e nano newsletter

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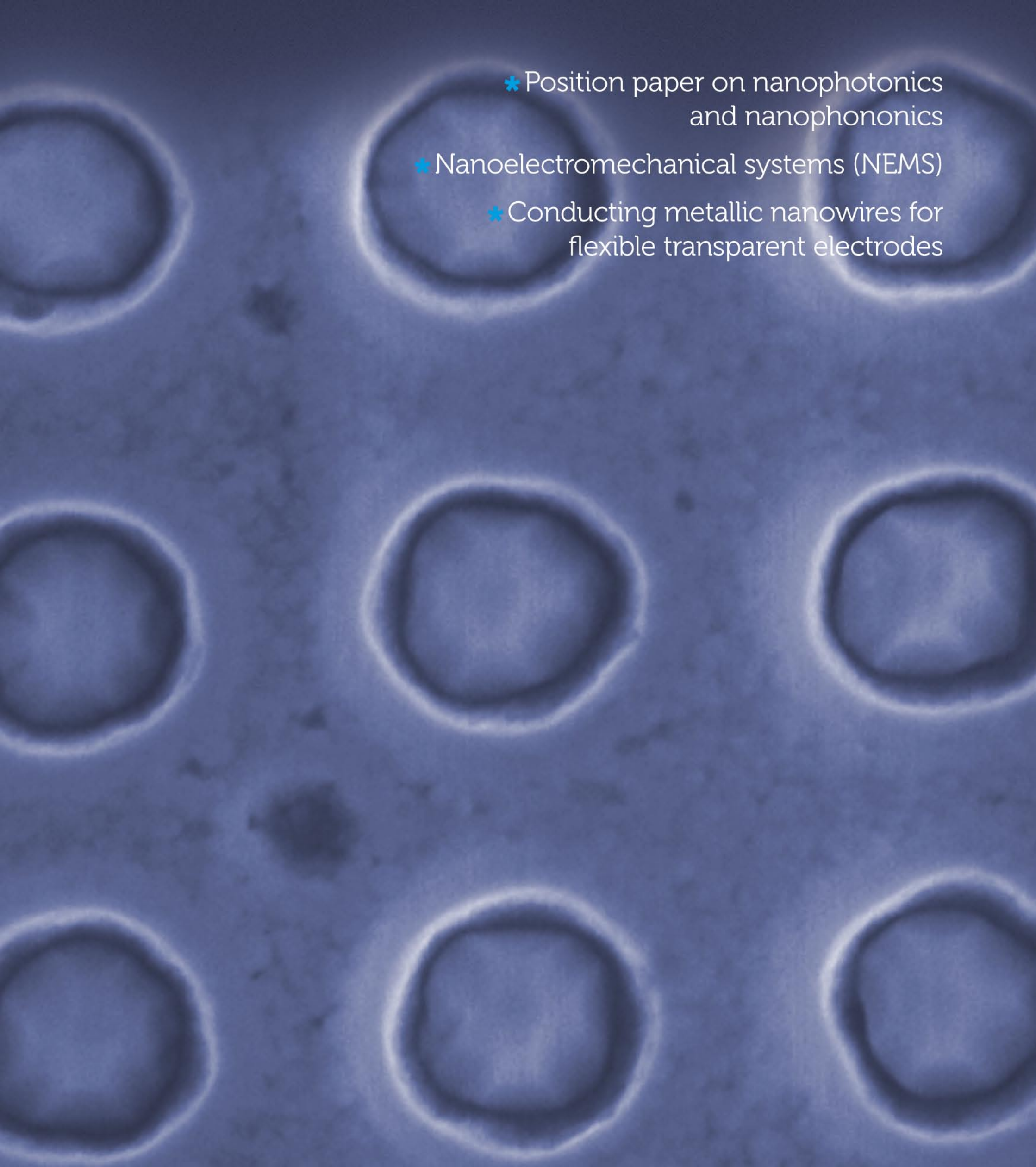
- Position paper on nanophotonics and nanophononics
- Nanoelectromechanical systems (NEMS)
- Conducting metallic nanowires for flexible transparent electrodes



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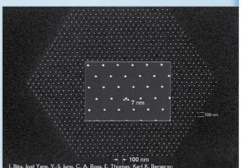
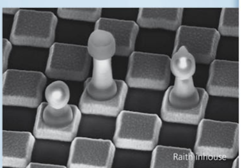


Ultra high resolution template for directed self assembly of block polymers



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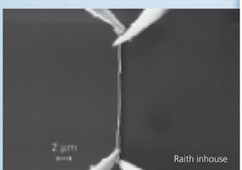

Direct 4-contact nanoprobing of an Au-capped Ni/NiO_2 nanowire

write

view

multi-application

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 appears 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 Nanophononics / Nanophotonics.

In previous issues, other topics such as Nanowires were also reviewed (see nº 17/18). In this edition, an article on "Conducting metallic nanowires for flexible transparent electrodes" is presented providing new insights in this relevant topic.

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).

2011 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.

> Dr. Antonio Correia Editor - Phantoms Foundation

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Position Paper on Nanophotonics and Nanophononics

CONTENTS

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Executive Summary

Nanophotonics and Nanophononics are knowledge areas essential for the development of novel technology and products in ICT, Energy, nanomanufacturing, environment, transport, health, security and several others. Photonics is recognised as a Key Enabling Technology and nanophotonics is likely to be at the base of the next wave of photonics innovation. Nanophononics is becoming more and more visible as the “energy issue” rears its head virtually in all research and development fields. In particular, heat transfer in the nanoscale is more than just thermal management since it underpins the science of fluctuations and noise, needed to develop knowledge at the system level all the way to quantum processes in biology, and is at the heart of information generation and transformation.

This latest NANOICT project position paper complements on the nanophotonics part, those previously published by the MONA and PhOREMOST projects and the recent one by the Nanophotonics Europe Association. It is probably the first one of its kind in the nanophononics field.

Concepts and technologies provide a base for the research topics in this document. In particular, scalable nanofabrication methods are presented, such as III-V semiconductor growth on Si, nanoimprint lithography, roll-to-roll printing and self-assembly, as potential enabling technologies in future value chains.

Cost and thermal management issues in nanophotonics appear as main concerns as far as integration and packaging is concerned. These are recognised as becoming acute

problems when going to the nanoscale and much of the heat transport science in the nanoscale is still at the basic research stage. Nevertheless, as progress is being made towards heterogeneous integration using nanoparticles and nanoscale materials, both issues acquire an urgent dimension in time if Europe will remain a main player in the next and (next+1) technology generations in ICT.

As the feature size goes from micrometres to nanometres, variability arising from several factors becomes crucial to reliability. Thus concepts developed in adaptive integration approaches, would control the impact of variability even during operation of optical circuits. Likewise, the missing link in Si photonics, namely a Si-based source, is closer than ever to meet the challenge of integration and performance. Special materials and nanostructuring techniques, aided by advanced and computation-intensive design, are seen as paramount to control the distribution of optical energy in nanoscale energy devices, metamaterials and non-linear nanophotonic structures to make photon management a reality.

Nanophononics forms a relative new research field, although related research topics tackling problems at macro scale have been around for some years. With reducing dimensions, understanding of thermal phenomena at microscopic level is becoming more and more important and new approaches are needed for modelling and simulations and for experimental methods. For example, thermal management at packaging level may not be enough for IC's in near future. Instead one has to solve heat dissipation related problems at device level, including fluctuations and non-linear phenomena. Thus, there is a need to amalgamate the currently somewhat fragmented activities and strengthen the research in of nanophononics in Europe.

Recommendations

1) Targeted European-level support for *fundamental research in application-relevant nanophotonics and nanophononics focusing first on common issues,* for example, heat dissipation at component level, using noise in ICT and ways to cope with the fluctuations in key parameters. The latter bound to be a more serious issue in the nanoscale than in the current micrometre scale but crucial for heterogeneous integration.

2) Bring together the experimental and theoretical communities of phonon physics, heat transfer (mechanical) engineering, statistical physics, biology (fluctuations), nanoelectronics, and (solid-state) quantum communications to start with a *focused research programme on heat control in the nanoscale in the first instance and on, e.g., harvesting fluctuations* as a follow-on or parallel focus.

3) A research infrastructure for *emerging cost-efficient nanofabrication methods* jointly with a multi-level simulation hub and a comprehensive nanometrology associated laboratory targeting nanophotonics and nanophononics applications, complementing the Si and the III-V photonic foundries. This infrastructure could then evolve into a potential foundry, with industrial participation, covering combinatory lithography, cost-analysis, packaging and training.

4) Targeted European-level support for research on ***material sciences*** to develop techniques able to achieve material control at the sub-nanometre and, in particular, in 3-dimensions. This includes, e.g., control of multilayer thickness of silicon-rich silicon oxide and of the barrier dielectric at the wafer scale level.

Foreword

This position paper is the result of an informal consultation among the contributing scientists, who acted on their personal capacity. It originates in the activities and discussions of the EU project NANOICT (www.nanoict.org) in the working groups Nanophotonics and Nanophononics.

On the nanophotonics part, discussions stared early in 2002 when it became known that the European Commission would be calling for a new "instrument" in FP6, the Networks of Excellence (NoE). Researchers then working in nanophotonics became members of several related networks, going through expressions of interests, full proposals and then the execution of the project themselves. One of them was the NoE "Nanophotonics to realise molecular scale technologies" (PhOREMOST) **(www.phoremost.org).** PhOREMOST started its discussion in 2002 preparing its expression of interest. The NoE was active from October 2004 until December 2008, when it evolved into the Nanophotonics Europe Association **(www.nanophotonicseurope.org).** A similar development took place with the NoE on Metamaterials which evolved into the virtual institute METAMORPHOSE.VI **(www.metamorphose-vi.org).**

Concerning nanophononics, an informal meeting was held in October 2005 at Commission's premises with representatives of the NMP and ICT, including ICT FET) priorities and the participation of Jouni Ahopelto (VTT), Clivia M Sotomayor Torres (then UCC Tyndall National Institute) and Bruno Michel (IBM Zuerich). This and other follow up initiatives, such as workshops and stimuli from outside Europe, helped to trigger the ICT FET proactive initiatives Towards Zero-Power ICT and MINECC. Among such contributing events and reports one can highlight the International Workshop on the Future of Information Processing Technology edition 2005[1], the report of the USA Semiconductor Research Council (SRC) to the MEDEA/ENIAC workshop in Montreux held on 22nd September 2006[2],which had phonon engineering among the top five most important research priorities for the SRC, and others.

Many discussions on the progress of the science and technology of both nanophotonics and nanophononics have taken and are taking place in a myriad of conferences, workshops and schools. In Europe we count with the series of the School Son et Lumiere[3], the conference series Eurotherm[4], the CA ZEROPOWER[5] and more recently with the workshops on Phonons and Fluctuations[6] among others.

This is a first non-exhaustive attempt to condense what researchers think are priorities and hot topics in both nanophotonics and nanophononics. Nevertheless, the views expressed here have been distilled from those of the contributors and are the sole responsibility of the editors.

We thank our colleagues and hope this paper is one step towards strengthening the European Research Area.

Clivia M Sotomayor Torres
Barcelona, December 2011

Jouni Ahopelto
Espoo, December 2011

1 Introduction

The NANOICT Coordination Action Nr. 216165[7] has as one of its missions to document the state of the art and trends in research areas related to the overlap between nanoscience and nanotechnology in ICT. It does so by gathering and publishing position papers in several areas, namely, nanowires, MEMS, carbon nanotubes, molecular electronics, theory, graphene and simulation, among other. All of which can be found in the project website.

At the start of NANOICT research areas such as nanophotonics had a smaller profile than, for example, MEMS/NEMS or nanoelectronics. Some even did not even have a name, such as nanophononics. The situation has changed dramatically since then, calling for a position paper on nanophotonics and nanophononics.

This is an attempt to document not so much the precise state of the art, but the scientific questions or key issues and the trends in some areas of both, nanophotonics and nanophononics. In nanophotonics, two examples of scholarly work are recommended: one by S. Gaponenko[8] and the other by Novotny and Hecht[9].

There have been a few recent reports covering areas of nanophotonics. One of these is the EU project MONA, which published a Roadmap on Nanotechnology and Optics[10] published in 2007. This was complemented by the roadmap of the EU Network of Excellence "Nanophotonics to realise molecular-scale technologies" (PhOREMOST) entitled "Emerging Nanophotonics", published in 2008[11]. Last November, the Nanophotonics Europe Association[12] (NEA) organised a Foresight exercise and the outcome was published as "Nanophotonics a Foresight Report"[13].

