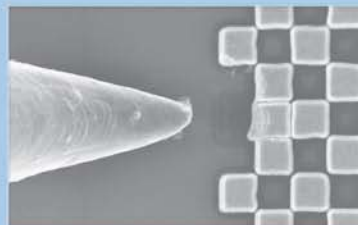
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- ...Nanoscale imaging
- ...EDX-chemical analysis
- ...Electron beam etching
- ...Electrical and mechanical probing
- ...Electron Beam Induced Deposition (EBID)



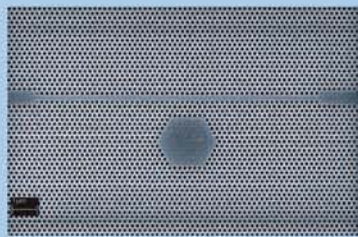
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## Nanoelectromechanical Systems (NEMS)

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### 1. Introduction

Micro Electro Mechanical Systems (MEMS) have been studied and developed for more than 3 decades [1]. They bring together silicon-based microelectronics with micro-machining technology, making possible the realization of complete systems-on-a-chip. The fundamental and characteristic element on every MEMS is a mechanical (movable) component with dimensions ranging from few microns up to millimeters in some cases. These systems have been proven to be very useful for a plethora of different applications, e.g. ink-jet heads for printers [2], accelerometers for automotive applications [3], micro-mirrors for beam splitting [4], chemical sensors [5], etc. Following the evolution of microfabrication technologies for integrated circuits, pushing downwards the resolution limits, the dimensions of the mechanical components in MEMS were also reduced below 1 μm, yielding the first Nano Electro Mechanical Systems (NEMS) [6, 7]. This is the way NEMS appeared following the so-called “top-down approach”. In parallel, the development of nanofabrication “bottom-up approaches”, based on materials growth or self-assembly, has constituted another alternative to fabricate NEMS.

NEMS are characterized by small dimensions, which determine the devices functionality. However, it is sometimes difficult to decide if a given device can be defined as a NEMS or not. Therefore, we consider necessary to establish a definition for the term in this paper.

#### 1.1. Definition

Nano Electro Mechanical System (NEMS) is a system:

- which involves electronic and mechanical elements

- whose main functionality is based on at least a mechanical degree of freedom
- whose size has the following characteristics:
  - at least two out of its three dimensions are below 1 μm OR
  - its functionality is given by a thin layer smaller than 10 nm
- which can include:
  - actuation
  - signal acquisition (sensing)
  - signal processing
  - vehicles for performing chemical, biochemical reactions and bioelectrical interactions

### 1.2. Interest

Since they first appeared in the literature [8, 9], several groups all around the world have been actively contributing in the field of NEMS. Besides the possibility of increased device density, the growing activity in the field has been mainly motivated by the benefits that these systems provide.

Among the interesting properties of NEMS, many can be explained using scaling laws. Let us consider a mechanical device and scale down its three dimensions: thickness (*t*), width (*w*) and length (*L*). The effect of scaling on important parameters can be illustrated through simple formulas given in **Table 1**.

Therefore, NEMS offer [11] fundamental resonance frequencies in the microwaves [12], high mechanical quality factors [13], active masses in the femtograms (1 fg = 10<sup>-15</sup> g) [14, 15], heat capacities below the yoctojoule (1 yJ = 10<sup>-24</sup>J) [16, 17], ultra-low operating power level (for 1 device 1 pW = 10<sup>-12</sup> W) [11], etc. All these properties make NEMS interesting for a series of different applications because they improve previous MEMS devices functionalities by orders of magnitude.

### 2. Applications

As it can be understood from the discussion above, the natural applications of NEMS can be mainly divided into three different groups: sensors, electronics (signal processing) and new tools for fundamental studies.

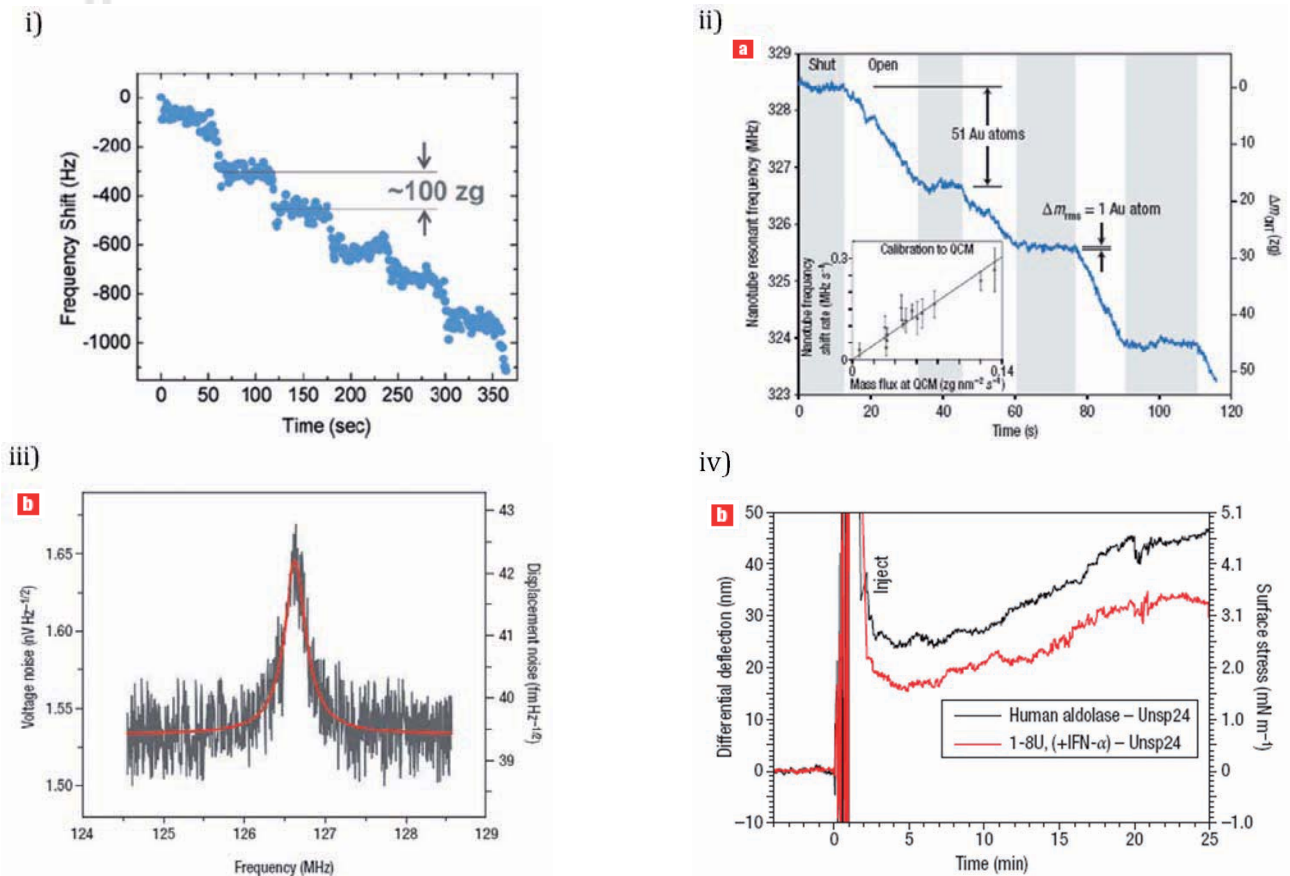
#### 2.1. Sensors

Mass and force sensors have been the most studied because they allow the detection of different species after proper connection to chemistry/biology by means of proper functionalization.

Mass	Elastic constant	Resonance frequency	Force noise
$m = \rho V \propto l^3$	$k = \frac{\beta E w t^3}{L^3} \propto l$	$f_{res} = \gamma \sqrt{\frac{E}{\rho}} \frac{t}{L^2} \propto l^{-1}$	$S_F = \frac{2k_B T k}{\pi Q f_{res}} \propto l^2, \quad \text{constant } Q$ $\Delta F^2 = \int_{BW} S_F df \propto l$

**Table 1:** Table summarizing how the properties of a mechanical system scale down with the reduction of its dimensions [10].





**Figure 1:** i) Resonance frequency shift of a nanosized free-standing beam while  $N_2$  molecules are deposited on the structure in an “on/off” configuration. The device is operated at cryogenic temperatures. Each step in the data corresponds to approximately a 100 zg mass (2000  $N_2$  molecules). The root mean square frequency fluctuations of the system correspond to a mass resolution of 20 zg for the 1 s averaging time employed. Extracted from [15].

ii) Resonance frequency shift of a CNT-based nanomechanical resonator as a function of time while gold atoms are being deposited in an “on/off” configuration. The device is operated at room temperature, and presents a mass sensitivity of  $1.3 \times 10^{-25}$  kg/Hz<sup>1/2</sup>, i.e. 0.40 gold atomsxHz<sup>-1/2</sup>. Extracted from [19].

iii) Output voltage noise spectrum a 127 MHz self-sensing undriven cantilever measured at 1 atm and 300 K (black trace). A d.c. bias of 100 mV is used during the measurement. The red line is a Lorentzian fit to thermomechanical noise combined with uncorrelated white background noise. Off-resonance, the displacement sensitivity attained is 39 fm/Hz<sup>1/2</sup>. Extracted from [22].

iv) Label-free gene fishing of an interferon-induced gene. The red line (ME15+) indicates the response of the cantilever coated with an interferon- $\alpha$ -sensitive human 1-8U gene fragment. The black line represents the differential mechanical response of the cantilever sensitized with the human aldolase A oligonucleotide. Extracted from [28].

For mass sensing, the race has been pushing down the limits of detection passing through the attogram (1 ag =  $10^{-18}$  g) [14, 18], the zeptogram (1 zg =  $10^{-21}$  g) (Figure 1.i, [15]) and finally ending with the detection of a single individual atom using a carbon nanotube (CNT) (Figure 1.ii, [19]). From a more applied point of view, nanomechanical resonators have been used for (bio)chemical detection [20] and it has already been possible to detect a single virus [21]. However, one of the most promising applications is still under development and this is the “Single-Molecule Mass Spectrometry (NEMS-MS)” [11].

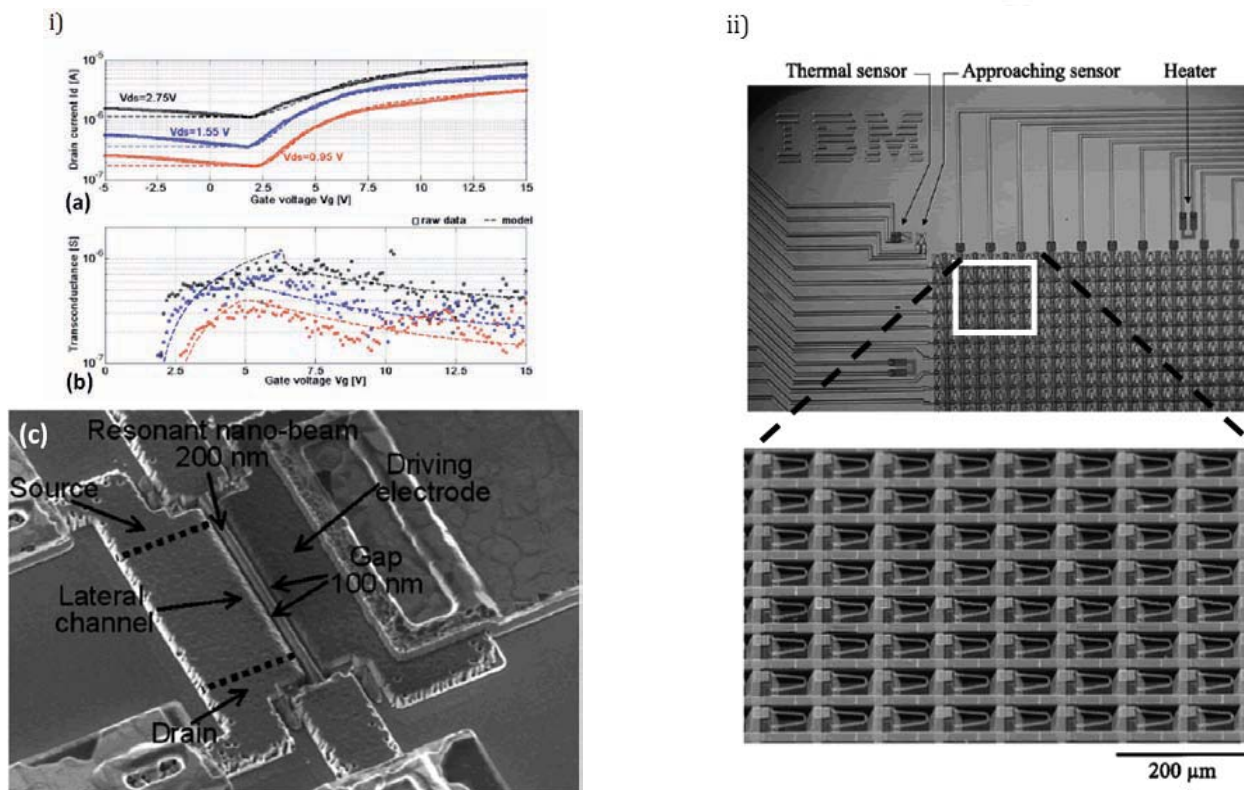
Regarding force sensing, the lower resolution limit attained by a NEMS up to date is within the femtonewton range at room temperature and atmospheric pressure (Figure 1.iii, [22]). However, the geometries that are proved to be more sensitive to force are much longer than standard NEMS [23, 24] and in some cases the search for higher measurement stability requires the systems to be much thicker [25-27]. Using those systems, a single base-mismatch in between two different DNA-strands of 18

bases has been detected [25] and also, as shown in Figure 1.iv [28], label-free detection of interferon-induced genes has been achieved.

## 2.2. Electronics

The trends in Integrated Circuits (IC) technology [29] can be divided into three groups: “More Moore” (referring to the continuous reduction of dimensions of MOS transistors with classical gate/source/drain architecture), “More than Moore” (including a series of additions to current and future CMOS technologies like Bulk Acoustic Resonators (BAR), Surface Acoustic Wave (SAW), metal contact switches, etc.) and “Beyond CMOS” that basically involves NEMS integration with CMOS.

The main advantage to include mechanical parts (both NEMS and MEMS) in circuits is on one hand, that the quality factors of mechanical oscillators are much higher than of electrical oscillators. This is highly demanded for filtering and communication applications [30, 31] and even more taking into account that they can be easily tuned [32, 33]. On the other hand, it is possible to build



**Figure 2:** i) Fabrication and modeling of a lateral resonant gate FET (NEMS-FET). (a)  $I_D(V_g)$  characteristics and (b) transconductance  $g_m(V_g)$  of the transistor shown in a SEM micrograph in (c). Extracted from [37].

ii) Optical picture and SEM micrograph zoom of a micro fabricated  $32 \times 32 = 1024$  2D cantilever array chip from IBM Zürich. It has been designed for ultrahigh-density, high-speed data storage applications using thermomechanical writing and readout in thin polymer film storage media. Extracted from [38].

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mechanical transistors and diodes [34] with a much lower power consumption when they are inactive [35]. When moving into the NEMS regime [36, 37] (Figure 2.i page 7), the obvious advantage of a higher integration allows more density for the devices, their high frequencies increase the circuit speed and their ultra-low operating power reduce the power consumption when the devices are active. As a consequence, a reduction in power consumption keeping a fast behavior is accomplished by integrating NEMS with CMOS.

A different approach is the one pursued by IBM within the Millipede project (Figure 2.ii, [38-42]) in which an array of small scanning probes is used to read and write bits of information from a substrate (data storage).

### 2.3. Fundamental studies

Another group of applications have a more fundamental origin. By their properties, NEMS constitute themselves new tools for scientific purposes. They can help in exploring scientific phenomena previously unobservable by other means. In particular, the fact that NEMS with given dimensions are mesoscopic systems could lead to the observation of quantum effects.

Initially, NEMS were aimed as an instrument to determine the quantum for the electrical (Figure 3.i, [43]) and thermal conductance (Figure 3.ii, [17, 44-46]). Currently, quantum electromechanical systems (QEMS) are aimed [47-52] which could represent a new source of experiments and a number of applications that cannot be envisaged at the moment. In the last years a quite complete theory on cavity optomechanics has been developed

which has been accompanied by several experiments demonstrating cooling of resonators down to their ground level by dynamical backaction (Figure 4.i page 9, [53-57]). An additional topic of extreme interest is the study of non-linear [58, 59] and/or complex systems [59-63], which can yield applications of localized energy modes [64, 65], as can be a selectivity increase [66, 67], or directly the oscillators synchronization (Figure 4.ii, [68]).

There are more examples on the use of NEMS as new tools for science: in [69], a specific type of NEMS mass sensor serves as transduction platform for the study of physical-chemical phenomena which are currently unobservable with any other tool. In [70], it is shown that Casimir forces, which are very difficult to observe experimentally, cannot be neglected anymore in very small NEMS and could be experimentally observed.

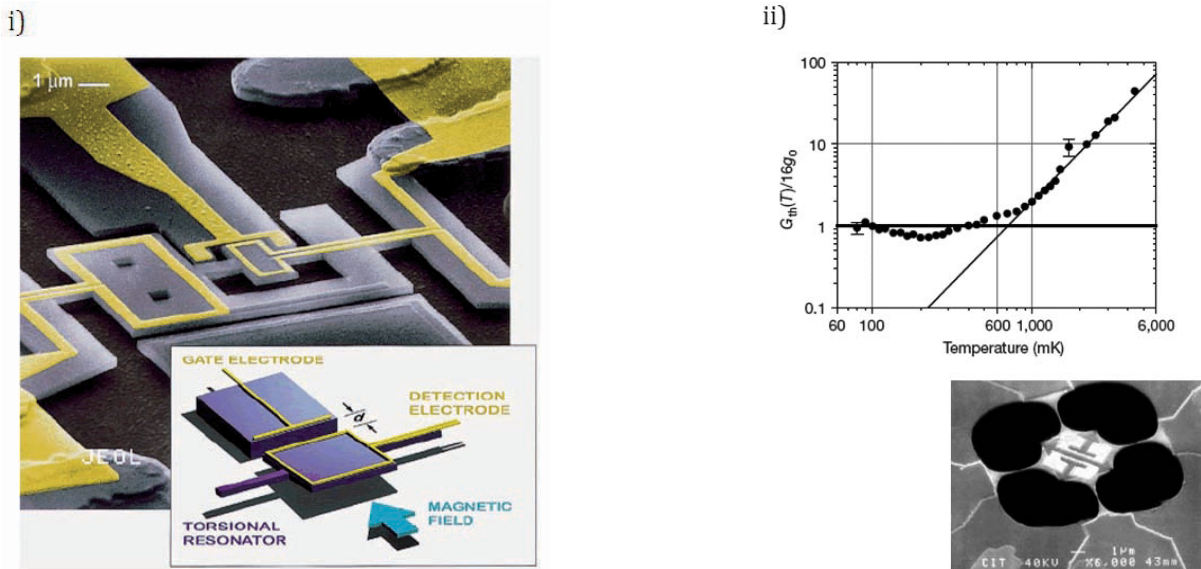
### 3. Challenges

The wide range of applications and the huge interest of NEMS have been demonstrated up to now. However, together with the plethora of interesting properties, a multitude of questions and challenges arise and constitute hot topics in NEMS research.

#### 3.1. High Quality factor

Achieving a high quality factor in a NEMS is of great importance because it means low energy dissipation, higher sensitivity to external forces, reduction of the minimum operating power level, etc.

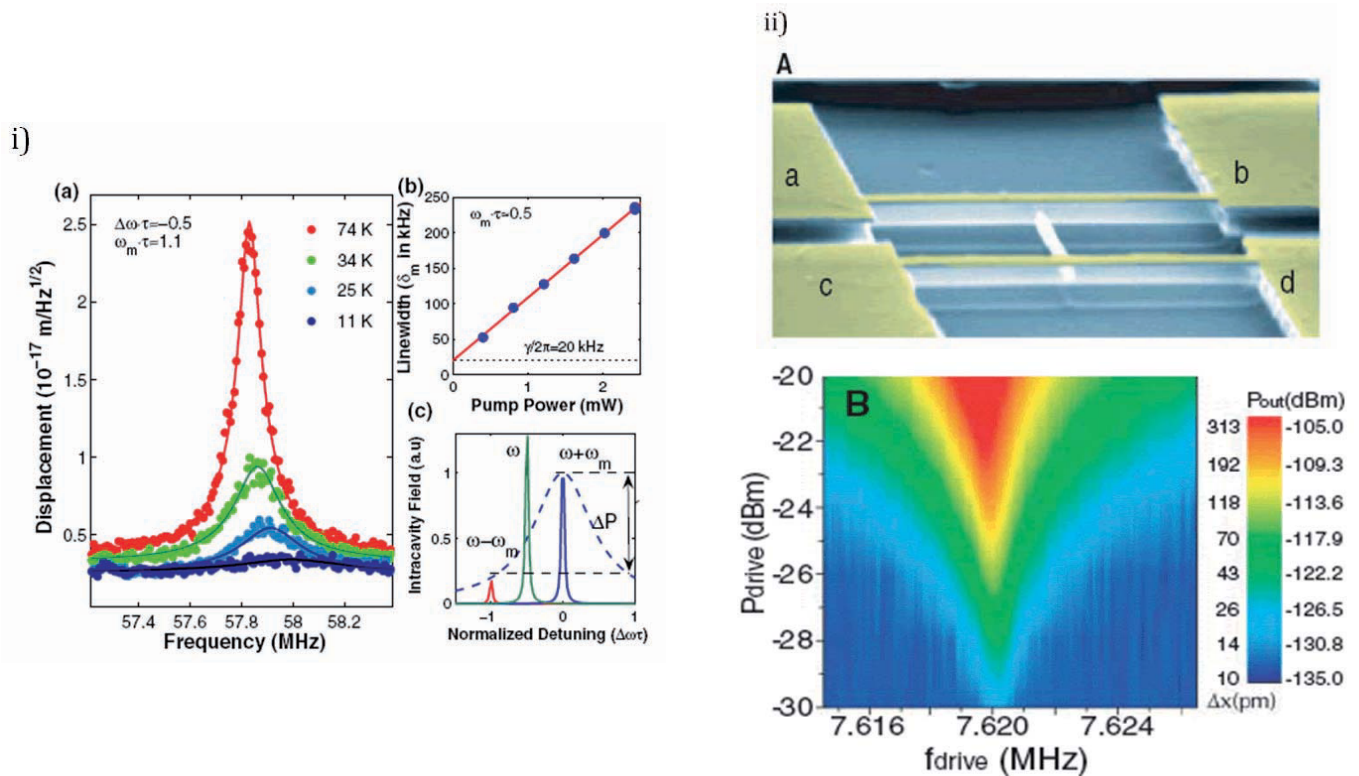
The energy losses of a resonator have internal and external sources [71, 72]. The latter includes losses due to gas



**Figure 3:** i) Nanometer-scale charge detector. The inset schematically depicts its principal components: torsional mechanical resonator, detection electrode, and gate electrode used to couple charge to the mechanical element. In this device the fundamental resonance frequency of the structure is 2.61 MHz, with a quality factor measured to be  $Q=6500$ . A charge sensitivity of  $0.1 e/Hz^{1/2}$  is achieved, with a thermal noise limit of the order of  $10^{-6} e/Hz^{1/2}$  comparable with charge detection capabilities of cryogenic single-electron transistors, but responding at higher temperatures ( $>4.2 K$ ) and over a larger bandwidth than other techniques. Extracted from [43].

ii) Thermal conductance data for a fabricated mesoscopic phonon system consisting in a free-standing structure. A quantized limiting value for the thermal conductance,  $G_{th}$ , at very low temperatures is observed at 16 occupied modes,  $16 g_0$ . For temperatures above  $T_{co}=0.8K$ , a cubic power-law behavior is observed, consistent with a mean free path of  $0.9 \mu m$ . For temperatures below  $T_{co}$ , a saturation in  $G_{th}$  is observed at a value near the expected quantum of thermal conductance for phonon transport in a ballistic, one-dimensional channel: at low temperatures,  $G_{th}$  approaches a maximum value of  $g_0=\pi^2k_B^2T/3h$ , the universal quantum of thermal conductance. Extracted from [17].