Why a position paper of nanophotonics and nanophotonics?

From the perspective of the editors, there is a need to consider some questions: What has been developed in these fields and to what level of maturity? What area has a higher probability of making an impact in the 5 to 15 year scale needing nanostructuring and nanopatterning down to controlled 10 nm feature sizes? Which are the potentially scalable nanophotonic technologies suitable for industrial production? Which will contribute to make a reality the ambition of photonics as a key enabling technology in a measurable time scale?

To date there is no public roadmap in nanophononics and yet a range of issues at the forefront of research in nanoelectronics, photonics, information technology, signal processing, depend heavily on phonon-mediated interactions.

Indeed, nanophotonics and nanophononics are closely related as we will show in the next pages and is the reason for combining these two topics in a single position paper.

To start with, the possibility to control heat transport by light has been demonstrated by Meschke et al.[14] who showed that at low temperatures in solids heat is transferred by photon radiation and the thermal conductance approaches the unique quantum value G_Q of a single channel. They studied heat exchange between two small pieces of normal metal, connected to each other only via superconducting leads, which are ideal insulators against conventional thermal conduction.

Mechanical vibrations have been recently coupled to photons in optomechanical crystals, leading to greatly enhanced light-matter interactions and facilitating new sensing applications and signal processing approaches.[15]

Mediated by careful design of band structures and density of states, the possible light-heat interaction points to a challenging and promising approach to handle information in nm-scale heterogeneous integration, where the matching of otherwise different length scales is enabled using, for example, plasmonic antennas.

In the language of ICT, the information is carried by state variables, charge, photons and other quasi-particles called state variables or "tokens"[16]. Tokens are exchanged in information processing operations and they do not have to be the same. They can be fermions or bosons or have mixed-character.

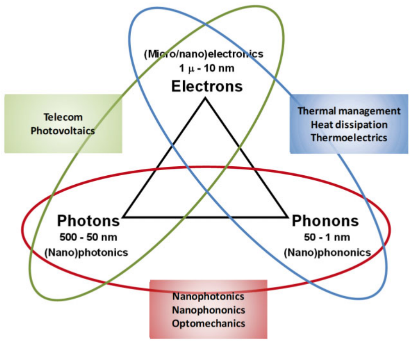

Fig. 1 > State variables for information processing. The length scales in the diagram also reflect the dimensions needed to manipulate the particles/waves./

It is broadly agreed that photonics cuts across several fields and the same holds for nanophotonics. Photonics is an intrinsic part of More than Moore and Heterogeneous Integration as in the ENIAC Strategic

Research Agenda and now the Vision, Mission and Strategy document[17]. In fact, the National Science Foundation workshop series documented in the Nanotechnology 2011-2020 report[18] included nanophotonics in the sections on Nanophotonics and Plasmonics, Metrology, Energy and Nanoelectronics.

Europe enjoys a strong, but not necessarily leading, position in nanophotonics and nanophononics, but the situation is precarious in view of the strong initiatives elsewhere, such as the USA multibillion dollar programs on Centers of Excellence in Basic and in Applied Energy Research. Europe is strong in some research areas including Si photonic integrated circuits (PICs), metamaterials, nanofabrication and nano-scale thermal transport, but the link to the value chain is at best weak since crossing the "valley of death" still has a very low success probability. It is expected that having Photonics labelled as a Key Enabling Technology[19], and the growing number of interaction among interdependent Technology Platforms, will improve the situation. The same is not so obvious in the fragmented academic research.

The academic communities are relatively well established and galvanised around, eg, the European Technology Platform Photonics 21 and the national mirror platforms, several networks of excellence, research infrastructure consortia and associations, eg, METAMORPHOSE VI, NEA; also in professional organisations such as the European Optical Society (EOS), to name but a few. Exciting new developments with a tremendous potential, mainly at conceptual level, eg., in transformation optics[20], need to be tested for the possibility of becoming a technology.

Activities, mainly academic at the moment, in nanophononics include the recently established network on "Thermal Nanosciences and Nanoengineering", led by Sebastian Volz, summer school Son et Lumiere community, Eurotherm meetings and ESF Network on Statistical Physics. Few recent ICT FET projects in FP7 have been addressing nanophononics related issues, including the CA ZeroPower, which focuses on energy harvesting. The integrated Project NANOPACK in FP7 also partially covered nanophononics. Altogether, a fragmented community which, while advanced in its specific areas, does not yet appear as a cohesive community like nanoelectronics and nanophotonics.

We conclude this document with recommendations concerning the research areas included in this report.

2 Concepts and technologies

2.1 Concepts

The main concept in common is the wave picture of photons and phonons in a finite or semi-infinite media. In reality these media can be periodic or semi-periodic and be described in reciprocal space in terms of Brillouin zones and energy bands. The dependence of these bands as a function of wavevector is called dispersion relation of the photon or phonon in that medium. The realisation of artificial nanostructures and or layered material to tailor the dispersion relations is termed dispersion relation engineering. Random nanostructures offer also advantages in novel nanophotonics as will be seen below.

The significance of dispersion relation of electrons and photons in solids as far as device-relevant properties are concerned is associated with the material properties directly related to these dispersion relations, including the effective mass, group velocity, band gaps and ultrarefractive (slow wave) properties.

Dispersion engineering has made major advances including, a significant reduction of optical losses, now down to a few dB/cm, and their understanding of a number of exciting demonstrations of nonlinear effects (see 3.5). The key advantage of the nanophotonic approach is the ability to balance material and structural dispersion in an intelligent way, allowing to control either a very large bandwidth, e.g. for supercontinuum generation[21] or a very small bandwidth for cavity-enhanced nonlinear optics, as in the project LECSIN.

Concepts belonging to solid state physics, optics, mechanics, statistical mechanics, non linear physics, quantum optics and chemical physics, among others, are brought in to use localisation, confinement, cavities or resonators, waveguiding, etc., in most of the applications of photons and, in the future, phonons in practical devices and systems.

2.2 Nanofabrication methods as enabling technologies

In Europe there are consortia which have over the years successfully achieved the setting up of a Silicon photonics platform[22] and a III-V, specifically InP, Components and circuit platform[23] accessible to academic groups, research organisations and SMEs.

It is argued that the key contribution to be made by "nano" is the reduction in switching power. Typical microphotonics achieves pJ/bit, whereas nanophotonics can do fJ/bit. It can be safely argued that power reduction is what drives the entire field.

While the Si and III-V foundries include growth, design, material and device characterisation, processing of devices and sometimes full circuits, there is one gap and that is in packaging. Information on their activities and research activities is in the respective project web pages.

Moving to integrated III-V semiconductors on Si an example is given below on the work at KTH. Since growth methods of Si and III-V separately are well documented and since the top-down nanofabrication as well, in this section we include less well known nanofabrication methods which have been singled out because of their promise and existing demonstrators.

III-V on Si for Si nanophotonics

This is an example of III-V growth on Si based on nanopatterning and selective area growth (SAG). Many electronics providers incorporate photonics to widen applications in several sectors. Hitherto bonding of III-V devices on Si has been successfully demonstrated for integrated silicon photonics. But the industries realize that in the long run heteroepitaxial solutions will be essential. This also would lead to innovative research in the field of generic, nanoscale monolithically integrated photonics-electronics on silicon. It is expected that low cost, scalable manufacturing processes of silicon can be extended to incorporate III-Vs and other related semiconductors. Epitaxial lateral overgrowth of III-Vs on Si using nanopatterns can be one of the approaches to filter defects and obtain high quality layers. Recently, it has been demonstrated that quantum dot templates can be fabricated through SAG on Si.

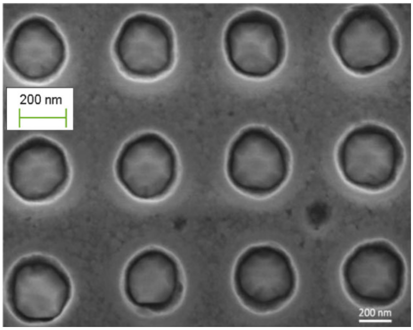

Fig. 2 > InP nano-pyramid templates grown on Si at KTH through nanoimprinting and SAG.[24]/

Applications: Masks for etching components, direct patterning of passive photonic components based on polymers and metals, microcavities, band edge lasers, waveguides, photonic crystals, polarisers, blue ray devices, memories, metamaterials, optofluidic and lab-on-a-chip devices, organic solar cells, diffractive optical elements, OLEDS and OFETs and anti-counterfeit structures.

Nanoimprint Lithography

Nanoimprint lithography (NIL) is a polymer patterning technique, based on a temperature-pressure cycle (thermal NIL) or a UV exposure-pressure one (UV-NIL). NIL is now used to pattern feature sizes of less than 30 nm in industrial applications for magnetic recording and diffractive optical devices, while structuring polymer films down to the 10 nm level has already been reported[25]. NIL is a radiation-free mask fabrication for pattern transfer and for directly patterning polymer, plain or functionalised, thus functionalising via material choice and patterning. It is a parallel or step-and-print technique which lends itself for volume production. Using appropriate overlay and stacking techniques, multiple layers can be processed. Furthermore, overlay accuracy down to 30 nm has been achieved using Moiré interferometry.

In the context of nanophotonics, patterning 2-dimensional photonic crystals in polymers loaded with light emitting centres close to a patterned metallic layer, has shown enhancement in the light extraction efficiency larger than a factor of 10, compared to unpatterned metal-free polymer films doped with emitting centres. This effect has been explained by a coupling effect of plasmons and excitons[26]. The possibility to realise 3-dimensional patterns is currently undergoing intense investigation. One major achievement has been the printing of 300 mm wafers using UV-NIL with a throughput of 20 wafers per hour, cf. 80 wafers/hr in the semiconductor industry[27].

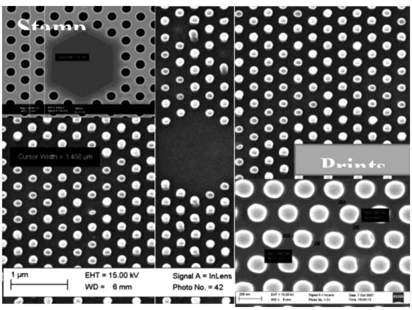

Fig. 3 > SEM micrographs of stamps and prints of a polymer microcavity. The stamp (top left) is a triangular array of holes with a pitch of 300 nm and hole diameters of 180 nm. The imprints were made on dye doped polymers. © V. Reboud (ICN, CEA LETI), to be published./

Applications: Masks for etching components, direct patterning of passive photonic components based on polymers and metals, microcavities, band edge lasers, waveguides, photonic crystals, polarisers, blue ray devices, memories, metamaterials, optofluidic and lab-on-a-chip devices, organic solar cells, diffractive optical elements, OLEDS and OFETs and anti-counterfeit structures.

Roll-to-Roll nanoimprinting

Recent nano manufacturing technology has advanced to the stage where inexpensive printing of high-performance devices on continuous rolls of polymer-based substrates promises to revolutionize advanced manufacturing. Roll-to-roll (R2R) processes will make it possible to generate high value-added technology products economically, at meters-per-minute rates on plastic film, paper and foil achieving feature sizes as small as 10 – 100 nm over areas containing millions of identical devices. In fact, R2R manufacturing of optical and electronic devices is increasingly progressing from the laboratory to the factory floor. For example, the potential of roll-to-roll nanoimprinting (R2RNIL) has been demonstrated in, e.g., fluidic devices, display illumination devices and printed electronics. A recent development is the production of transparent conducting electrodes using graphene for touch-screen panels by R2R[28] in a web of 30 inches. Feature sizes of 100 nm can easily be reached when a flexible mould is used in continuous R2RNIL as a part of the manufacturing process[29].

Many nano-applications, such as OLED, TFT, nanofluidic device and protein patterning have been proposed[30] and are the target devices for R2R nanomanufacturing, and while low-cost fabrication of anti-reflection films has been demonstrated[31], a high volume manufacturing methods is still needed.

Interest in R2R is also becoming strong in other countries: In the USA, a recent workshop on Roll-to-roll technologies and prospective applications took place last September where bottleneck and applications were discussed among academic, industrialist and government agencies[32].

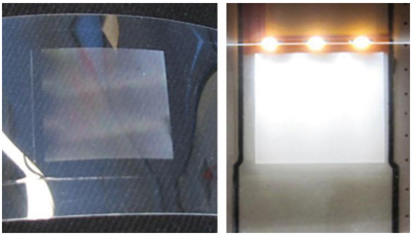

Fig. 4 > Optical micrographs of roll-to-roll nanoimprinted, transparent 3 cm x 3 cm size backlight device. The device consist more than 60 000 optical binary grating elements. The quality of elements influence directly the light diffraction of the device and therefore excellent edge quality is needed (T. Mäkelä et al, VTT Microsystems and Nanoelectronics, to be published)./

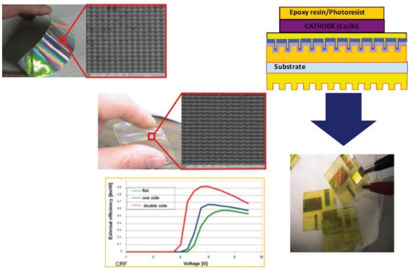

Fig. 5 > An example of a double-sided printed OLED structure with feature sizes below 1 µm consisting of a high efficiency LED with substrate patterned on both sides by roll-to-roll and NIL. The device exhibited 65% external efficiency. (V Lambertini, T Mäkelä and C Gourgon, unpublished data)./

Applications: Low-cost manufacturing, displays, optical sensors, sensing, fluidics, solar cells, photovoltaics, diffractive and plasmonic nanostructures, touch-panel screens.

Self-assembly

Self-assembly techniques are researched as alternative to electron-beam lithography and interference lithography. They have been identified as a research need in the ENIAC SRA 2007[33] but were absent in the Multi-annual Plan of the ENIAC Joint Undertaking[34], reflecting that self-assembly is a research area with applications envisaged beyond the five-year time frame.

Scalable self-assembly combined with soft lithography has been shown to produce several cm square of ordered nanoparticles in monolayers as well as in patterns[35]. This has been taken to the limit of nanoparticle printing with single nanoparticle resolution in well specified sites[36].

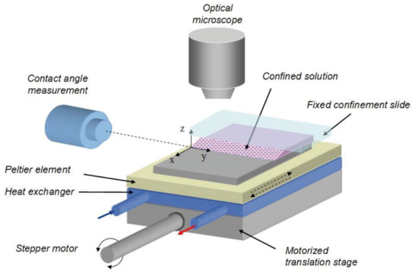

Fig. 6 > Illustration of the experimental setup developed for controlled convective and capillary assembly of particles on surfaces. The assembly is performed by dragging the liquid meniscus of a colloidal suspension droplet between a fixed slide and a moving substrate actuated by a stepper motor. The temperature of the substrate is controlled by a Peltier element. (after ref 35 © American Chemical Society 2007)./

The use of silicon patterned substrates to engineer the capillary flow has resulted in the self assembly of 3-dimensional photonic crystals in a process which is fully scalable and compatible with silicon fabrication[37]. Efforts towards developing methodology as a measure of quantitative order have been demonstrated[38].

Recent development in self-assembly include directed self-assembly of di-block copolymers in order to reach the sub 20 nm size regime. The FP7 project LAMAND[39] investigates the use of this nanofabrication approach for scalable high resolution nanopatterning for ICT.

Applications: heterogeneous integration, opto-biotechnology, environmental sensor, medical sensors, artificial nano-scale materials, bio-circuits, energy harvesting, artificial tissues and organs, high resolution lithography.

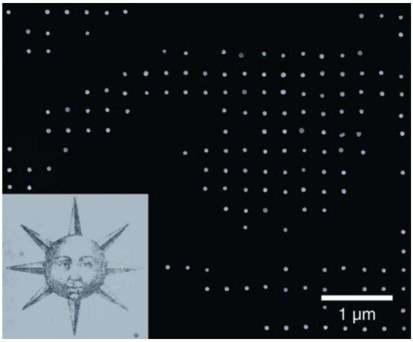

Fig. 7 > Optical micrograph (inset) and SEM image of 60 nm Au nanoparticles positioned by capillary assembly and transferred to a silicon wafer (after [40] © Macmillan 2007)./

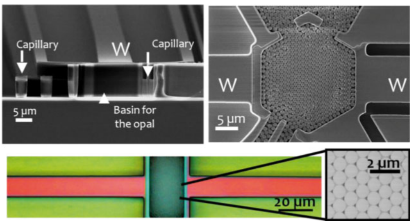

Fig. 8 > Top left: Cross-sectional view of the capillary channels entry points. Top right: Sub-micrometre spheres deposited using capillary forces in an optimised pattern in a basins and waveguides fabricated in Silicon. Bottom: Waveguide and 3D photonic crystals by self-assembly © S. Arpiainen and J. Ahopelto, VTT. Further details in reference 37 (Arpianen et al)./

2.3 Conclusions

Novel concepts in nanophotonics have been slow to appear as commercial products and probably the main reason is the long and hard way denoted by Photonics21 as the "valley of death". Sophisticated concepts carry with them special terminology which is poorly understood outside a small circle of specialists who, in addition, interact little with the rest of actors in other parts of the value chain. An effort is needed in making as realistic as possible projections of these new concepts so that targeted programs can be set up. An invaluable European asset is the creativity of a large nanophotonics community in Europe working in photonic crystals, nanoplasmonics, non-linear optics and metamaterials, to name but a few.

Concerning nanofabrication technologies, the emphasis in cost is balanced by the improved performace of nanophotonic structures and, in the future, of nanophononic ones.

In general, they all need high resolution lithography, be electron beam or deep UV lithography at some stage. These are already used in the Si and III-V photonics foundries in work to prove and up-scale device and circuit concepts and architectures. They are also needed for stamp (mould) fabrication of masters for UV and thermal NIL, R2R and directed self assembly[41], which offer the versatility needed in heterogeneous integration, among others. One way to lower costs is to improve master replication for these techniques and research in new materials and methods for this are essential. Completing the value chain in Si and III-V nanophotonics must consider the ability to test a set of generic packaging concepts when fabricating devices, an area of research activity which will need serious investment in such platforms, perhaps co-financed by stake holders.

A common research need in nanofabrication for nanophotonics and nanophononics is encompassed under the field of dimensional (nano)metrology. The importance of this cannot be over emphasised: nanometrology[42] is the link to test the validity of simulations and critical dimensions needed for a specific function. Nanometrology is an ubiquitous factor defining the uptake of a new product and or technology. But the dimensional nanometrology methods and tools have to be non-invasive, cost efficient and have the capability of being used in-line, use efficient data file size, since these have to be transferred quickly across a factory platform for measures to be taken in case of unacceptable deviations. Thus dimensional (nano)metrology is a key step in the way to overcome the valley of death. Once we have metrology under control, participation in European Standards bodies, and there are maybe too many, and in the Intelligent Manufacturing Systems (IMS)[43] program discussions on standards, will become an easier task.

Below some of the more specific key issues and research needs are mentioned.

Heteroepitaxy: To be useful it is necessary to achieve defect-free growth of thin III-V on Si to allow the integration of components on Si. This will need not only advanced epitaxial growth but also advanced characterisation and simulation. For advanced heteroepitaxy large area nanopatterned substrates are perceived as a bottleneck but perhaps NIL and interference lithography can meet this need.

Nanoimprint lithography: The bottleneck is the cost of stamps and stamp wear. While the former could in principle be solved by stamp replication, the latter needs chemical treatments and or new materials developments to allow 1000s of prints without changing an anti-adhesive coating on the stamp. Work is still needed in nanorheology and in improving our understanding of demoulding forces for a rich variety of designs[44]. For this time-efficient simulations are needed[45]. One of the most promising research areas if combinatory nanofabrication, for example combining NIL and or flexoprinting and or gravure and self-assembly, which will enable much progress in heterogeneous integration.

Roll-to-Roll printing: Going to sub 20 nm feature size and or alignment accuracy remains a huge challenge, specially the alignment procedures which, as part of quality and yield process control, constitute a go-no go type of milestone. For this, in-line metrology is required with application-defined tolerances to print complete devices on a platform. Furthermore, registration of multiple layers on flexible substrates is another milestone.

Self-assembly: Since this method uses liquids, although not in all its variants, control of convection forces and surface energy is an important issue. Moreover, quantification of order and metrology is required here, in addition to dimensional, chemical and biological metrology, depending on the nature of nanoparticles or moieties being assembled. While some routes are envisaged for dimensional metrology down to 3 nm, biological and chemical metrologies lag significantly behind. Methods to ensure and control ordering by, e.g., use of external fields[46] are likely to help achieving high levels of order in self assembled structures. The control of classical and quantum fluctuations inherent in liquid processes is an area of research which is wide open and has probably the highest return in process know-how. Last but not least, the scalability of self-assembly as a nanofabrication technology remains to be demonstrated.

3 Nanophotonics

While this is a position paper on European research it is helpful to look at other attempts to prioritise research in nanophotonics. One of this was the EU-NSF Workshop on Nanotechnology 2020 (nano2), which took place in Hamburg in June 2010, one of the four global workshops organised by the NSF and the NNI. The conclusions of the Photonics and Plasmonics session came up with the following important applications and goals for 2011-2020:

- The all-optical chip
- Metamaterials operating in the visible
- Single-(bio)molecule detection
- Artificial photosynthetic systems for energy conversion

One point emphasised several times was that progress will depend on key access to state-of-the-art computational tools, optical and structural characterisation tools and 1 nm precision nanofabrication.

In this section we focus on topics which have been left out or treated briefly in other position papers.

3.1 Integration of nanophotonics in Si Photonic circuits

In Europe the integration of photonics into silicon technologies is pursued within European, national and industry-led, projects, by researchers at universities, research organisations and few SMEs. There are several approaches to integrate Si nanophotonics in photonic integrated circuits. Two examples are those of IBM and of the University of Ghent/ IMEC. Luxtera, ST Microelectronics and Intel, among others have their own approaches. In the IBM concept, routers based on ring oscillators[47] have been proposed, while the IMEC/Ghent approach is less explicit about the work-horse of the optical layer but contains the key layers of thermal, electronic, photonic and sensing functions.

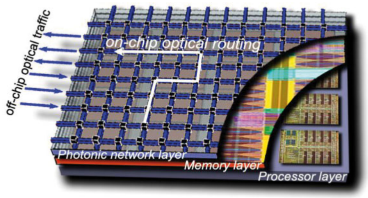

Fig. 9 > Artist impression of a 3D silicon processor chip with optical IO layer featuring an on-chip nanophotonic network. From: www.research.ibm.com/photonics/

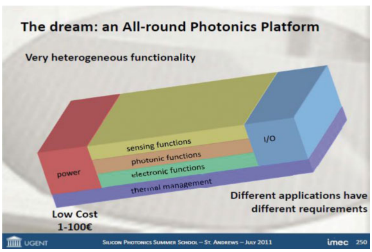

Fig. 10 > One approach to an all-optical circuit (From: W Bogaerts, Photonics Research Group, Ghent Univ - IMEC, Silicon Photonics Summer School July 2011 St Andrews)./

In what follows examples will be given of research areas which have not been included in the recent NEA report or that here are presented from a different angle. Not all of them are strictly speaking nanophotonics but bring with them opportunities for nanophotonics to be deployed there.

3.2 Adaptive Integration Photonics

Heterogeneous integration technologies and miniaturization allow a wider functionality and complexity of circuits, but complexity needs control. Moving from single devices to complex photonics circuits, an overall management of all the building blocks and constitutive parts is mandatory, especially in view of the convergence between photonics, electronics and bioscience. Parameters deviation from ideal values due to fabrication tolerance, functional drifts induced by aging, mutual crosstalk effects (thermal, optical, electrical) must be corrected either in the manufacturing phase or/and during operation, in order to achieve the desired circuit functionality and adapt it to application specific requirements.

Trimmable silicon waveguides with induced stresses or covered with a chalcogenide glass cladding[48] have already been demonstrated an effective tool for post-fabrication manipulation of photonic integrated circuits, with remarkable advantages with respect to classical heathers. Also, feedback control signals extracted through transparent optical probes are an unavoidable requisite to locally inspect the status of a generic PIC, and to drive and control the working points of its functional elements.

Applications: generic programmable arrays of optical building blocks[49]; tunable, adaptive, reconfigurable and programmable PICs; (re) writable waveguides and circuits[50]; devices robust against nonlinearities, temperature and aging; sensors with locked working point; increase yield by compensating fabrication imperfections and aging effects.