**Figure 4:** i) Cooling of a 58 MHz micromechanical resonator from room temperature to 11 K is demonstrated using cavity enhanced radiation pressure. (a) Normalized, measured noise spectra around the mechanical resonance frequency and varying power (0.25, 0.75, 1.25, and 1.75 mW). The effective temperatures were inferred using mechanical damping, with the lowest attained temperature being 11 K. (b) Increase in the linewidth (damping) of the 57.8 MHz mode as a function of launched power, exhibiting the expected linear behavior. (c) Physical origin of the observed cooling mechanism due to the asymmetry in the motional sidebands. Extracted from [56].

ii) SEM micrograph of the fabricated device (A) consisting in two parallel resonating beams whose movement is recorded by magnetomotive detection technique and an additional transversal beam coupling both oscillations. (B) Synchronization at subharmonic driving. A signal generator drives one beam (at frequencies close to  $f_{\text{res}}/2$ ), and the response of the second beam is measured with a spectrum analyzer (at  $f_{\text{res}}$ ). The contours represent the response in dBm. The synchronized regions become visible in the contour plots when the response exceeds the noise level of -136 dBm. One of the beams is driven at a frequency  $f_0/h$  while the response of the second beam is recorded. This could be fundamentally important to neurocomputing with mechanical oscillator networks and nanomechanical signal processing for microwave communication. Extracted from [68].

damping, clamping losses and coupling losses related to the transducing scheme. Air damping affects the vibration because the mechanical structure must displace some material in order to perform its movement. That is the reason why this contribution decreases when the pressure decreases [73]. In addition, a resonator can lose energy via acoustic coupling to its clamps [74], which can be minimized by engineering them, e.g. free-free beams present higher quality factors than clamped-clamped [75, 76] ones. The last contribution to the external losses can come from the transducers, so this contribution will be different depending on the read-out technique and it has to be studied individually as it has been done for magnetomotive detection [77] or for SET-based detection [78]. Internal losses can also be classified in two groups: losses generated in a perfect defect-less crystal and losses due to impurities and/or defects in the bulk crystal lattice structure and in surfaces. Within the former group, Thermo Elastic Damping (TED) [79] and Akhiezer effect [80] are setting a top limit for the Q. Surface defects are shown to be much more important than bulk ones as suggested by the quality factor decrease when increasing the surface to volume ratio [11, 81]. In addition, experiments led in ultra high vacuum (UHV) have shown that surface

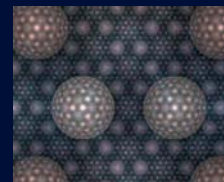
oxides, defects and adsorbates increase energy dissipation but, on the opposite, annealing under UHV increased the Q in one order of magnitude [71, 82, 83].

More recently, however, Craighead's group has shown that it is possible to increase the quality factor of a doubly clamped beam by increasing the tensile stress of its material (Figure 5 page 11, [84, 85]), in this case silicon nitride. Moreover, silicon nitride has additional advantages such as chemical inertness (difficult to oxidize) and high robustness (difficult to break).

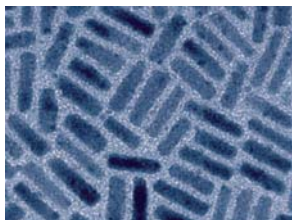
### 3.2. Modeling

On the modeling side, the major issues involve multi-scale problems, inclusion of quantum effects and incorporating the electric environment on individual device models (i.e. circuit modeling).

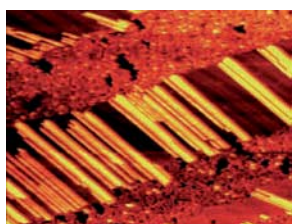
The first problem is exemplified by "sticking" which is an atomic scale phenomenon with a typical timescale in the femtosecond range ( $1 \text{ fs} = 10^{-15} \text{ s}$ ): the typical operational time scale of a device is in the nanosecond range ( $1 \text{ ns} = 10^{-9} \text{ s}$ ), and incorporating these two in a secure way is currently undoable from the point of view of simulation time. Even on a larger length scale, there are problems with the large fields in the small length scales:



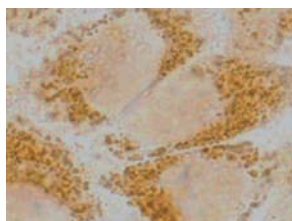
## MOLECULAR NANOSCIENCE



## SCANNING PROBE MICROSCOPIES AND SURFACES



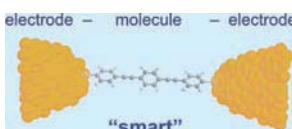
## NANOMAGNETISM



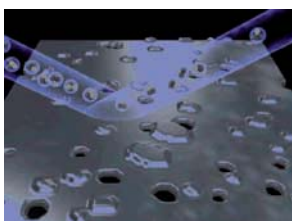
## NANOBIOSYSTEMS: BIOMACHINES AND MANIPULATION OF MACROMOLECULES



## NANOELECTRONICS AND SUPERCONDUCTIVITY



## SEMICONDUCTING NANOSTRUCTURES AND NANOPHOTONICS



## HORIZONTAL PROGRAM ON NANOFABRICATION AND ADVANCED INSTRUMENTATION



IMDEA-Nanociencia is a private Foundation created by joint initiative of the regional Government of 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), which is located in the campus of the Universidad Autónoma de Madrid, 12 km away from Madrid downtown with an excellent communication by public transportation with the Madrid-Barajas airport (25-30 min) and Madrid downtown (15-20 min).

The Institute offers attractive opportunities to develop a career in science at various levels from Ph.D. students to senior staff positions.



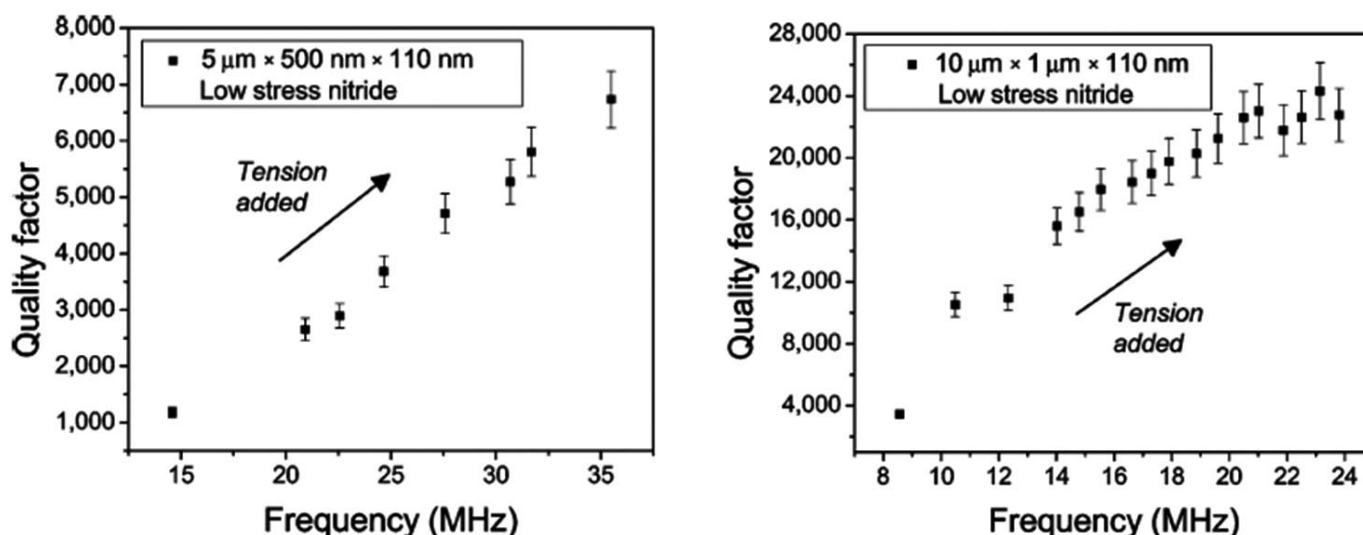
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**Figure 5:** Results of added stress on low-stress silicon nitride beams. A  $5 \mu\text{m} \times 500 \text{ nm} \times 110 \text{ nm}$  device with initial  $f$  and  $Q$  of 14.6 MHz and 1200 respectively was stretched to an increased  $f$  and  $Q$  of 35.5 MHz and 6700. A  $10 \mu\text{m} \times 1 \mu\text{m} \times 110 \text{ nm}$  device, with an initial  $f$  and  $Q$  of 8.6 MHz and 3400, was stretched to an increased  $f$  and  $Q$  of 23.8 MHz and 23000. The arrows indicate the direction of the experiments in which stress was added to increase both frequency and quality factor. Extracted from [85].

classical expressions such as  $Q^2/2C$  are meaningless if  $C$  is too small.

In addition, the basic theory and models only stand for simple beams or cantilevers. For more complex geometries, only Finite Element Modeling (FEM) is available. Dissipation mechanisms, electro/mechanical modeling and circuit architecture modeling are also important issues that need to be addressed and solved.

Finally, it would also be interesting to incorporate quantum effects in device models (e.g. describing the coupling between two closely-located nanoscale objects simply through capacitances is certainly incorrect but the only way to do it currently).

### 3.3. Transduction in the nanoscale

Actuation and detection (transduction) are two of the major issues when considering a mechanical system. By transduction we refer to the conversion of one type of energy to another type, e.g. converting the mechanical energy of an oscillator into an electronic signal that can be interpreted by subsequent circuitry.

Transduction has already been a "hot spot" for MEMS technology and different techniques became popular, e.g. optical detection (laser beam deflection, interferometry...) and electrical detection (capacitive, piezoresistive, piezoelectric, gate effect...). However, when moving down to NEMS, the transduction techniques are not as efficient because of the size reduction [86]. The optimal transduction technique should present actuation and read-out that strongly interact with the mechanical element but with really weak couplings between each other, a large operation bandwidth and ultrahigh sensitivity [11].