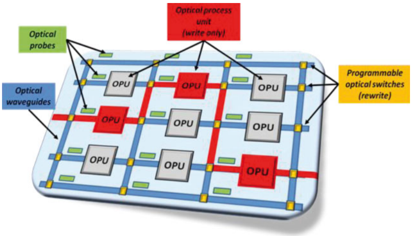

Fig. 11 > Example of programmable optical circuit. A set of Optical process Units (OPU) interconnected with reconfigurable switches and optical waveguides (Courtesy of Prof. A. Melloni, Politecnico de Milano)./

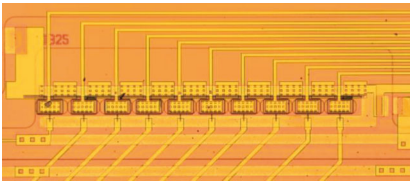

Fig. 12 > Example of optical process unit combining electronic, photonic and microwave. Coupled ring resonators tunable delay line (Courtesy of Prof. A. Melloni, Politecnico de Milano)./

3.3 CMOS-compatible colour filters

An example of integration of a device inspired in nanophotonics is the colour filter which can be integrated with CMOS image sensors. Band pass filtering can be achieved in thin metallic layer drilled with a sub wavelength array of holes. To address several issues related to filtering for optical image sensors, i.e., metal layer thickness with respect to colour filtering, wavelength dependence, incident angle dependence, polarization behaviour, cross talk, process compatibility with CMOS constraints among others, a double-breasted rectangular hole array in aluminium has been chosen due many advantages compared to square, rectangular, circular holes or infinite slits in metallic layers (figure 13).

Colour filtering functions, especially in the visible spectrum, are associated with high resolution features and high density pattern etched in a metallic layer. New

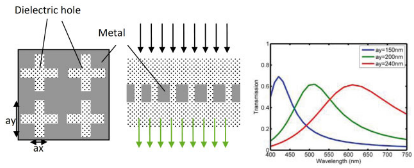

Fig. 13 > Diagram of symmetric cross holes of sides ax and ay perforated metal film and corresponding FDTD transmission spectra for normal incident plane wave. Parameters are: period = 250 nm, metal: 40 nm thick Aluminium, ax = 60nm. (Courtesy of Stefan Landis (CEA-LETI)./

lithography strategies are often needed to manufacture such stamps for large scale manufacturing up to 200 mm wafers. Figure 14 shows a recently developed pattern shape modification strategy, mainly used in Optical Proximity Correction to manufacture optical mask[51], for electron beam lithography and the corresponding SEM picture of the stamp and the resulting imprint and thin aluminium layer etching.

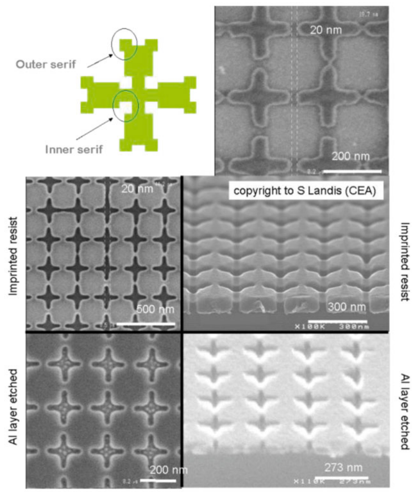

Fig. 14 > Pattern design and SEM top view stamp picture. SEM cross section pictures of imprinted resist patterns with cross array on silicon substrate and etched aluminium layer. Left images are SEM top view, right images are cross sectional views. © S. Landis CEA, LETI-Minatec Campus./

3.4 Silicon nanoemitters

The still-missing device in silicon photonics[52] is an integrated silicon light source which is efficient and can be easily integrated in CMOS photonics. Few concepts have been proposed, among which there is the use of low dimensional silicon quantum dots formed in a dielectric matrix. Reliable CMOS manufactured devices have been produced which show bright reddish emission when electrically driven. Figure 15 (bottom) shows an example of an orange emitting device. There are still open problems associated with the efficiency of the process (maximum power efficiency is 0.2%). In addition, the emission wavelength can be tuned by using suitable rare earth ions which can be electrically excited. Figure 15 (top) shows a fully processed wafer where electrically driven erbium doped silicon nanocrystals amplifiers have been fabricated. In figure 15 (middle) an image of an active optical resonator is shown.

In the project LECSIN[53] surprisingly high efficiency luminescence has been observed from silicon based on Purcell enhancement and mode engineering in photonic crystal cavities. Furthermore, a large effort in nanoparticle-based emission work is conducted in Catania (Matis CNR INFM and ST Microelectronics Catania) mainly on Erbium-doped photonic crystals.

Applications: optical interconnects, silicon photonics, datacom, telecom, integrated biosensors, light emitting device, lighting, photovoltaics.

3.5 Photon Management

Photon management refers to the ability to engineer materials and devices structures at the nanometre scale to control the spatial distribution of optical energy and mould the flow of propagating light. The huge progress in fabrication of nanostructured materials has enabled new strategies for photon management in a range of photovoltaic devices and lighting devices.

Fig. 15 > Top: a silicon photonic integrated circuits with active emitters for electrical driven Er coupled to Si-nc optical amplifiers. Centre: an electrical driven active optical resonators. Bottom: a CMOS LED with emitting silicon nanocrystals. (Courtesy of Pavesi et al, UNITN and LETI unpublished data)./

The ultimate success of photovoltaic cell technology requires great advancements in both cost reduction and efficiency improvement. Photon management is able to simultaneously face these problems thanks to the great advances made in light trapping schemes in photonic materials. Indeed, light trapping schemes allow the design of devices with a very thin layer of active absorbing materials, reducing the amount of material used and improving cell efficiency.

Photon management is also of fundamental importance to optimize the performance of light emitting diode (LED) for lightning applications. In this case the target is to maximize the out-coupling of light to the external environment.

The optimal technological platform to manage and conceive new trapping mechanism, control far-field patterns, polarization properties, up- and down-conversion of absorbed light, are thin dielectric membranes (planar waveguides), where scatters are included in the material, with standard growing/processing technique. Varying the size, the density, the refractive index, which can be also metallic and/or non-linear, of the scattering centres it is possible to mould and manage the photonic properties at will.

Ordered arrangements of scattering centres (photonic crystals) have been extensively studied in this last decade. On the other hand, quasi-ordered, completely disordered and correlated disordered arrangements have been and are the subject of extensive studies in this last two-three years because they retain many features of the ordered counterpart with the advantage of not suffering of structural disordered imperfections during the growing process, being the disorder part of the game.

Applications (key words): photon management, photonic crystals, photonic quasi-crystals, disordered photonic materials, correlated disorder, light trapping schemes, thin film photovoltaics, light emitting diode, far field radiation.

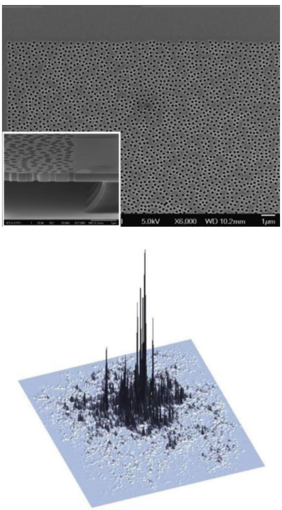

Fig. 16 > Example of a new device structure for light trapping in thin dielectric membrane. (top) Scanning Electron Microscopy image of a completely disordered photonic system realized on a thin dielectric membrane of Gallium Arsenide (thickness 300 nm). Air holes (220 nm of diameters, filling fraction of 0.3) are the scatterers. The inset shows a detail of the suspended membrane. (bottom) Surface Intensity distribution of a typical trapped mode inside the membrane. (© LENS Firenze, Italy)./

3.6 Metamaterials

These are artificial materials with superior and unusual electromagnetic properties not found in nature, currently being fabricated for targeted applications. The materials follow specific designs of electromagnetism and in the visible regime pose a major nanofabrication challenge, however, there are several potential new technologies to manufacture these materials from top-down to bottom up. The tremendous potential impact of the applications should they become a reality make this field uniquely attractive. Comprehensive reviews can be found at http://www.metamorphose-vi.org/.

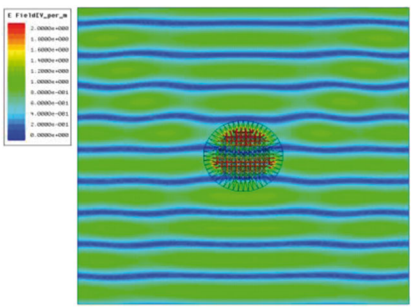

Fig. 17 > "Invisible" cylinder (copyright Pekka Alitalo, Aalto University)./

Applications: In ICT: Smart and adaptive integrated electronic and optical circuits and devices, sub-wavelength optical information processing systems, low-cost low power consumption communication and control systems, magnetically and electrically controllable components. In Energy: Low-loss electronic and optical components, advanced solar cells harvesting at all frequencies, materials for thermal flow control, intelligent control of power consumption and generation. In Health: Sensors including biosensors, on-body communication systems, in-body drug delivery and control devices, implanted actuators. In environment: Monitoring and imaging devices. In transport: Car radars, sensors, road safety monitoring systems, road monitoring and vehicle tracking. In Security: Security control devices, sensors, imaging and monitoring devices.

3.7 Nonlinear nanophotonics

The research toward compact and efficient nonlinear photonic devices has greatly improved in the recent years in view of potential application in many areas where the integration is a key issue, including new spectroscopy techniques. Given the general structure of the nonlinear interaction between light and matter, in term of polarization $\vec{P} = \chi(1)\vec{E} + \chi(2) : \vec{E}\vec{E} + \chi(3) : \vec{E}\vec{E}\vec{E}$, one may act on the susceptibilities χ or on the field enhancement. This translates into a research of new materials and new geometries ranging from the UV to the THz domain.

Novel effects can be obtained when material properties are modulated at the sub-wavelength scale, that is, by exploiting molecular structures or nanostructures.

The tight confinement of the electromagnetic field is achievable in the vicinity of metal dielectric boundary, commonly referred to as surface plasmon polaritons. As a consequence nonlinear effects are greatly enhanced: Raman scattering[54], CARS, optical switches, surface enhanced second harmonic generation, high-harmonic generation by coupling nanoantennas[55] and, recently, two-photon emission has been also demonstrated[56]. The field confinement allows the visibility of nonlinear magneto-optical effects, such as Magnetization-induced Second Harmonic (MSHG), where a nonlinear rotation of the e.m. polarization plane is achieved[57]. The combination of geometry and materials (here metals are referred as nonlinear metamaterials) gives other interesting nonlinear effects at the nanoscale and the promise of new ones. In this last case it is possible to "play" with the conformation of the metamolecules changes, providing novel mechanism of nonlinearity[58] and improving the nonlinear response related to the chirality of the medium[59].

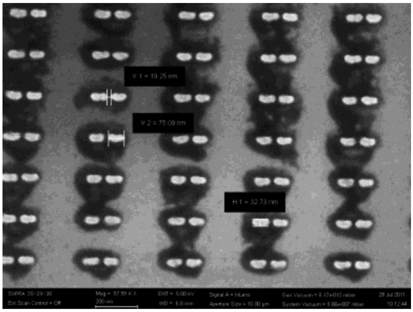

Fig. 18 > SEM micrograph of Au nanoantennas/GaN to enhance the second harmonic generation signal in the visible (400 nm). (F. Bovino and A. Passaseo et al, Selex –SI, CNR-Italy, Univ. Roma La Sapienza, to be published)./

Recently, a number of exciting demonstrations of nonlinear effects have been made, especially in terms of third harmonic generation[60] and four wave mixing[61]; efficiencies previously unthinkable have now been demonstrated for mW-level pump powers and miniaturised devices. This is a major advance over the time when nonlinear optical experiments required high power lasers and entire optical benches, and this opens new opportunities in on-chip all-optical signal processing and on-chip quantum circuits.

In this context, research for new materials and combination of them is of great importance.

Applications: Surface and interface nonlinearity for high resolution spectroscopy; bio applications and sensing. Nonlinear magnetism in the optical range for bio sensing. Improved new devices, in space and time, for optical information processing such as modulators and switch. Integrated circuit for quantum optical information, including quantum sensing. New integrated parametric sources (UV –THZ).

3.8 Conclusions

Among the commonly mentioned key issues in nanophotonics research is design for specific applications including a subset of generic architectures and device performance in the nanoscale. Power efficiency, both as in power management and wall plug efficiency, are also shared key issues and both are followed closely by the need of technologies and standards suitable for very large scale manufacturing. More specific research needs and key issues can be found below.

Si photonic circuits: Being one of the areas with a higher Technology Readiness Level, the research needs are seen in technology development, in interconnects and design rules for monolithic and vertical integration.

Silicon nanosources: The key issues include the low power efficiency of silicon nanocrystal emitters, the low areal density of silicon nanocrystals and the low ratio of Er ions directly coupled to silicon nanocrystals, which prevents reaching lasing thresholds. To mitigate these issues research needs are seen in alternate system for light emission monolithically integrated in silicon, in deposition methods able to control the density of silicon nanocrystals independently of their size, e.g., sol-gel deposition and in fabrication techniques which should be able to control at the sub-nanometre level the deposition of dielectrics acting as tunnelling barrier for charge injection into the active centres.