Optical detection is affected by diffraction effects, which limit the smallest size of the mechanical device. Some authors have shown successful extension of Michelson or Fabry-Pérot interferometers into the NEMS domain [87],

but the technique however is mainly convenient for NEMS-based force sensors (or surface stress) because their sizes are larger than the wavelength of the laser. On the other hand, optical actuation by means of photothermal effect or radiation pressure has been demonstrated [88-90], which makes this technique more interesting provided that a fully integrated scheme is accomplished. A transduction scheme that behaves properly for NEMS, both for detection and actuation is the magnetomotive technique [77], which involves the application of an external magnetic field and an AC current through the mechanical device. Therefore a Lorentz force arises, which will drive the mechanical element and, in addition, generates an electromotive force in the circuit that can be transduced as a read-out voltage. Highly sensitive measurements with very low noise have been made using this technique, e.g. zeptogram detection [15], hydrogen detection [91] and modes synchronization [68]. However, there are major drawbacks for this technique: (i) it cannot be integrated and (ii) very low temperatures and very high magnetic fields are required.

Piezoresistive detection is affected by the reduction of the resistors dimensions, which implies a huge resistance, meaning high Johnson noise and high losses by non-matching impedance. This issue is more important if we take into account that the piezoresistivity response of Si or Ge decreases with dopants concentration [92]. However, high resolution measurements have been performed using resonating piezoresistive structures with silicon resistors [23, 93]. It was at the beginning of 2007 when Roukes' group published some results which meant a cornerstone for this type of detection [22], using metallic resistors with a very low piezoresistive coefficient as transducers. In this case they were overcoming the initial issue of a low sensitivity with an ultra low noise and proper matching impedance, finally yielding an unprece-

dent ed resolution for a NEMS operating at room temperature and atmospheric pressure. On the other hand, electrothermal actuation using small metallic resistors has also been demonstrated [94] up to several MHz (1 MHz =  $10^6$  Hz) thanks to the small thermal mass of these devices. However, this technique features a major drawback in the sense that the resulting power dissipation is high and locally elevates the temperature which can be problematic for mass sensing and other applications. In forthcoming years, very small structures may feature novel interesting properties that could result in improved transduction schemes [95], as it recently happened for Si nanowires (Si-NWs, below 200 nm diameter) and their newly discovered giant piezoresistive effect [96].

Capacitive transduction, which is really convenient for MEMS as it allows a simple two ports detection and actuation scheme, is really affected by the size reduction, mainly because the dynamical capacitance changes, i.e. changes in the capacitance due to the motion of the resonator, are very low ( $10^{-18}$  F) and therefore are obscured by parasitic capacitances, that are some orders of magnitude higher. Some specialized measurement techniques have been developed [13, 97-99] in order to cancel the effect of those parasitic capacitances. Some other solutions involve the use of geometries allowing high capacitive coupling but still preserving NEMS properties [100] or using the resonator not only as a capacitor's plate but also as, e.g. the gate of a MOS transistor [35, 37]. Monolithic integration of capacitive NEMS with CMOS circuitry greatly enhances the detection efficiency [101, 102].

Less effort has been devoted to piezoelectric transduction, but it has also been explored both for sensing and actuating NEMS. The read-out is based on the measurement of the polarization fields caused by the vibration of the lever. Those changes in polarization can be detected by working at the location where the variation is the largest as the gate of a transistor [103]. In addition, this technique can be used to drive resonators, as has been recently demonstrated [104] by Roukes group.

Apart from the aforementioned techniques, it is possible to find several other techniques that are less conventional but that have proven to be useful or interesting in some cases and whose potential in some cases is still unknown.

Atomic Force Microscope has been used to detect the vibration amplitude of some systems with an unprecedented spatial resolution [105-108], although this is mainly limited to research samples. Detection of motion based on tunneling effect has also been used in many cases, in some cases pursuing monolithic integration [109] and in some other cases just seeking for the best transduction technique. This has been particularly successful in the case of CNTs, where a nanotube-radio has been built [110] and with which the detection of a single gold atom has been performed [19]. As for the actuation, an alternative technique could be Kelvin polarization force [111], which can be used on insulating materials, unlike electrostatic actuation.

### 3.4. Fabrication

As it has already been introduced, two different approaches can be chosen for NEMS fabrication, i.e. top-down and bottom-up. In the first case, there are three basic fabrication steps: the deposition of material (easy to go for thin layers down to 10-20 nm), the removal of material (by anisotropic Reactive Ion Etching, RIE, whose loss of lateral dimensions can be minimized down to the same amount of 10-20 nm) and the definition of the zones where the material is going to be deposited and/or removed. This last step is called lithography and the most standard is optical UV. Due to diffraction effects and to other particular considerations of each mask aligner, the lateral resolution achieved using this technique can barely reach 1  $\mu$ m. Therefore, as soon as one of the lateral dimensions of the structure goes into the sub-micrometer range, complications arise because nano-lithographic processes are needed. These lithographic processes (see Figure 6) can be either serial (more flexible) or parallel (higher throughput). Different examples can be EBL [6, 7], Direct Laser Writing lithography [112], AFM lithography [113], etc. for the serial approach; and DUV lithography [36, 37], NIL [114], nano-Stencil lithography [115], etc. for the parallel approach. Each of the lithographic processes mentioned present advantages and disadvantages which are discussed in detail here. However, if an eventual mass production is pursued, serial processes should be discarded. In fact, the major challenge from the fabrication point of view is not the selection of the optimum lithographic process but the achievement of a reproducible and stable fabrication process with a fair control of the final mechanical properties of the fabricated devices. As an example of how difficult it can be to attain such reproducibility, one can take the example of the most controlled fabrication processes, i.e. CMOS circuitry fabrication. In this case, transistors and circuits are generally working in a digital mode and therefore two states only have to be distinguished (0 or 1), and consequently there is a relatively large tolerance with the individual properties of each transistor. On the other hand, a very small variation in the length of a cantilever, e.g. 5 %, would become a variation of the resonant frequency of a 10%, which might result unacceptable in some applications.

For the bottom up approach the aforementioned problems also apply in some cases, as for example the growth of

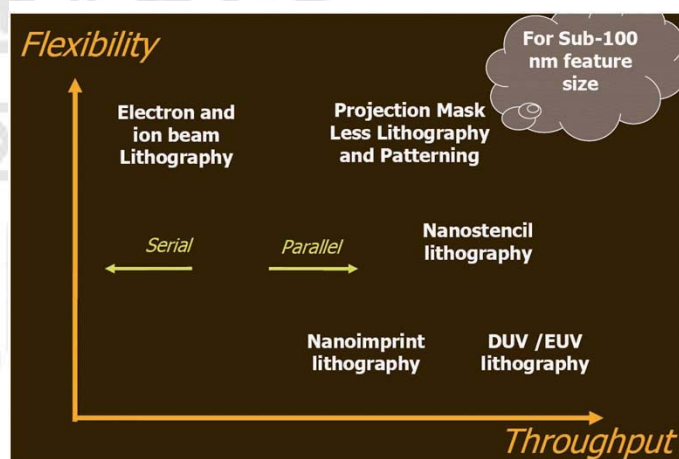


Figure 6: Scheme taken from [123] summarizing the different lithographic techniques for nano-patterning definition.



nanowires or nanotubes out of catalytic nanoparticles whose size must be controlled prior to growth. However, the main problem still remains the integration of the nanostructures with connections to the macro-world or even circuitry. Two approaches are followed to accomplish this integration. The first one involves the deposition of the catalytic particles on a substrate where the circuits (or similar) are already present, the growth of the CNTs [116] or the NWs [117-119] being subsequently performed. The second one involves the growth of the nano-elements in a separate substrate and then, with the use of electrical fields, placing them in between two electrodes [120-122].

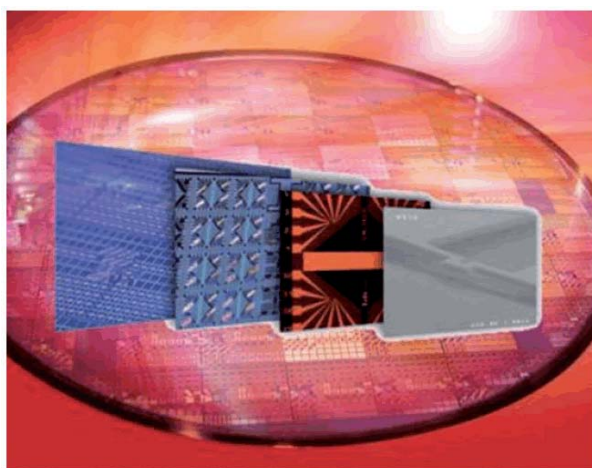
### 3.5. System Integration

Maybe the most important issue that NEMS are facing now and will be facing in the near future is how to turn these promising devices into effective, real systems. Most of the works we have referenced up to now can be considered as handcrafted and just facing the applications from a research point of view. There are still a lot of steps to overcome in order to make these 'stand-alone' resonators (with discrete electronics around them) evolve towards complete systems that can be produced in masse for an eventual commercialized application.

Integration of NEMS with CMOS seems to be one of the most promising approaches. One approach can consist in using CMOS steps to define the resonators and at the end finishing with a post-processing step to release the mechanical structures [36, 37, 124].

Industrial foundries are generally reluctant to this so-called In-IC approach since it can perturb the stability and the 'cleanliness' of the CMOS process. However, in a near future, this method could progressively become more applicable because of the increasing convergence between nano-transistors and NEMS in terms of size.

The other approach consists in post-processing pre-fabricated CMOS substrates in order to fully define the mechanical structures [113, 115]: this solution can be



**Figure 7:** Picture of the first 200 mm wafer fabricated within the "Alliance for NEMS-VLSI" [125]. In one single wafer, 2.5 million NEMS are included, which represents more than the total amount of NEMS fabricated during the previous 15 years. The process consists in a 4 lithographic levels with a hybrid DUV and EBL approach and all the devices present thermoelectric actuation and piezoresistive detection [22, 94]. Extracted from [126].

useful to reduce fabrication costs if an advanced CMOS is not available or required.

Up to now, the biggest step for the integration of NEMS as a system has been achieved by the collaboration between LETI-CEA in France and the California Institute of Technology (Caltech) in the US [125, 126] which are directly aiming at the large integration of NEMS into a system (Figure 7).

### 4. Conclusions

We have shown that NEMS have unique and useful properties that make them suitable for a plethora of different applications in various fields, ranging from Information and Communication Technologies (ICT) until bio-chemical detection, including some applications that are not yet known but that for sure will emerge together with the development of these systems. They have the potential to become a revolution for the market in the same way that MEMS have caused an enormous impact during the last 20 years. However, there are some important issues to be solved before NEMS can have actual applicability, e.g. integration of the mechanical part with circuitry into a complete system, reduction of fabrication costs in order to make them competitive against existing sensors, etc.

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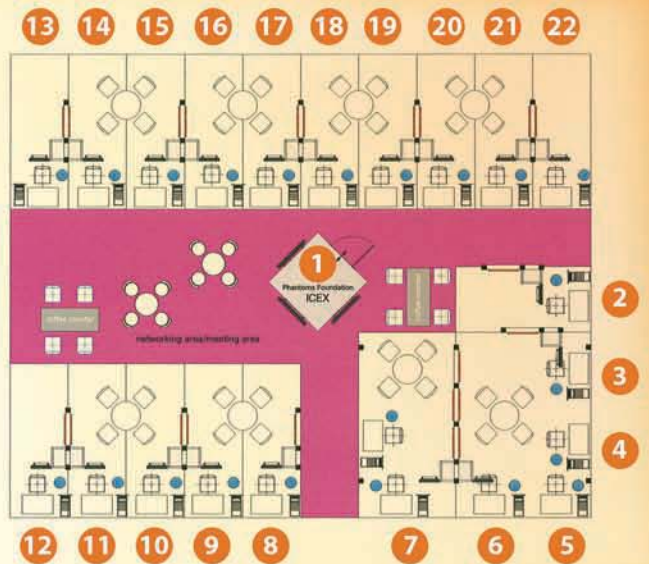


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- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- 9
- 10
- 11
- 12
- 13
- 14
- 15
- 16
- 17
- 18
- 19
- 20
- 21
- 22



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### ⌘ PostDoctoral Position (CNB-CSIC, Spain): *"Single Molecule techniques and their application to DNA break repair"*

Our group, holder of one of the European Research Council Starting Grants, has one Postdoctoral Open Position with an EU contract for two years to study the action of molecular machines involved in DNA repair at the single-molecule level. We use and develop Magnetic, Optical Tweezers, and Atomic Force Microscopy to unravel the mechanisms of action of nanomachines involved in Homologous Recombination and DNA-End joining pathways to repair DNA damage in bacteria. To do that, our group develops projects in collaboration with Dr. Dillingham group at University of Bristol.

**The deadline for submitting applications is April 28, 2009**

For further information about the position, please contact: Fernando Moreno-Herrero ([fernando.moreno.icn@uab.es](mailto:fernando.moreno.icn@uab.es))

### ⌘ PhD Position (CEA Grenoble, France): *"Atomistic modeling of the transport properties of semiconductor nanowires"*

Semiconductor nanowires are attracting much attention due to their promising properties and due to their possible applications in opto and nanoelectronics. The diameter of these nanowires ranges from a few to a few ten of nanometers, while their length can reach microns. These nanostructures provide many opportunities: for example, it is possible to vary the composition of the wires along their axis to introduce quantum dots or tunnel barriers whose width and position are well controlled. These nanowire "heterostructures" can then be connected to electrodes for charge transport measurements. Many such original experiments are being performed today to explore the potential of semiconductor nanowires for nanoelectronics.

**The deadline for submitting applications is April 26, 2009**

For further information about the position, please contact: Yann-Michel Niquet ([ylniquet@cea.fr](mailto:ylniquet@cea.fr))

### ⌘ PostDoctoral Position (CEA, France): *"Carbon nanotube-based flexible and high frequency electronic devices"*

The Molecular Electronics Laboratory has an open position for a postdoctoral fellowship. The contract is for 18 months and can start immediately. The Molecular Electronics Laboratory (LEM) is a multidisciplinary group of ~15 research scientists. It belongs to the Condensed Matter Physics (SPEC) department of the IRAMIS Institute (Institut Rayonnement Matière de Saclay), one of the Institutes for fundamental research of the CEA in Saclay (Paris area).

**The deadline for submitting applications is March 31, 2009**

For further information about the position, please contact: Vincent Derycke ([vincent.derycke@cea.fr](mailto:vincent.derycke@cea.fr))

### ⌘ PostDoctoral Position (CEA-Grenoble, France): *"Pattern directed chemical functionalization of silicon substrates"*

The Laboratory has an open position for a postdoctoral fellowship. The contract is for one year. The laboratory, in collaboration with two technological research oriented groups of the CEA, has been involved in Si functionalization related activities for several years. Hybrid Si molecules devices are fabricated in order to evaluate the possibility to use such technology to provide miniaturized memories. Surface functionalization procedures are optimized on large Si samples (~cm<sup>2</sup>). Then, in a second step, these methodologies are transferred to the functionalization of the Si cells (~100mm<sup>2</sup>) devices devoted to electrical characterizations to reach proof-of-concept parameters. Surface analyses (MIR-IR, XPS, ellipsometry) are performed at the Nanocharacterization Platform of Minatec.

**The deadline for submitting applications is March 31, 2009**

For further information about the position, please contact: Florence Duclairoir ([florence.duclairoir@cea.fr](mailto:florence.duclairoir@cea.fr))

### ⌘ PhD Position (DRFMC-CEA-GRENOBLE, France): *"Non-contact atomic force microscopy investigations of self-organized pi-conjugated molecular wires"*

Nowadays, near field microscopy techniques are essential tools for fundamental and technological research in the field of organic and molecular electronics. A thorough knowledge of the molecular conformation, self-organization and electronic properties on surfaces is indeed mandatory for the realization of electronic and optoelectronic devices with smart functionalities such as molecular-based nanometric organic field effect transistors (OFETs). The candidate must have a master degree in physics, and a great motivation to carry an experimental work in an interdisciplinary group, where physicists and chemists are working in close collaboration. A former experience in near field microscopies (STM/AFM) is not mandatory but some knowledge of basics concepts will be appreciated.

**The deadline for submitting applications is March 30, 2009**

For further information about the position, please contact: Benjamin Grévin ([benjamin.grevin@cea.fr](mailto:benjamin.grevin@cea.fr))

### NANO Vacancies - <http://www.phantomsnet.net/Resources/jobs.php>

#### ✦ **PhD Position (Institut de Ciència de Materials de Barcelona (ICMAB-CSIC):** *"Modification of Surfaces with Functional Organic Molecules"*

We are looking for highly talented and motivated graduate candidates for PhD positions. Candidates must hold an excellent university degree (Master) in Chemistry or Materials Science. An interdisciplinary outlook is desired and will be encouraged. Experience in organic chemistry and surface self-assembly will be positively valued. The successful candidates will be prepared to work in an international environment and travel to other European countries to develop the project.

**The deadline for submitting applications is March 14, 2009**

For further information about the position, please contact: Concepció Rovira ([cun@icmab.es](mailto:cun@icmab.es))

#### ✦ **PostDoctoral Position (Institut de Ciència de Materials de Barcelona (ICMAB-CSIC):** *"Modification of Surfaces with Functional Organic Molecules"*

We are looking for highly talented and motivated postgraduate candidates. Candidates must hold an excellent doctoral degree in Chemistry or Materials Science. An interdisciplinary outlook is desired and will be encouraged. Experience in organic chemistry and surface self-assembly is highly recommended. The successful candidates will be prepared to work in an international environment and travel to other European countries to develop the project.

**The deadline for submitting applications is March 14, 2009**

For further information about the position, please contact: Concepció Rovira ([cun@icmab.es](mailto:cun@icmab.es))

#### ✦ **PostDoctoral Positions (University of Liège, Belgium):** *"Two postdoctoral positions in Cancer Biology: Angiogenesis and lymphangiogenesis in mouse and zebrafish and The oxygen metabolism in pathological angiogenesis and particularly in pre-eclampsia"*

Two postdoctoral positions are immediately available in Professors Jean-Michel Foidart and Agnès Noël's lab at the Department of Tumor and Development Biology in the University of Liège (GIGA-cancer).

Research projects focus on 1) angiogenesis and lymphangiogenesis in mouse and zebrafish and 2) the oxygen metabolism in pathological angiogenesis and particularly in pre-eclampsia.

**The deadline for submitting applications is March 12, 2009**

For further information about the position, please contact: Agnès Noël ([Agnès.noel@ulg.ac.be](mailto:Agnès.noel@ulg.ac.be))

#### ✦ **PostDoctoral Position (Cincinnati Children's Hospital Medical Center, United States):** *"The role of stem cells in tumor development"*

Postdoctoral Fellow positions are available at the Cincinnati Children's Hospital Medical Center (CCHMC, Director: Christopher Wylie), Developmental Biology Department in the lab of Geraldine Guasch (<http://www.cincinnatichildrens.org/research/div/dev-biology/fac-labs/guasch/default.htm>) to investigate the role of stem cells in tumor development.

**The deadline for submitting applications is March 12, 2009**

For further information about the position, please contact: Geraldine Guasch ([geraldine.guasch@cchmc.org](mailto:geraldine.guasch@cchmc.org))

#### ✦ **Staff Scientist (CIC nanoGUNE Consolider, Spain):** *"nanoGUNE is welcoming applicants with an outstanding track record of research in electron microscopy"*

CIC nanoGUNE Consolider, located in San Sebastian, Basque Country (Spain), is a R&D center created recently with the mission of conducting basic and applied world-class research in nanoscience and nanotechnology, fostering training and education excellence, and supporting the growth of a nanotechnology-based industry.

At the present time, nanoGUNE is welcoming applicants with an outstanding track record of research in electron microscopy. While all professional profiles will be considered independent from the field of specialization, we are particularly interested in a "hands-on" type scientist, whose true expertise and passion is in leading-edge experimentation in the field of transmission electron microscopy. Proficiency in spoken and written English is compulsory; knowledge of Spanish is not a requirement.

**The deadline for submitting applications is March 15, 2009**

For further information about the position, please contact: Director ([director@nanogune.eu](mailto:director@nanogune.eu))



## NANO News - <http://www.phantomsnet.net/Resources/news.php>

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[http://www.nanospain.org/files/news/nanotech2009\\_press\\_release.pdf](http://www.nanospain.org/files/news/nanotech2009_press_release.pdf)

After a very successful 2008 edition, the Phantoms Foundation and the Spanish Institute for Foreign Trade (ICEX), in cooperation with the Embassy of Spain (Commercial and Economical Office) in Tokyo, will promote the Spain Pavilion at nano tech 2009, as an initiative under the program "España, Technology for Life".

Keywords: *Scientific Policy / Nanotechnologies*

☄ Nitrogen-doped carbon nanotube catalyst systems for low-cost fuel cells (05-02-2009)

<http://www.nanowerk.com/spotlight/spotid=9177.php>

Vertically-aligned nitrogen-containing carbon nanotubes (VA-NCNTs) produced by pyrolysis of iron(II) phthalocyanine (FePc, a metal heterocycle molecules containing nitrogen) could be used as effective ORR (oxygen reduction reaction) electrocatalysts.

Keywords: *Energy / Nanotubes*

☄ Nanotube memory flashes past silicon (05-02-2009)

<http://www.newscientist.com/article/dn16540-nanotube-memory-flashes-past-silicon.html>

A new design that is 100,000 times faster than previous efforts has paved the way for nanotube flash memory to be a part of future electronic and computing devices.

Keywords: *Nanotubes / Nanoelectronics*

☄ Building walls with bottom-up nanotechnology (16-01-2009)

<http://www.nanowerk.com/spotlight/spotid=9020.php>

New work by a team of scientists in Korea demonstrates the position- and shape-controlled growth of nanoarchitectures using the selective growth of nanowalls with conventional lithography and catalyst-free metal organic vapor-phase epitaxy (MOVPE).

Keywords: *Nanofabrication / Nanoelectronics*

☄ FET Newsletter Issue 04 (16-01-2009)

[ftp://ftp.cordis.europa.eu/pub/fp7/ict/docs/fet/fet-nl-04\\_en.pdf](ftp://ftp.cordis.europa.eu/pub/fp7/ict/docs/fet/fet-nl-04_en.pdf)



This issue contains interesting news stories from the world of FET - in particular, the announcement of the first-ever FET Conference, which will be held in Prague from 21-23 April 2009.

Keywords: *Nanoelectronics, Scientific Policy*

☄ Nano-welding facilitates bottom-up nanotechnology fabrication (12-01-2009)

<http://www.nanowerk.com/spotlight/spotid=8844.php>

Researchers at the University of Sheffield in the UK have now demonstrated the ability to reliably weld individual nanowires and nanoobjects into complex geometries with controllable junctions.