Adaptive Integration Photonics: The research issues identified include hitless monitoring of optical signals to provide feedback, waveguide activation to provide tuning and permanent trimming and programmable and adaptive circuits. As specific research needs the question of light detection without photodiodes and the functionalisation of waveguides through new material combination to obtain electro-photo sensitivity are mentioned.

Colour filters: Two main issues are crucial, namely, omnidirectionality and process compatibility to enable the integration. Simulations of critical dimension fluctuations impact on performance are essential.

Photon management: Key issues include numerical characterization, characterization of electrical properties of the dielectric membranes with scattering inclusions and the role of the correlations between scatters positions. As specific research needs the partnership with research growing facilities and with original equipment manufacturer (OEM) is seen as crucial.

Metamaterials: The research needs in this field include fundamental research on exotic-property and non-classical optical and microwave materials; theoretical modelling and design of artificial electromagnetic materials; engineered non-linearity of materials; approaches to targeted synthesis and design of electromagnetic materials; material architectures providing design control over material parameters, losses, spatial dispersion, nonlinearity, reconfigurable photonic metamaterials, conceptually novel architectures for electrical, magnetic, and optical control of the properties of engineered materials; develop and implement active optical materials with compensated loss; develop nano-structured light and microwave energy harvesting materials; research on field-transforming metamaterials (cloaks, concentrators, dividers) and in-situ and non-destructive characterisation of artificial electromagnetic materials.

Non linear nanophotonics: Key issues are: the definition of the operational wavelength for specific applications (deep UV for oceanic sensing, which needs an enhancement of the non-linearity, and MID-IR for sensing in general), new materials with high nonlinear coefficients, design of suitable antennas geometry, better time response of the nonlinearity. Furthermore, loss reduction, especially in slow light waveguides in silicon or III-V's to reduce further the pump power for nonlinear interactions. Reduction of nonlinear losses by, eg., working in the mid-IR or by developing novel materials, to increase the efficiency of nonlinear interactions. The research needs include also materials with reconfigurable nonlinearity and nonlinear meta-molecules. For most of the above sources and detectors are needed. A need to improve the local enhancement of the nonlinearity for quantum information processes, for bio sensing in the THZ and optical range is also seen as a priority.

4 Combining nanophotonics and nanophononics

Recent advances in nanofabrication have made it possible to realise structures in which photons and phonons can be coupled. These optomechanical structures open new avenues for very interesting research and, also, to new applications for sensing and signal processing.

4.1 Optomechanics

A single cavity can confine simultaneously both phonons and photons and increase the interaction among them (slow light and sound) and produce well known physical effects like stimulated Raman and Brillouin scattering, supercontinuum generation or light octave spanning at the chip scale[62]. In general, optomechanics addresses the coupling of optical (photons) and mechanical (phonons) vibrations via radiation pressure. Typically, light is in the near infrared regime, usually at wavelengths around 1.55 micrometres, whereas mechanical resonances vary from some MHz to some GHz depending on the structure. A key aspect of cavity optomechanics is the possibility of laser sideband cooling of the cavity down its ground state of motion, which should ultimately lead to the observation of quantum effects and to extremely sensitive mechanical sensors.[63] But the real advantage of the dual confinement of such cavities and waveguides, known as optomechanical crystals[64], lays in the fact that light and sound act as mutual driving forces at the meso and nanoscale through both the back-action effect[65] and the optical gradient force[66]. That means that phonons can be used with an extremely high efficiency (0.7 photons/phonon) to drive photon modes, and the reversal effect has been already proposed for a photon-phonon transducer. The potential applications range from quantum computing and information technology to study of quantum mechanical systems in their ground state. Especially remarkable is the aim of producing a coherent source of phonons, the first building block towards the sound equivalent of a laser, a SASER (Sound Amplification by Stimulated Emission of Radiation) that could be realised on a CMOS compatible platform using optomechanical concepts. Different geometries have already been proposed and experimentally characterised, including ring micro-resonators, slabs and nanobeams. All these structures have good optomechanical coupling, but do not have a complete stop band or band gap for both photons and phonons, which is a crucial point to avoid energy leakage, especially in the mechanical domain.

Experimental demonstrations of optomechanical effects in high-Q optical cavities have made used of large, in terms of optical wavelengths, cavities such as toroids or microspheres. In order to enhance further the optomechanical interaction, cavities with size comparable to the wavelength of photons and phonons have to be used. This has led researchers to implement novel cavities by using photonic-phononic crystal membranes, i.e., periodic structures which possess band gaps for both photons and phonons simultaneously. This has resulted in the concept of "optomechanical crystals",[67] or "phoxonic crystals".[68] In addition to the possibility of enhancing optomechanical, or acousto-optic, interaction by building smaller cavities, optomechanical crystals possess other important features in comparison with other implementations of optomechanics: i) flexibility in the design of the structures owing to the maturity of the photonic/phononic crystals fields, ii) structures built on planar substrates by conventional top-down lithographic means, ultimately using mainstream CMOS processes, with the possibility to create arrays of devices on a same chip, iii) possibility to create additional optomechanical structures, e.g., waveguides to guide phonons and photons simultaneously and phonon sources,[69] iv) possibility of new ways of photon-phonon interaction such as via electrostriction.

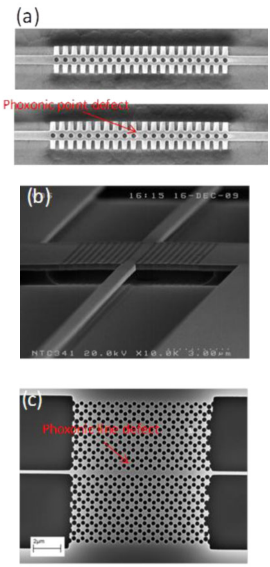

Fig. 19 > SEM images of suspended silicon phoxonic crystal membranes. (a) Corrugated waveguide with holes that support a bandgap for TE-polarized photons around 1.55 micrometres and 4 GHz phonons (top panel). The introduction of a λ/4 defect (bottom panel) should lead to the localization of photons and phonons in a nanoscale volume. (b) Removal of the buried oxide leads to a suspended phoxonic crystal that facilitates the excitation and propagation of GHz phonons. (c) Top-view of a line defect created in a honeycomb-lattice. The structure can confine and guide slow photons and phonons simultaneously (Courtesy of A. Martinez, U Polytechnic Valencia, and Vincent Laude, CNRS-FEMTO)./

Applications: optical delay lines, highly sensitive sensors, modulators, optical memories, optical isolators.

4.2 Photothermal effects

Combining thermal waves with photonics gives rise to photothermal modulation. In photothermal techniques a heat pulse propagates through medium and the backscattered photothermal signal is monitored.[70] The method can be used for example to investigate inhomogeneous and layered materials. The problem of the photothermal modulation of optical beams is extremely complex due to the inhomogeneously modulated refractive index combined with multiple optical reflections inside the sample. A treatment for normal-incidence optical probing of photothermally modulated layered thin-film samples with arbitrary optical constants has been given.[71]

Applications: Contactless experimental techniques to study thermal transport in inhomogenous media.

4.3 Conclusions

Optomechanics is a relatively new research field which have potential for new sensing applications and signal processing approaches. To capitalise this potential, better understanding of the physics behind photon-phonon coupling at nanoscale is needed, together with well-established fabrication processes for the optomechanical structures. One missing building block is a phonon source that can be integrated with the photonic/phononic crystals.

Photothermal techniques are a good candidate for non-invasive characterisation method for nanomaterials and composites. Here again understanding of coupling between photons and phonons or thermal waves is crucial.

5 Nanophononics

The control and manipulation of acoustic/elastic waves is a fundamental problem with many potential applications especially in ICT. One can mention confinement, guiding and filtering phenomena at the scale of the wavelength (and even below) which are useful for signal processing, advanced nanoscale sensors and acousto-optic on-chip devices, acoustic metamaterials for sound isolation and for focusing and super-resolution.

Phonon engineering can be achieved for example by periodically patterning a Si membrane (phononic crystal, PnC, membrane)[72], which is a strategy that is being exploited to provide a means for a controlled influence on phonon transport properties including functions like generation, propagation, storage, manipulation and detection. Optomechanical crystals for simultaneous control of both phonons and photons and cavities for enhanced phonon-photon coupling expand the prospect for novel applications of nanopatterned membranes[73,74,75].

5.1 Phononic crystals

Phononic crystals, which are artificial materials constituted by a periodic repetition of inclusions in a matrix, can be used to achieve these objectives via the possibility of engineering their band structures. Due to the contrast between the elastic properties of the matrix and the inclusions, the phononic crystals can exhibit absolute band gaps where the propagation of acoustic waves is prohibited in any direction of space and for any polarization, see Fig 20.[76] The structure behaves like a perfect mirror in the frequency range of the band gap. Then, it is possible to create waveguides, for example by removing or changing a row of inclusions, that are able to produce localized modes inside the band gaps and therefore confine, propagate and bend waves at the scale of the wavelength.[77] Confinement inside cavities (point defects) and coupling between waveguides and cavities can also be used for filtering and multiplexing operations. [78]Another possibility of opening a gap, especially at low frequency as compared to the Bragg gap, is to use inclusions exhibiting local resonances, the so-called locally resonant sonic materials useful for the purpose of sound isolation and/or absorption.

Phononic crystals of finite thickness, such as a periodic array of holes in a plate or a periodic array of dots on a membrane, have only been studied recently, since it was demonstrated that they can also exhibit absolute band gaps and thus provide the possibility of the above functionalities in small size integrated structures working at high, GHz to THz telecommunication frequencies.

The progress in the field of phononic crystals goes in parallel with their photonic counterpart, although they involve a larger variety of materials that have the possibility of high contrast among the elastic properties, large acoustic absorption and the solid or fluid nature of the constituents. Since the band structure is scalable with the dimensions of the structure, a great deal of work has been devoted to macroscopic structures in the range of sonic (kHz) and ultrasonic (MHz) frequencies where the proof of concepts of band gaps and manipulation of sound (such as waveguiding, confinement, sharp bending) have been established with simple demonstrators. Yet, there are a continuous interest in the engineering of bands with new structures and materials.

With the advancements of nanotechnologies as well as self-assembling techniques, the interest on nanophononics is increasing. Phononic circuits, including waveguides and cavities, inside sub micrometre phononic membranes and working at a few GHz are started to be studied but still remain mostly at the level of demonstrations. The band structure of these so-called hypersonic crystals can be studied by light (Raman and Brillouin) scattering techniques, in particular to investigate tunable systems in which the properties can be changed drastically with external stimuli such as stress or temperature (for example the phase transitions of a polymer infiltrating the holes of a phononic crystal).

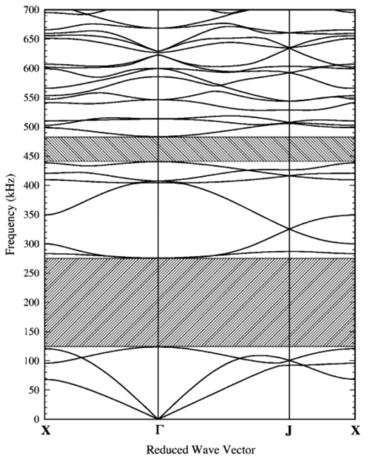

Fig. 20 > Plane wave expansion calculation results for the band structure of the two dimensional *XY* modes of vibration in the periodic triangular array of steel cylinders in an epoxy resin matrix for a filling fraction f=0.4. The reduced wave vector $\boldsymbol{k}(kX,\ kY)$ is defined as $\boldsymbol{K}a/2p$ where $\boldsymbol{K}$ is a two-dimensional wave vector. Absolute band gaps are represented as hatched areas. (Reprinted with permission from J. O. Vasseur et al., Phys. Rev. Lett. 86 (2001) 3012, © 2001 American Physical Society)./

The configuration being normally considered is the insertion of periodic holes in silicon plates, where the opening of band gaps is the consequence of the coherent destruction of phonon modes by Bragg scattering, but also geometries based on the periodical arrangement of cylindrical cavities on top of a membrane (see Figure 21). The latter allows for a superior control of the phonon dispersion, and almost dispersionless phonon branches, which are not related to the opening of band gaps, exist on large wavevector domains. While coherent scattering phenomena in phononic crystals have been shown to affect the low frequency phonons, recent reports address the possibility of extending these effects to the high frequency THz phonons that dominate heat transfer process[79,80] Thus, future functionalities of PnC membranes related to heat management need the development of cutting-edge nanofabrication techniques allowing to downscale the characteristic sizes to a few nanometer scale.