Keywords: *Nanofabrication*

☄ European Future Technologies Conference, Prague, Czech Republic (09-01-2009)

[http://cordis.europa.eu/fetch?CALLER=EN\\_PRESS\\_EVENT&ACTION=D&RCN=30302](http://cordis.europa.eu/fetch?CALLER=EN_PRESS_EVENT&ACTION=D&RCN=30302)



Under the title 'Science beyond fiction', the focus of this event will be on creating new visions and actions for future information and communication technologies (ICTs), based on the scientific opportunities which are available today.

Keywords: *Nanoelectronics, Scientific Policy*



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[http://cordis.europa.eu/fp7/ict/programme/fet\\_en.html](http://cordis.europa.eu/fp7/ict/programme/fet_en.html)

## NANO News - <http://www.phantomsnet.net/Resources/news.php>

### ⌘ Swedish scientists make breakthrough in nanowire growth control (05-01-2009)

[http://cordis.europa.eu/search/index.cfm?fuseaction=news.document&N\\_RCN=30298](http://cordis.europa.eu/search/index.cfm?fuseaction=news.document&N_RCN=30298)

Scientists in Sweden have discovered new ways to control the growth and structure of nanowires at the single-atom level. Their findings, which provide major insights into materials physics, have come out of the EU funded NODE project.

*Keywords: Nanomaterials, Energy, Nanofabrication*



### ⌘ Computing in a molecule (02-01-2009)

<http://cordis.europa.eu/ictresults/index.cfm?section=news&tpl=article&ID=90295>

Atomic-scale computing, in which computer processes are carried out in a single molecule or using a surface atomic-scale circuit, holds vast promise for the microelectronics industry.

*Keywords: Molecular Electronics*



### ⌘ Photonics emerges from the shadows (29-12-2008)

[http://cordis.europa.eu/ictresults/pdf/factsheet/INF70100\\_ICT\\_%20Results\\_Fact\\_sheet\\_08\\_November\\_PHOTONICS.pdf](http://cordis.europa.eu/ictresults/pdf/factsheet/INF70100_ICT_%20Results_Fact_sheet_08_November_PHOTONICS.pdf)

European study has documented a fast-growing sector of more than 2100 companies and 700 research laboratories that employs a quarter of a million people and is worth almost €50 billion a year.

*Keywords: Nanophotonics & Nano-Optoelectronics*

### ⌘ IBM Scientists Develop World's Fastest Graphene Transistor (19-12-2008)

<http://www-03.ibm.com/press/us/en/pressrelease/26302.wss>

IBM Researchers announced that they demonstrated the operation of graphene field-effect transistors at GHz frequencies, and achieved the highest frequencies reported so far using this novel non-silicon electronic material.

*Keywords: Nanoelectronics, Graphene*

### ⌘ Measuring conductance of carbon nanotubes, one by one (15-12-2008)

<http://www.physorg.com/news148580751.html>

A team of Cornell researchers has invented an efficient, inexpensive method to electrically characterize individual carbon nanotubes, even when they are of slightly different shapes and sizes and are networked together.

*Keywords: Nanoelectronics, Nanotubes*

### ⌘ Intel to produce 32nm chips (10-12-2008)

<http://www.physorg.com/news148134336.html>

Intel Corp., the world's biggest computer chip-maker, said Wednesday that it has developed a manufacturing process that shrinks the circuitry in a chip to just 32 nanometers.

*Keywords: Nanoelectronics, Nanotechnology Business*

### ⌘ EU funded nanoICT CA publishes two position papers on carbon nanotubes and modelling at the nanoscale (09-12-2008)

[http://www.phantomsnet.net/nanoICT/files/nanoICT\\_Press-release%20\\_Dec08.pdf](http://www.phantomsnet.net/nanoICT/files/nanoICT_Press-release%20_Dec08.pdf)

E-Nano newsletter 13th issue contains two position papers from the EU funded nanoICT Coordination Action corresponding to the Working Groups on carbon nanotubes and modelling at the nanoscale, areas currently very active worldwide.

*Keywords: Nanotubes, Theory & Modeling, Scientific Policy*



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[http://cordis.europa.eu/fp7/ict/programme/fet\\_en.html](http://cordis.europa.eu/fp7/ict/programme/fet_en.html)



## Mono-molecular electronics on a surface: challenges and opportunities

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### 1. Introduction

Technology continues to produce functioning transistors on ever smaller scales. The day will come soon, however, when there will not be enough atoms on the surface of a semi-conductor to define the structure of a transistor and, consequently, of complex electronic circuits. At this stage, new approaches and new technologies are necessary for building computers, memory or telecommunication devices [1]. Anticipating this challenge, researchers in a few laboratories around the world are now looking for the maximum number of atoms required to fabricate, for example, a calculating unit able to perform a computation by itself. This problem of creating an atom based technology is not limited to electronics or to telecommunication and encompasses all types of devices, including mechanical machines and transducers.

Meeting the atom technology challenge for ICTs requires new understanding in four now well identified fields of science and technology:

1. Learning the kinds of architectures for molecule-machines (or atom surface circuits) which will permit to perform for example complex logic operations stabilized at the surface of a solid where the required interconnection will be constructed.

2. Creating a surface multi-pads interconnection technology with a picometer precision, respecting the atomic order of the surface which is supporting the nano-system assemblage.

3. Cultivating molecular surface science accompanied with molecule synthesis (respectively atom by atom UHV-STM fabrication on a surface).

4. Creating a packaging technology able to protect a functioning atom-technology-based machine, while at the same time insuring its portability.

Those 4 topics were discussed during the 1<sup>st</sup> nanoICT mono-molecular electronics Working Group meeting in Toulouse, France between the 8<sup>th</sup> and the 10<sup>th</sup> of December 2008.

### 2. The architecture

Molecular devices i.e. hybrid molecular electronics are on the agenda of the micro-electronics roadmap since the seminal Aviram-Ratner paper in 1974 [2]. Until the turn of the century, such a futurist possibility of using molecules instead of solid state devices for electronics was just considered as a game for exploring the limits of calculating machines and memory devices. Approaching the end of the ITRS roadmap, things are now changing. Thanks to an intense experimental and theoretical effort, molecular electronics has now positively evolved from concepts to the first measurements and comparison with calculations [3]. There is now a real shift towards the full integration of a computing power in a single and the same molecule i.e. the mono-molecular approach [4]. This is now followed by exploring also the possibility of using atomic circuit fabricated on the surface of a passivated semi-conductor surface for implementing quantum dot based computer approach [5] and may be one day a mixture of both approaches.

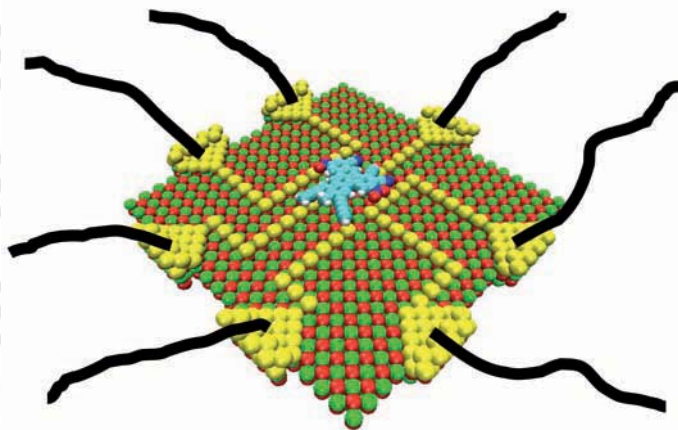
The different possible architectures for a single molecule (or an atomic circuit) to compute include the design of single molecule circuits in a standard electrical architecture, electronic wave-like atomic or molecule circuits located on the surface of a semi-conductor or quantum Hamiltonian like computing architectures. All those approaches are now studied by quantum chemistry software able to take into account the surface electronic structure, the interconnects and the local quantum structure of the computing circuit. Let us take the simple example of a logic gate. There are 3 ways of designing a logic gate at the atomic scale:

(1) The use of surface missing atom to fabricate an atomic scale circuit mimicking the topology of a macroscopic electronic circuit. Those surfaces are generally passivated semi-conductor surface with a relatively large gap. Atoms are extracted one at a time to create a specific surface electronic structure in the electronic surface gap. This new electronic structure will form the surface atomic circuit [6]. The STM vertical manipulation of the single surface atoms

can automated and proceed in parallel.

(2) The full molecule, instead of the surface can be the electronic circuit. In this case, it is the  $\pi$  system of such an extended molecule which will define the circuit and the  $\sigma$  skeleton will ensure the full chemical stability of the molecular architecture [7]. Such a molecule will have to be directly chemisorbed to the required number of nano-metallic pads or in a very dedicated approach to surface atomic wires more able to interact with specific part of the  $\pi$  molecular orbitals.

(3) Molecular orbitals (from a large molecule or defined from a specific surface atomic circuit) can be manipulated by chemically bonding on a  $\pi$  conjugated board specific chemical groups able to shift the corresponding molecular states [8]. Switchable lateral group can be very active playing donor or acceptor group to modify very locally the nodes distribution of a give molecular orbital. Such an effect can be used to design single molecule logic gate (See **Figure 1**) without forcing the molecule to have the topology of an electrical circuit [9].



**Figure 1:** A possible surface implantation of a molecule logic gate. The presented molecule fi adder was designed following a Quantum Hamiltonian Computer approach [9]. The interconnection architecture is constructed using metallic atomic wires. The logic inputs are located directly on the molecular board, supposing 2 switchable chemical group current driven inputs.

Solutions (1) and (2) have been proposed long ago but are not very compatible with the quantum level where those atom circuits or molecule logic gate are supposed to work. For solution (3), a quantum Hamiltonian design of AND, NOR and even fi adder logic gates have been designed followed by proposal of chemical structure functioning on the manipulation of molecular orbitals [9]. Extreme care has to be taken here for the optimisation of the chemical structure of those molecule-gates taking into account their future adsorption for example on a passivated semi-conductor surface [10]. In particular, the optimisation of the electronic contact between the surface atomic wires and the molecule will be obtained by selecting with care the chemical composition of the end group of the molecule [11] for running current through the gates with the objective to reaching peak values in the range of 10 to 100 nA. All those architectures give us an indication of the rich-

ness of quantum behaviour to design molecule like logic gate up to the complexity of a digital 2 by 2 full adder. At the Working Group meeting, the question was: to what extend the complexity of such a logic function embedded in a single molecule or in a small amount of dangling bond created on purpose on a surface can be increased up for example to a  $N \times N$  full adder. There is no theoretical answer yet to this question. But the interesting fact is that a careful quantum design will certainly shift up the elementary unit of a logic circuit from the transistor level to the logic function level. For example, no gain at the gate level is required in the Hamiltonian logic gate approach. This will simplify a lot the interconnections. But at the same time, cascading the building block at the logic gate level will certainly require some power gain. This will consequently increase the complexity of the interconnection procedure in between the logic gate units. The quantum designer will have to define the most interesting building block complexity (of course beyond the transistor) to find an optimum between the computing power on board of a molecule and the required interconnects. There is no solution yet for designing dynamic memory cell at the atomic scale.

### 3. N-Interconnects

Creating ultra precise interconnects on a single molecule has often been a bottleneck for molecular electronics [4,12]. But there are now two well-known avenues to realize a full interconnection scheme depending if the supporting surface is a small or large electronic band gap semi-conductor. The first tentative characterization of a single molecule switch was reported already in 1988 using the HV-STM machine [13]. Since then, a lot of progresses have been accomplished using the end atom of the STM tip apex as a pointer to contact one atom [14], one molecule [3,15] and to practice single atom or molecule manipulation [16,17]. The first measurement of the conductance of a single molecule was realized in 1995 using an UHV-STM machine [3].