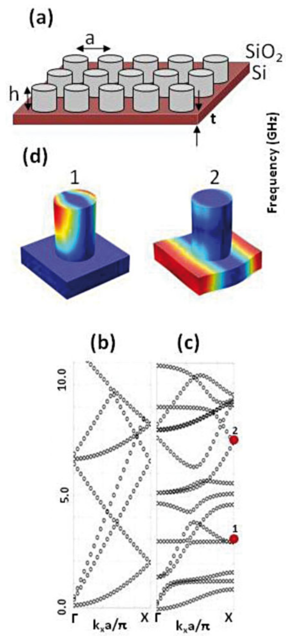

Fig. 21 > Schematic of the proposed structure with periodic pillars on a Si membrane (a). (b): Calculated phonon dispersion curves of 100nm thick Si membrane (b), and of the phononic structure with SiO_2 pillars (c). (d) Displacement field of the modes at the points marked with red dots in (c) (J. Gomis et al., unpublished)./

Besides the topics related to the existence of absolute band gaps, there is growing interest on refractive properties of phononic crystals, in particular: negative refraction phenomena and their applications in imaging and sub-wavelength focusing in phononic crystals, self-collimation and beam-splitting in relation with the shape of the equifrequency surfaces, controlling the propagation of sound with metamaterials with emphasis on cloaking and hyperlens phenomena.

Thermal transport in nonmetallic nanostructured materials can be strongly affected by the specific phonon dispersions as well as by different scattering mechanisms. The existence of band gaps and flat dispersion curves can reduce the thermal transport and be useful for thermoelectric applications. On the other hand, channels for propagation of heat can be envisaged either inside the phononic crystal or by avoiding the escape of heat outside a thin film surrounded by a phononic crystal. Different frequency domains of phonons can be involved depending on the temperature and on the wavelength dependent mean free paths. Some insights into the latter can be derived from molecular dynamic calculations.

In conclusion, the field of phononic crystals should acknowledge a continuous growth in relation with the fundamental understanding of the wave phenomena in these heterogeneous materials and with their numerous expected technological applications. The latter cover a broad range of frequencies from the sonic regime for sound isolation and metamaterial behaviors, to GHz regime for telecommunications and to THz regime for phonon-photon interaction and thermal transport phenomena.

5.2 Heat transport through interfaces and in nanoscale structures

An important field where nanophononics will a have striking impact is the heat transfer area, as much better thermal insulators and much better thermal conductors are required if one wants to meet the energy challenges of the 21st century. The electronic conductivity σ spans over more than 30 orders of magnitude ($[10^{-22}-10^{8}]$ Ω m^{-1}), something which has led to the development of electronics, whereas the thermal one κ spans barely over 5 orders of magnitude ($[10^{-2}-10^{3}]$ $Wm^{-1}K^{-1}$)[81]. The typical phonon wavelengths have a broad distribution around 2 nm at room temperature, and wavelengths are much longer at liquid helium temperature. The phonon mean free paths are known to be longer than 100 nm, even at room temperature.

At the Fourier scale, in addition to the 'volume' transport represented by the conductivities, the interface effects known as 'boundary resistances' R_b, also sometimes called Kapitza resistances, can be dominant in the effective transport coefficients $\kappa_{eff}=\kappa+R_b/d$ at small scale (d→0). The impact of the boundaries at the nanoscale has been studied since the beginning of the 2000's, especially for the purpose to develop more efficient thermoelectric materials, as lower thermal conductivity imply higher thermoelectric figure-of-merit ZT.[82] The partial phonon diffuse reflection at the surfaces implies loss of coherence, which integrated over all frequencies, is represented by a so-called 'specular coefficient' p. As the roughness is not always easy to analyse, it is often a fit parameter that allows to reproduce numerically the experimental data. An additional significant challenge is the control of the surface states.

The confinement of phonons leads to discretisation of the phononic density of states. Similar to concepts developed for photonics, such as periodic structures, superlattices, etc, one can consider manipulating phonons or thermal energy, including storage, conversion, emission, absorption and rectification. So far the confinement induced effects have hardly been treated for simple geometries. The extension to more complex geometries will provide a grand challenge.

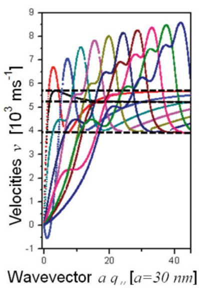

Fig. 22 > Calculated thermal phonon group velocities (heat propagation velocity) due to confinement in a30 nm-thick Si membrane. Dotted black lines: planar bulk reference (E. Chavez et al, to be published)./

In addition to continuum models, phonon behaviour has been analysed also using atomic-based simulation methods, such as molecular dynamics, Green's function and ab-initio methods. These methods are not suitable for structures with intermediate sizes in the range of 10-100nm due to computational restrictions. To bridge the acoustic scale, continuum elasticity based methods and the atomic scale more extensive use of the Boltzmann transport equation (BTE) will be required.

One main property that distinguishes phonons from other bosons such as photons is that they interact between themselves[83] and, consequently, their lifetimes, or relaxation times, are strongly correlated to their distribution. Recent numerical calculations[84] have shown that the bulk phonon mean free paths might be much larger than previously expected, so that nanoscale models might already be needed at the 1 μm scale.

The calculation of the phonon lifetimes relies on formalisms based on the Fermi's golden rule that were developed in the 1950s mainly for bulk phonons.[85,86] Some of the main results are obtained in the framework of isotropic approximation, whereas others require anisotropy to be explicitly taken into account as the main cause of damping, as in the Herring mechanism.[87] The impact of non-resistive phonon interaction, called normal processes, is not well understood, and although atomic simulations allow extracting some of these lifetimes, the simulations do not provide means to control them. The extension of the formalism to the phonons existing in nanostructures appears to be of highest importance if one wants to understand how to modify phonon conductivity by dimensions and geometry. In particular, phonon momenta conservation rules ($q_1=q_2+q_3$) relax at small scales. The current deterministic approach is therefore incomplete and more statistics-based ones are required.

It is very difficult experimentally to correlate the thermal macroscopic effective conductivity coefficients, e.g., conductivity and specific heat, to the phonon spectra. One can measure thermal conductivity relevant for bulk or thin films samples with various methods such as the 3-omega method or photothermal spectroscopy. The thermal diffusivity, i.e., the ratio of the thermal conductivity to the specific heat, can be measured by various time-domain methods probing the dynamics of the studied systems.[88] These include the laser flash method, the more-recently developed thermal transient grating technique and time-domain thermoreflectance. All these techniques give access to macroscopic effective coefficients. If the medium is strongly out of equilibrium, as in many times is the case with graphene or carbon nanotubes, and no local temperature can be defined, as in ballistic regime, such parameters are not meaningful and the transport should be represented for instance by conductances.

Regarding spatial resolution, scanning thermal microscopy has been proven to possess the highest one. Raman spectroscopy or fluorescence-based methods can reach sub-10 μm resolution. Dispersion relations can be measured using neutron diffraction, or using inelastic light scattering, i.e., Brillouin and Raman spectroscopy. The latter gives a limited part of the room temperature momenta range. Ultrafast phonon spectroscopy has been used up to ~2 THz, the very beginning of the room-temperature spectrum. One approach is to use passive detection, i.e., to measure thermal THz radiation using microbolometers. This technology has been used, for example, to realise real-time THz cameras for security screening.[89]

Applications: Thermal management for ICs and heterogeneous integration applications, THz cameras for security and medical applications.

5.3 Issues relevant to micro and nanoelectronics

Heat dissipation has become one of the most important limiting factors toward increasing density, performance and reliability of modern electronic devices, including:

microprocessors, high-power radio frequency transmitters, photovoltaic cells and power electronic modules; and it is particularly critical in 3D chip stacks of integrated circuits, where the inherent difficulty of supplying power to and removing heat from individual dies has become a crucial factor for the future growth of the semiconductor industry that could potentially reduce the design window of 3D products.

In these devices, heat generated during their normal operation is dissipated through dissimilar interfaces comprising metals, semiconductors, oxides, thermal interface materials (TIMs) and fluids (air or water); and from small areas which are continuously reduced to lower manufacturing cost. The reduction of the spatial characteristic dimensions not only allows faster switching and better electrical performance, but also changes the thermal properties of the constituent materials from their bulk values. It is well known, that at scales comparable to or below the mean free path of phonons (as in current and future transistor designs), the scattering of phonon with boundaries is one of the main sources of thermal resistance leading to a significant reduction in the thermal conductivity of semiconductors. Phonons are subject to complex scattering mechanisms, i.e., phonon-phonon, phonon-impurities, phonon-boundaries and phonon-defects, which play a crucial role in describing how the heat is transported in the material. Furthermore, the difference between the thermal properties of bounding materials translates to a significant mismatch in their thermal impedances and in low phonon transmission rates, which also promotes high thermal interface resistances. The latter, not only reduce the efficiency of cooling systems, leading to larger carbon dioxide emissions, but also hinder the reuse of the thermal energy.

While in some situations the reduction of the thermal conductivity can be beneficial, such as for thermoelectric devices using, for example, silicon nanowires; this reduction significantly deteriorates the thermal performance and reliability of other devices, such as: SOI, UTB FD-SIO, III-V, FinFET and nanowire transistors. It is estimated that future III-V and nanowire-based transistors will be subject of serious heat dissipation problems. In particular, since: i) III-V semiconductors have thermal conductivities which are 5 to 30 times lower than that of silicon (e.g. $In_{50}Ga_{50}As$ or $In_{50}Al_{50}As$), ii) additional insulating layers with very low thermal conductivity will be used to control current leakage and iii) the inherent low dimensionally of the involved structures will promote phonon-boundary scattering; restricting in this way heat dissipation and inducing large thermal stresses. Note that most of the failure mechanisms in transistors are temperature-dependent.

Despite the design of current transistors relying almost exclusively on charge transport models, the ITRS 2009 has defined that future nanoscale device simulators, coupling electronic band and phonon spectra interactions, are necessary to enable future transistor architectures. In particular, to predict the limit of CMOS-based transistors, to design and evaluate devices beyond traditional planar CMOS, to assess the performance new devices subject to electrical and thermal fluctuations, and to propose physical models for the evaluation of novel materials (e.g. high-k stacks, III-V channels, etc.) in these new architectures.

From the thermal point of view, to model the thermal behavior of these devices considering all scales involved is a complex task. The complexity lies: in the large variation of the participating spatial (from nanometers to centimeters) and temporal scales (from picoseconds to hours), in their intricate operation and in the physical behavior and nature of each scale. Even though the formulation of the thermal transport at the sub-continuum level has long been established, no mathematical method is able to fully resolve the thermal response of electronic devices from nano to macro scales and hierarchical models are required for this purpose.90 purpose.[90] Traditionally, different numerical tools have been used: to characterize the thermal properties of materials and interfaces, to estimate phonon properties (i.e. relaxation times), to describe the transient transport of phonon in 2D and 3D domains, to conduct thermal device simulations at macroscopic scales, etc. These include molecular dynamics (MD), lattice dynamics (LD), phonon Monte Carlo (MC), phonon Boltzmann transport (BTE), Cattaneo equation and Fourier law, among others. Quantum based approaches, other than LD, have been typically neglected due to the computational time involved, the requirement of large computational facilities, i.e., thousands of processors, and the difficulty to model large molecular systems.

5.4 Molecular dynamics modelling of interfaces and heat transport

Molecular dynamics (MD) is one of the few methods used to characterize the thermal properties of materials and interfaces, partially due to a positive balance between the accuracy of results and the computational time involved. The method, which has a classical nature, solves the Newton's second law to describe the dynamics of atoms subject to one or more interacting potentials. MD has been used extensively to estimate a broad range of thermal properties of the materials. For thermal characterization purposes, the method offers many advantages at the expense of no quantum effects since: i) it does not require previous assumptions about the nature of the thermal transport, ii) it captures the anharmonic interaction between atoms, iii) it does not require simplification on the underlying molecular structure, iv) well documented inter-atomic potentials for common semiconductors are available, v) it can be applied to relatively complex geometries and vi) can be used to model solid, liquid and gas phases.

MD has been particularly valuable and useful: i) to estimate the thermal conductivity of semiconductors,[91] ii) to calculate the phonon transmission and reflection probabilities at smooth and rough semiconductor interfaces,[92] iii) to determine the phonon relaxation times of silicon and germanium,[93] iv) as part of hierarchical modelling approaches, v) to determine the thermal conductivity of silicon-germanium core shell nanowires,[94] vi) to study molecular mechanisms to enhance heat dissipation and thermal rectification at solid-liquid interfaces,[95] vii) to determine the metal-nonmetal thermal interfaces resistance subject to phonon and electron interactions,[96] viii) to determine thermal properties of carbon nanotubes and graphene sheets,[97] and ix) to thermally characterize the matrix-filler thermal interface resistance in TIMs.[98] An example of a calculated thermal profile in a solid-liquid interface is shown in Fig. 23.

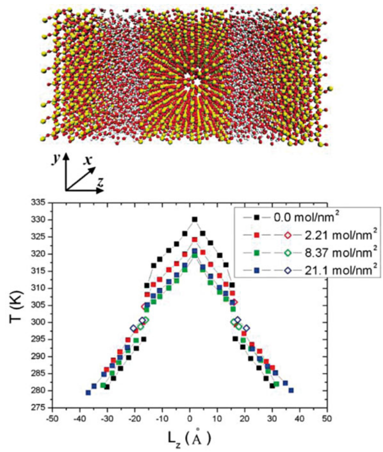

Fig. 23 > Top panel: a snapshot of quartz-confined water model structure. The quartz slabs are in the middle and on two sides. Water is confined between quartz slabs. Bottom panel: steady-state temperature profiles for heat flux of 6400 MW/m^2 for four selected fully hydrophilic cases at 300 K. The solid squares are for quartz and the open diamonds are for water. Reprinted with permission from M. Hu et. al., Nano Lett. 2010, 10, 279-285. Copyright 2010 American Chemical Society./

Despite all these advantages and progress towards the characterization of materials and interfaces, the lack of quantum effects[99] and the difficulty to include realistic electron-phonon interactions limit the application of MD and its results. Novel approaches for the incorporation of these two phenomena in MD are currently in progress.[100] However, larger efforts in this area are mandatory to facilitate the design of future transistors.

5.5 Heat transport between particles

Nanofabrication provides means to control thermal properties of nanomaterials and nanosystems, with impacts on, for example thermoelectric materials and thermal interface materials.[101] The physical mechanisms are mostly related to heat carrier scattering between two bodies through interfaces or gaps or at surfaces. Developing tools to quantify and design the corresponding thermal resistance remains a crucial task. Recent work has proposed a general derivation of the inter-body thermal resistance based on fluctuation-dissipation theorem.[102] It has provided relevant predictions of the near-field radiation based thermal resistance between two nanoparticles. For example, the heat transfer between two silica nanoparticles is enhanced by orders of magnitude at distances less than twice the diameter of the particles. This near-field interaction was then experimentally proven for microscopic objects.[103] Further studies have then extended the derivation proving that the inter-body thermal resistance is identical to the energy carrier mean relaxation time.[104] This analysis not only provides a simple and direct means to study and design the thermal resistance of nanostructures, it might also indicate a new degree of freedom to control heat transfer in nanostructures through the tuning of the carrier relaxation.

Moreover, larger solid bodies separated by a small vacuum gap can exchange energy and momentum (and information) by various mechanisms[105,106,107]. It has been considered that the most significant exchange channel is formed by inter-body photon coupling. Surface excitations involving optical phonons and plasmons can also play an important role. These polariton effects can enhance the coupling close to the maximal fundamental limit. When the different bodies represent thermal baths the heat exchange is via near-field heat transfer effects and considerable efforts have been devoted to understand the heat transfer via photon and polariton channels. Advances in experimental techniques have also enabled near-field heat transfer measurements from µm down to nm body distance[108].

Acoustic phonons are the major heat carriers in dielectrics, but their effect on heat transfer through a vacuum gap has been considered to be negligible, because they couple weakly to photons. Recently, it was theoretically demonstrated[109] that significant energy transmission and heat flux is possible if the acoustic phonons can induce an electric field, which then can leak into the vacuum [see Fig. 24]. Such mechanism is provided, for example, by the density response of free carriers due to phonons, by the piezo-electric effect or by response of built-in fields. The built-in field refers to fields that occur, for example, due to work function differences. The solid-vacuum-solid acoustic phonon transmission phenomenon can be thought of as an acoustic phonon tunnelling through vacuum.

Altfeder et al.[110] explained the outcome of their near-field heat transport experiment (between Au and Pt/Ir STM tip) by lattice vibration induced temporal changes in the built-in fields. They observed an extremely large heat flux, which is significantly larger, ~6 orders of magnitude, than the flux suggested by the photon based near-field heat transport theories, where the heat is essentially transmitted due to electron density fluctuation induced photons and/or polaritons. Such magnitude led them to interpret that their experiment actually involves phonon tunnelling. Detailed theory of this experiment is lacking and this leaves room for speculations.

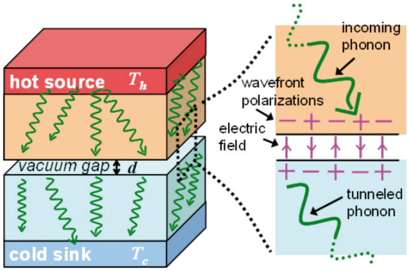

Fig. 24 > Illustration of the phonon transmission/tunnelling effect through a vacuum gap. Hot source radiates phonons towards cold sink and vice versa. Single phonon carries an electric field, illustrated by + or - signs of wavefront polarization. The polarization induces an electric field into the vacuum gap. The field enables finite transmission over the gap (M. Prunnila et. al., VTT)./

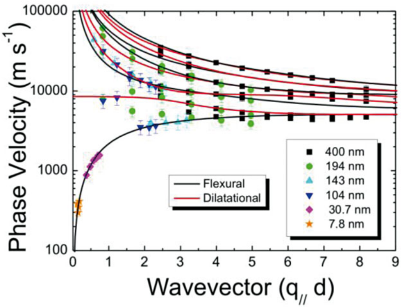

Fig. 25 > Phonon dispersion relation of Si membranes (with thicknesses, d, from 400 nm down to ~8 nm) measured by inelastic light scattering and plotted on one curve by representing the phase velocity as a function of the dimensionless q//·d. The ultra-thin nature of the membranes results in a slow phase velocity for the fundamental flexural modes, with a phase velocity downs to 300 m s^{-1} recorded for the ~8 nm membrane. This is 15 times smaller than the comparable Rayleigh Wave (J. Cuffe et al. to be published)./

5.6 Phonon dispersion in ultra-thin membranes

Phonon confinement is an important component of phonon engineering as the density of states of confined phonons, their frequency and symmetry depend on the geometrical shape of the cavity, as well on the acoustic characteristics of the cavity constituents. Thus, confined phonons are particular to a specific acoustic cavity and depend on the configuration of the structure. In this context, free-standing ultrathin Si films, which can be building blocks for many future applications and, especially, for nano-electrical mechanical devices, represent an excellent example to study experimentally the effect of the reduction of the characteristic size on the phonon dispersion relation (see Fig. 25). This knowledge is crucial in order to identify the role of confined phonons in device performance, for example, phonon-limited electron mobility and thermal transport. In addition, cavity design already represents a means to tailor the phonon dispersion relation for phonon manipulation, given that an effect of confinement in membranes is the manifestation of phonon modes presenting zero and negative group velocity[111].

5.7 Low temperature effects

In the low temperature limit several new issue emerge.

Thermalization of electronic nanodevices at low temperatures is an interplay between electrons, phonons and photons. Ultimately, the performance of the electronic device is determined by the level of coupling to the low temperature bath by phonons and photons, and by decoupling the electronic system from the high *T* thermal photons, e.g., microwaves travelling via the wiring[112,113]. Noise of heat current is showing interesting behaviour at low temperature. The curious property is that the noise, at least for certain mesoscopic realizations, is non-vanishing in the *T* -> 0 limit. This observation, so far only theoretical, puts in doubt the validity of the fluctuation-dissipation theorem (FDT) of heat current in the quantum regime. Mesoscopic phonon heat transport is one of the examples where this non-vanishing noise might be observable experimentally, another system is electron-phonon heat transport. The second interesting topic in terms of noise of heat current is testing the validity of the Jarzynski equality and fluctuation-dissipation relations (FDR) for small systems and conversion of information to energy. The realizations using the combined electron-phonon –systems seem feasible. Statistical physics of both electron and phonon systems in nanostructures looks like an interesting avenue for future research[114]. The thermal wavelength of phonons, exceeding tens of micrometres at practical low temperature conditions, exceeds in many cases (some of) the dimensions of the heat conductor. This has both fundamental and practical interest in engineering of thermal detectors and on-chip refrigerators[115]. It has been shown, for example, that the phonon thermal conductance can be reduced drastically at low sub-5 K temperatures by geometrical design, i.e., introducing serpentine structures in nanowires to block the propagation of ballistic phonons.[116]

Applications: Micro-coolers, detectors, quantum computing.

5.8 Improving the efficiency of thermoelectric materials

One application of nanophononics is to improve the performance of thermoelectric materials. The figure of merit

$$ZT = \frac{\sigma}{\kappa_{ph}+\kappa_{el}} S^2 T$$

can be enhanced by reducing the thermal conductivity κ_{ph} by increasing the scattering of phonons. This can be done by alloy scattering, by introducing superlattices or, very efficiently, using nanoparticles.[117] In Fig. 26 is shown a Si/SiGe nanodot multilayer with which the minimum room temperature thermal conductivity achieved was below 1 W/mK.[118] The materials are fully compatible with CMOS fabrication process and the approach potentially provides a mean to integrate TE energy harvesters with ICs.

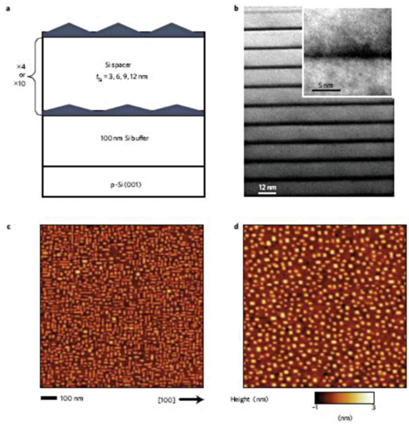

Fig. 26 > **a** Schematic of the self-assembled nanodot multilayers fabricated by molecular beam epitaxy. **b** Bright-field TEM image of a sample with t_{Si}=12 nm. The dark areas correspond to the Ge layers. The inset shows a high-resolution TEM of a nanodot. **c** AFM image of a single Ge/Si(001) dot layer before overgrowth with Si. **d** AFM image of the topmost layer of a sample with t_{Si}=3 nm. Reprinted with permission from G. Pernot et. al., Nature Materials **9** (2010) 491. Copyright © 2010 Macmillan Publishers Limited./

Applications: Energy harvesting, cooling, heat blocking layers for thermal insulation

5.9 Conclusions

An increasing number of groups are working in various fields of nanophononics, covering, e.g., modelling of phononic crystals and heat transport at macro and atomic scale. It is important to intensify the collaboration between the various activities and create a more unified value chain for nanophononics ranging from design and modelling to heat transport calculations to experimental verification of the models. The latter requires advanced nanofabrication techniques sometimes well beyond the state of the art. An interesting nuance here is that the THz frequency range covered by nanophononics is the only unoccupied frequency band available due to the lack of practical THz sources and detectors.

A large effort is being put into solving thermal management related issues in microelectronics at package level. It has become clear that the next step should be to go inside the transistors and try to find ways to control heat dissipation at micrometre and nanometre level. Here, new models for heat transport are needed to close the gap between continuum models and molecular dynamics modelling. Extensive experimental work is needed to support and qualify the new approaches, meaning also development of improved experimental techniques. Finally, it is obvious that phonons and vibrations have an important role in biological processes. This area remains still unexplored and would potentially open new avenues to understand the interplay of phonons, photons and electrons in environments where functions have been refined and optimised through evolution in millions or billions of years.

Phononic crystals: There are several groups working on band structure calculations of phononic crystals. The calculations should be extended to cover phonon propagation to understand and predict heat transport in these structures. Fabrication of phononic crystals is rather demanding due to small dimensions and well controlled surfaces, and various nanofabrication approaches have to be tested and, in the longer term, up-scaled to wafer level.

Heat transport at nanoscale: There is a clear need to develop modelling and simulation tools for heat transport for mesoscopic structures, i.e., tools for structures with dimensions from a few nm up to a few hundred nm, a range that is difficult for continuum models and, due to huge computational power needed, impractical for atomistic models. Also, there is a need to develop experimental methods for investigation of thermal properties of nanoscale structures, methods that are commensurable and can be compared with physical models. At low temperatures the demands are more relaxed and low temperature measurements can provide a first route to experimentally test the models.