In parallel, nanolithography has been developed to quit the vertical STM interconnection configuration for a fully planar configuration. In year 2001, what is considered now as the nanolithography limit was reached. The world record of an inter-electrode distance of 2 nm was obtained between 2 metallic nano-electrodes fabricated on a silicon oxide [18]. But this nanotechnology technique was progressively abandoned because (1) it is limited to a maximum of 2 to 3 electrodes [19] and (2) the use of resists and chemical in the process to define the nano-fabricated pattern is not clean enough with respect to the size of a single molecule and the order of the surface atoms. As a variant, break-junctions are also now used because of the very unique precision in the tuning of inter-electrode distance [12,20]. But it was analysed by the participants of the meeting that this fantastic technique will progressively be abandoned because there is no way to determine the number of molecule in the junction, because the conformation of the molecules located in this junction is unknown and because it is difficult to foresee a multi-





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nano-electrodes version of the break junction technique.

In 1999, a new planar nano fabrication technique, the nanostencil was introduced in an attempt to solve the surface cleanliness problem [21]. Then, nanostencil was proposed as a new way to interconnect electrically a single molecule. Nanostencil has a great advantage over nanolithography because it is supposed to preserve the atomic cleanliness of the surface supporting the planar interconnection electrodes. By varying systematically all the parameter of the nanostencil technique, including the testing of a large variety of surfaces from SiO<sub>2</sub> to NaCl or mica, it was demonstrated that on the good surfaces, this technique reaches its limits in the 20 nm range with no possibility to master the atomic structure at the end of the so fabricated nano-pads [22].

Facing this interconnection problem, lab scale experiments were performed: the fabrication of a pseudo-planar interconnection on metal surface taking benefit from native mono atomic step edge and designing specific Lander molecules with legs to level up the molecular wire as compared to the mono atomic step edge [11,15,23]. Those low temperature UHV STM experiments unambiguously demonstrated the need for an ultra clean atomic scale mastered interaction between for example the molecular wire end and the conducting contact entity [24].

Following the Working Group discussions, it seems that all the standard planar interconnection strategies explored since the end of the 80's like e-beam nano lithography, nano-imprint and Nanostencil will soon be abandoned. A new surface science approach respecting the exact atomic order of the surface with an interconnection precision better than 0.1 nm between the atomic wire (or the molecular wire) and the atomic scale pads will have to be developed. This challenge triggers a new approach for interconnects, a formal generalization of the technique developed at Bell labs in the 50's to interconnect a bar of a Germanium semiconductor material (See **Figure 2 page 29**). At that time, 4 probes measurement were practiced using 4 metallic tips approaching the semiconductor bar under an optical microscope. The bar was manipulated by micro metric screws together with the tips and stabilized by metallic springs [25].

In our days, atomic scale interconnection machines are starting to be built in a few labs around the world. There are basically low temperature (LT) UHV machines made of 3 LT UHV interconnect separated chambers, one for the atomic scale preparation of the supporting surface, one for single atom or molecule manipulation and one for the atomic scale to mesoscale or more interconnection procedure. Depending on the surface, the navigation on the surface is still using an optical microscope completed by a

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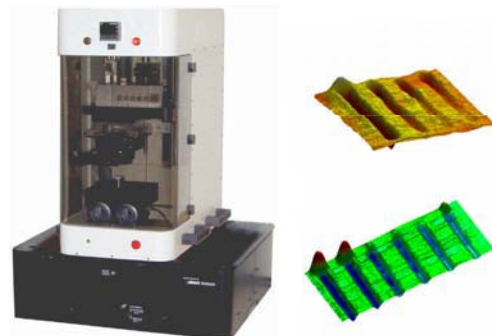
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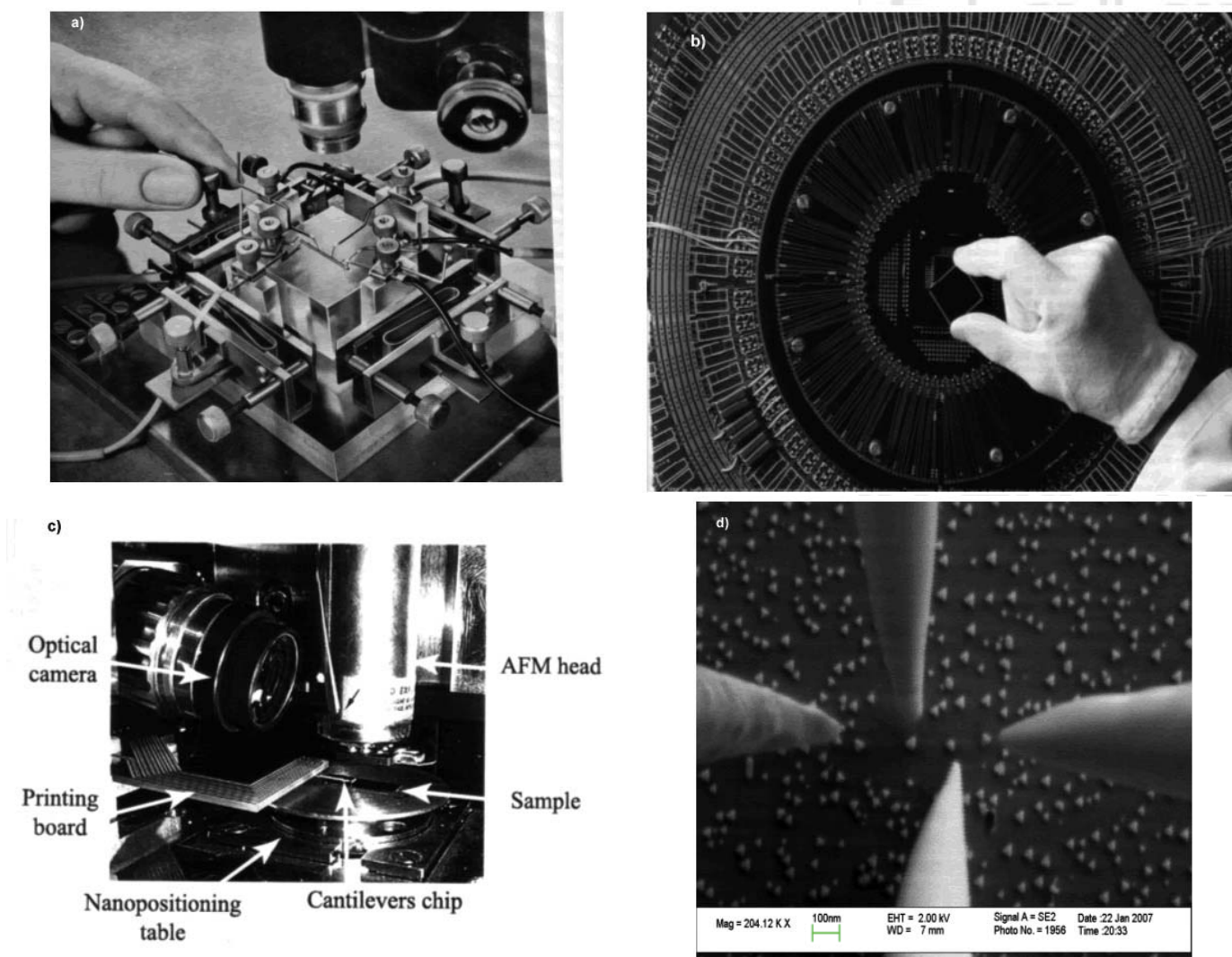
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**Figure 2:** History of planar multi-electrodes interconnects. (a) 1950's Bell Labs system equipped with an optical microscope and 4 electrodes for germanium interconnects [25]. (b) the 20<sup>th</sup> century multi-probes chip interconnects technology (courtesy of IBM). (c) A new generation of interconnection system involving an optical microscope plus an AFM microscope using 10 metallic cantilever positioned under the AFM head [28]. (d) A more recent version where the optical microscope had been substituted by an UHV scanning electron microscope and the metallic cantilevers substituted by nanoscale apex STM tips [26] (courtesy of the A\*STAR VIP Atom tech project, Singapore).

NC-AFM for a large surface electronic gap (See Fig. 2). For small gap passivated semiconductor surface, the navigation is ensured by an UHV-SEM with a resolution generally around a few nanometers (See Fig. 2). For the nano interconnection step, well faceted and ultra flat metallic nano-island are now in use. Those nano-interconnect pads are positioned at will with an 0.1 nm precision on the surface using the manipulation ability of the STM [26]. For the nano to meso and more interconnection stage, one technique for small gap semiconductor is to use multiple conducting STM tips in a top or back surface approach. For large gap surfaces, the nanostencil technique can still be used at its 20 nm in width limit and in its dynamic form [27].

Those interconnection machines are so new that it is not clear how one can build up a roadmap to anticipate how many contacts it will be possible to achieve. In the case of multiple STM tips positioned under the SEM, 4 is the actual limit for stability of the interconnects (See Fig.2).

For the optical microscope-NC-AFM case, 10 seems to be a good number [28]. There is here clearly a need to roadmap the computing power capacity increase embedded in a single molecule or with a surface atomic circuit and the number of possible interconnects converging towards this ultra small computing unit [19]. For example, it may happen that a well designed molecule offers too much computing power locally in regards with the maximum number of interconnects that one can physically be achieved in parallel on a surface. Then, a multiplexing like approach may be more appropriate, asking for more bandwidth and pushing the technology towards optical interconnects. Thus, efforts should be made in the future to extend experiments which aim to combine optics and local probe microscopy in an ultra clean environment with a prospect of a fully planar technology.

#### 4. Atom and Molecule Surface science issues

The stabilization of an atomic scale computing machinery

## Research

on a surface (be it self stabilized by its chemical structure or by the surface itself) requires a gigantic effort in exploring the properties of a large molecule of a surface at the atomic scale. During the Working Group meeting, a lot of questions were asked starting from the choice of the surface. Of course, the discussions were targeting lab scale logic gate handling and interconnects. For a fully packaged molecule logic gate, a more realistic choice of surfaces is actually out of the range of what can be discussed (see the corresponding section below).

Depending of the atomic scale interconnection machine to be used, a first delicate problem is the choice of the supporting surface. A list of criteria were discussed during the meeting: the electronic surface gap, the stability of the atomic surface structure, the stability of metallic nano-island on the surface. For example, we know 2 extreme cases of passivated semi-conductor surface: SiH(100) and MoS<sub>2</sub>. SiH(100) has a surface gap around 2.1 eV. The surface H atoms can be vertically STM manipulated one at a time to create p dangling bond like surface atomic wires or Hamiltonian computing structures [5,6]. But depending on the bulk doping, those H surface atoms are not so stable with temperature which precludes a thermal growth process to shape the contacting metallic nano-island. The lamellar MoS<sub>2</sub> compound has a self passivated semi conducting surface with a surface gap around 1 eV. The surface S atoms are extremely difficult to vertically STM manipulate [29]. But if manipulated, they

also offer the possibility to create surface atomic wires with a band structure much more complicated than the SiH(100) [30]. The surface MoS<sub>2</sub> surface is extremely stable up to 1200 °C [31] and metallic nano-pads can easily be shaped and manipulated to construct any multi-electrode interconnections pattern with an atomic scale precision [26]. But the low surface gap of this material will certainly preclude its direct use as a supporting interconnection surface. A better exploration of the surface properties of diverse semi-conductor surfaces (See for example **Figure 3 page 31**) and their possible passivation is here urgently needed.

Large electronic gap surface are even less explored than their semi-conductor counter parts. The nice property of those surfaces is the fact that leakage surface current between 2 metallic nano-pads adsorbed on the surface will be very low, well below the fA range, an advantage as compared with the above mentioned semi-conductor surface. The drawback is that there is no easy solution to fabricate or stabilize atomic wire on those surfaces. During the Working Group meeting, two solutions were discussed to bypass this problem: the use of molecular mold to stabilize metallic atomic wires or the use of long molecular wires between the metallic nano-pads and the central computing units. This second solution may be a good way to boost the research on long molecular wires characterized by an extremely small tunneling inverse decay rate [32].

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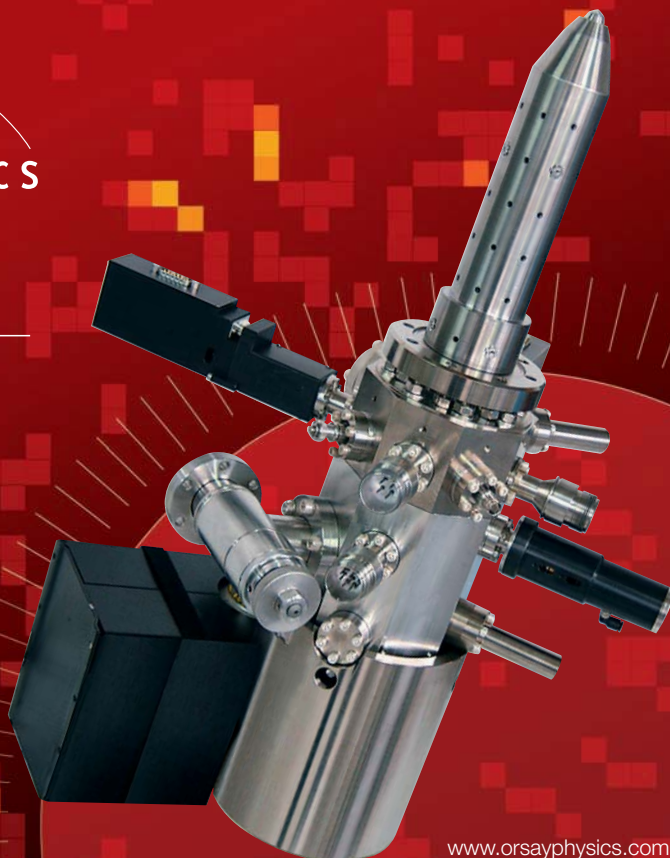
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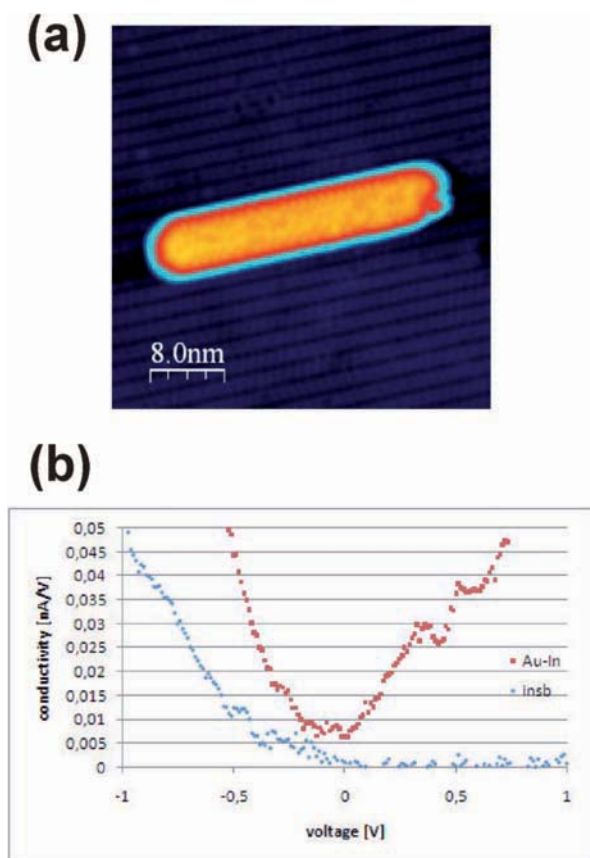
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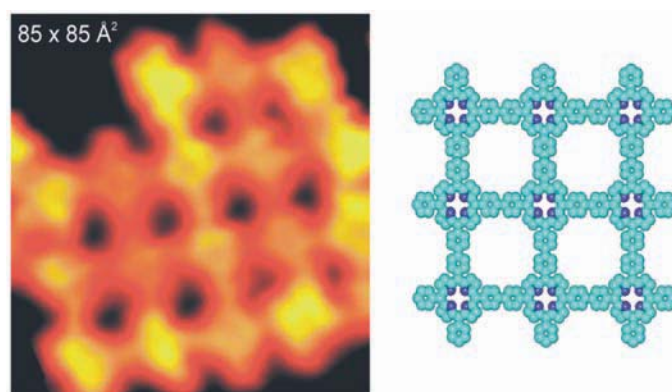


**Figure 3:** Exploring the surface science of interconnects: fabrication of Au nanowires on the InSb(001) surface in the UHV to be interconnected on a Fig. 2D UHV interconnection machine. (a) High resolution STM image of Au alloy nanowire formed on InSb(001) surface by a good selection of the surface annealing temperature. Bias voltage:  $-0.5\text{V}$ , tunnelling current:  $25\text{pA}$ . (b) STS conductance measured using an STM tip as a function of bias voltage on an Au alloy nanowire (red dots) and directly on the InSb substrate (blue dots) (Courtesy of the Jagiellonian University, Krakow).

Graphene, the new comer was also discussed in Toulouse as a mean to pass directly from the mesoscopic to the atomic scale with a “perfect” chemical like continuity between the 2 scales. This will be another choice of surface self supporting the interconnection and the computing unit. The open question is whether or not progresses in the fabrication techniques will allow an atom by atom fabrication technique respecting the absolute atomic scale precision required for such a circuit [33].

It is also not clear how far can we go by playing with a single and large molecule adsorbed on a surface be it the one of a semi-conductor or of a bulk insulating materials. There is the difficult challenge of sublimating of a large molecular weight molecule on a surface in an ultra clean manner respecting the integrity of the molecule [34]. May be better to perform the chemistry in situ sublimating only the monomers and playing with them after to construct or assemble the final large molecule (See **Figure 4** and [35]). It remains to be explored if such an approach can be performed for example at the surface of a semi-conductor.

Discussions in Toulouse about molecular surface science indicate how far we are from a very good understanding of molecular processes and behaviors of a large molecule on



**Figure 4:** Playing with single molecules on a surface. Instead of sublimating a large molecule on a surface, it may be better to bring first the monomers and to make them self reacting with each others by controlling the spontaneous 2D diffusion. STM image (left) of a molecular network on a Au(111) surface with the corresponding scheme (right). The network is grown from single porphyrin (TPP) molecules monomers (“on-surface-synthesis”) by forming covalent bonds between the individual building blocks [35].

a surface at the atomic scale. There is here a wide range of understanding and know how which need to be acquired before creating a full atomic scale technology for molecular computing.

## 5. Packaging

At the nanoICT meeting, packaging was not on the official agenda. Off site discussions about packaging indicate that we are far from being ready to study those questions simply because even the lab scale interconnection machines are just about to be assembled. Packaging is always associated with the number of interconnects which have to be stabilized with the encapsulation technology selected for the circuit [19]. There is not yet a clear path on how to create a packaging technology for surface mono-molecular electronics. A specific mono-molecular NanoICT seminar may be dedicated in the future to this very strategic problem. But it is so advance and so strategic [36] that it may turn out to be very difficult to trigger an open discussion about packaging.

## 6. Conclusion

The first mono-molecular nanoICT Working Group seminar was the occasion to cluster in a very Cartesian way all the 4 major issues under grounded in the mono-molecular approach of molecular electronics. In all areas of technology, the construction of a complex system by assembling elementary pieces or devices leads to a Moore’s law like trend when analyzing the complexity growth of the system per year, a trend which appears threatened in the near future for microelectronics. The mono-molecular approach of molecular electronics with its compulsory atomic scale technology offers way to push past possible limitations in miniaturization, and to gain further increases in computing power by orders of magnitude by relying of a full development of an atom or molecule based technology for both electronics and machines. To

## Research

reach this stage, each of the 4 issues well identified during this seminar will require a specific discussion and more than that a specific research and technological development program.

### Acknowledgements

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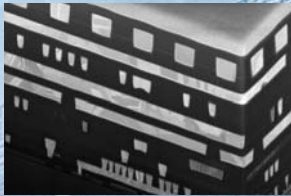
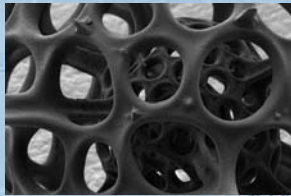
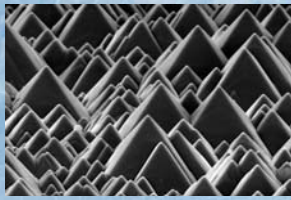
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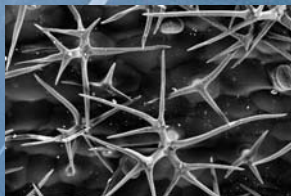
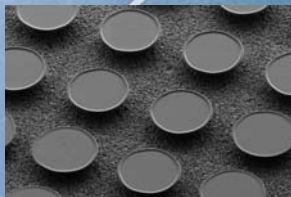
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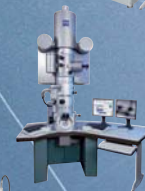
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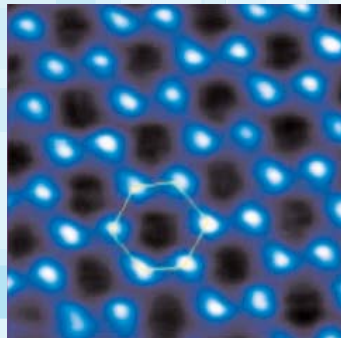
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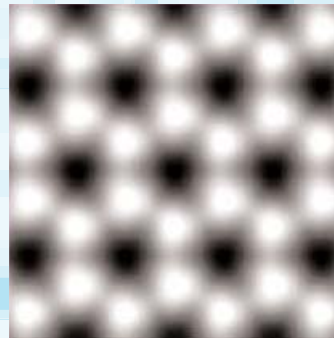
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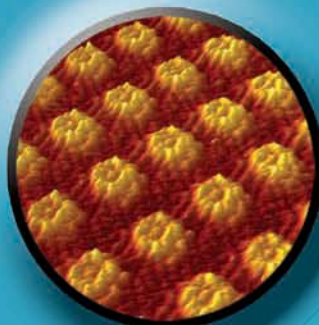
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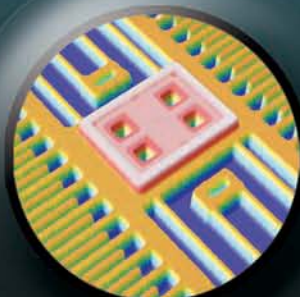
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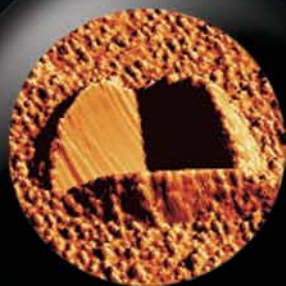
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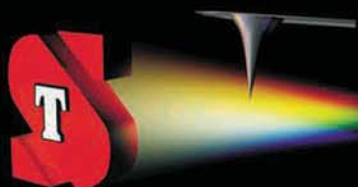
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