6 Conclusions and recommendations

Nanophotonics and nanophononics underpin basic science to develop know-how and methods to overcome scientific and engineering challenges in nanoscience and nanotechnology, impacting specially ICT. This is supported by the numerous applications mentioned throughout this position paper spanning not only communications but also energy, health, transport and the environment.

Nevertheless, the increasing complexity in the science of light-matter and phonon-(electron, spin) interactions in the nanoscale is resisting a reductionist approach. There are several sub-communities using highly specialised terminology and approaches which need to become more accessible to each other to enable qualitative progress in nanophotonics and nanophononics in their quest to become relevant ICTs.

Sustainable progress requires a strong synergy with new materials, instrumentation, modelling methods and nanofabrication. However, a much stronger interaction with components, nanomanufacture, design and architecture consortia is needed to make serious inroads into completing the value chain.

Although this paper does not include bio-photonics nor bio-phononics, we have much to learn from fluctuations in biology where there are ample opportunities to develop, e.g., optical, methods to study them.

Recommendations

a. Targeted European-level support for *fundamental research in application-relevant nanophotonics and nanophononics focusing first on common issues,* for example, heat dissipation at component level, using noise in ICT and ways to cope with the fluctuations in key parameters. The latter bound to be a more serious issue in the nanoscale than in the current micrometre scale but crucial for heterogeneous integration.

b. Bring together the experimental and theoretical communities of phonon physics, heat transfer (mechanical) engineering, statistical physics, biology (fluctuations), nanoelectronics, and (solid-state) quantum communications to start with a *focused research programme on heat control in the nanoscale* in the first instance and on, e.g., *harvesting fluctuations* as a follow-on or parallel focus.

c. A research infrastructure for *emerging cost-efficient nanofabrication methods* jointly with a multi-level simulation hub and a comprehensive nanometrology associated laboratory targeting nanophotonics and nanophononics applications, complementing the Si and the III-V photonic foundries. This infrastructure could then evolve into a potential foundry, with industrial participation, covering combinatory lithography, cost-analysis, packaging and training.

d. Targeted European-level support for research on *material sciences* to develop techniques able to achieve material control at the sub-nanometre and, in particular, in 3-dimensions. This includes, e.g., control of multilayer thickness of silicon-rich silicon oxide and of the barrier dielectric at the wafer scale level.

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Nanoelectromechanical systems (NEMS) Position paper- update 2011

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1. Introduction

The vibrant activities in the nano-scale research for producing finer nanostructures of various novel 1D and 2D materials, as well as advanced in on-chip integration and signal transduction supply strongly the development of NEMS. Several years of a highly interdisciplinary NEMS community at this stage yields extensive and important findings. This paper offers an update of activities in the research and development of NEMS over the last years. The following sections will describe the achievements and highlights the work done on fundamental studies using NEMS, their transduction and nonlinear behaviour, NEMS fabrication and incorporation of novel materials, including carbon-based 1D and 2D structures. Applications in the fields of electronics using linear and non-linear NEMS, bio-NEMS as well as energy scavenging will be covered.

The following text is an update of the position paper published in 2008 in E-Nano Newsletter nº 14 [http://www.phantomsnet.net/Foundation/Enano_newsletter14.php].

2. Fundamental studies

NEMS fundamental and characteristic properties, e.g. high surface-to-volume ratios, extremely small masses and small onsets of nonlinearity, make of them an outstanding scientific tool to study different physical phenomena that would otherwise be not accessible. In particular, over the years NEMS have extensively been used as tools to probe quantum physics. Originally aimed to detect individual quanta of electrical [1] and thermal conductance [2-5], we have experienced in the last few years an exciting race to cool down systems to their mechanical ground state. Even though this was finally attained by using micron-sized devices [6-7], smaller devices, in the sub-micron range and even below 100 nm, are still of the greatest interest because they are more susceptible to be affected by back-action of the surroundings, like detection or actuation techniques. Interaction with a superconducting qubit [8] or coupling to electronic conduction are some of the examples that have been recently proved [9-10].

NEMS small mass makes them ideal for mass sensing experiments. Usually, mass detection experiments seek the detection of mass landing on to the device [11]. But they can also be used to study adsorption-desorption and diffusion of particles on the device surface [12], leading to deeper understanding of the microscopic dynamics of deposited materials, together with understanding of the limitations of mass sensing with NEMS [13]. In [12], the authors used a system to perform mass spectroscopy measurements in order to monitor the landing of Xe atoms on top of the NEMS. The landing of atoms can be switched on/off via a shutter (Figure 1a). By continuously running a phase locked loop, the frequency is monitored over time for different temperatures of the device. The frequency stability can be therefore plotted as a function of temperature and different models for adsorption desorption can be checked. The data indicates that diffusion along the beam, an effect neglected up to date, is the dominant effect at lower temperatures (Figure 1b).

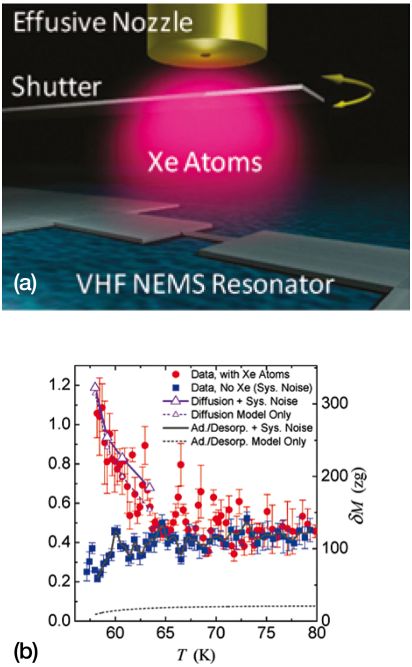


Fig. 1 > Experimental determination of the nature of frequency noise in NEMS [12] (a) Schematic showing the system utilized for the experiment with a clamped-clamped silicon carbide beam in a cryostat with a nozzle that ejects Xe atoms on the sample. (b) Frequency stability as a function of temperature with and without Xe atoms landing on the device. The noise cannot be interpreted as being caused by only adsorption/desorption of particles, but by the inclusion of diffusion of particles./

An additional topic of interest is the study of nonlinear and complex dynamics with NEMS. Their reduced dimensions make their onset of nonlinearity to be quite small, readily accessible, and easily predicted theoretically. In addition, their high quality factors and even higher frequencies make them easy to analyze quasi Hamiltonian systems and also to experimentally measure stationary states reached in very short times, i.e. few milliseconds. Finally, their small size facilitates array fabrication, which increases the complexity and the interest of the systems to be studied [14]. Numerous theoretical studies have been undertaken and published in recent years dealing with nonlinear behavior and its implications for certain applications. Euler instability in clamped-clamped beams [15] and diffusion induced bistability [16] are some of those examples.

Experimentally, the verification of the predicted behavior of a system of two coupled resonators has been shown screening rich nonlinear dynamics and even chaos [17]. A novel detection system has been proposed, based on symmetry breaking close to a Hopf bifurcation (Figure 2) [18]. But it has also been proven that it is not necessary to have arrays of individual beams to observe such behavior. Due to the nature of the nonlinearity in NEMS, it is also possible to observe such effects on one single beam using the existing coupling between several vibrational modes, which is of great importance when considering frequency-based sensing or similar applications [19]. Finally, NEMS have also been used to observe nonlinear damping in mechanical resonators, something that had not been observed before and which origin is not understood, predicted or modeled [20].

3. Transduction at nanoscale

The reduced size is what makes NEMS appealing from a fundamental and applications point of view. But everything comes at a cost, and the trade-off we need to pay in order to have such outstanding, e.g.,

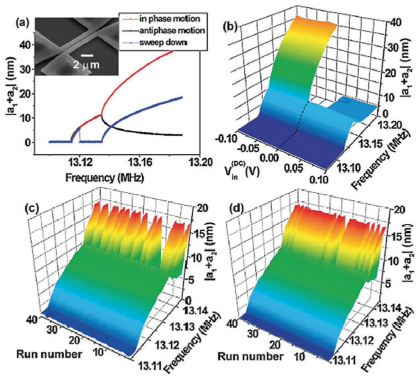


Fig. 2 > Bifurcation Topology Amplifier [18] (a) Experimental measurement of the parametric response of two uncoupled NEMS beams, confirming the predicted pitchfork bifurcation. Inset: pair of coupled clamped-clamped beams to perform the experiment. (b-d) Amplitude response of the coupled system as a function of frequency. When the voltage difference between the beams is zero (b) the system presents a perfectly symmetric behaviour and the upper branch is chosen 50% of the time. If the voltage is slightly negative (c) or positive (d) (±3 mV) the symmetry gets broken, as predicted by theory. This symmetry breaking can be interpreted as a very effective signal amplifying sensor./

sensing capabilities is very low transduction efficiencies.

In order to use a NEMS, it is necessary to make it move (actuation) and to detect such motion (detection). The combination of actuation and detection is what is usually referred as transduction. Finding an optimal transduction technique that works universally for a wide variety of NEMS has been pursued by many different research groups.

We can divide transduction mechanisms in two big groups, those based (or using) optics and those based (or using) electronics. The first group had been traditionally overlooked for NEMS, as diffraction effects were assumed to be detrimental when going deep into the sub-micron regime. However, recent experiments have shown that it is possible to not only detect motion [21-23], but also to actuate NEMS devices using optics (Figure 3) [24-26]. Another point against optical transduction methods was that they could not be integrated on-chip, which limited the future applicability of such methods. However, this has also been disproved, and integrated solutions for optical transduction have been proposed [24, 27].

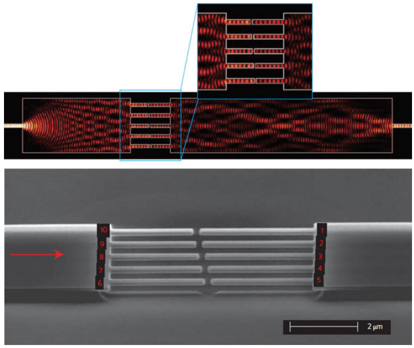


Fig. 3 > Novel transduction mechanisms for the nanoscale- photonic circuit. Simulation of the light propagation through an array of NEMS, shown in SEM image below, when no motion is present. As soon as the cantilevers start moving, misalignment occurs, and therefore the output intensity gets modulated [24]./

But even though optics seems to be catching up, electronic transduction is usually preferred, mainly due to on-chip integration possibilities. A plethora of methods have been used over the years: magnetomotive [28], thermoelastic [29], piezoelectric [30-31], capacitive [32], ferromagnetic [33], Kelvin polarization force [34], etc. A common problem for any of these methods is the fact that the motional signal produced by the NEMS is minute when compared to the parasitic cross-talk coming from the actuation signal. This is mainly caused by the great size difference between the NEMS and the necessary elements to connect it to the macroscopic world like metal pads, wire bonds, etc. This undesired effect creates a background on the response of the device that hides the actual mechanical signal and makes it very difficult to be distinguished, which in turn affects the stability of the closed-loop systems, used for frequency-based sensing. A number of solutions have been proposed to solve this issue, most of them based on the use of some mixing mechanism that moves the frequency of the detected signal away from the frequency of the actuating signal. Down-mixing [35], amplitude modulation [36-37], frequency modulation [20, 38], use of superior harmonics actuation [39], parametric actuation [40] are some of the mentioned techniques used to cancel the effect of the background and have given much more stability and superior performance than more traditional approaches as direct bridging of the signal [41-42].

However, even though these techniques have proven very useful from a research point of view, the most promising option for future integration and with wider applicability is the use of an on-chip amplifier located very close to the NEMS [43], or even within the mechanical device itself [44-47]. The amplifier boosts the motional signal, making it bigger and less susceptible to the parasitic effect mentioned before. At this point the problem then stops being the NEMS and becomes electronic (how to lay-out best a series of transistors to obtain the biggest gain with the smallest noise) and/or technological (how to integrate on-chip the mechanical device with the adjacent electronic circuitry).

4. Materials, Fabrication & System integration

Most of the fabrication methods used for investigating the ultimate performance of NEMS devices still rely on silicon based technology. The reason is the combination of good mechanical properties and well-established processing methods. Mechanical resonators require materials that provide high quality factors and high resonance frequency. For this reason, the most relevant progress in the exploitation of the functional properties of NEMS devices has been obtained with devices made of silicon [48-49], silicon nitride [50-51], silicon carbide [52-55] or related materials like SiCN [56], addressing a range of diverse aspects like ultra-high frequency operation [49], information processing [48], parametric amplification [51-52] or sensing [53, 57]. Remarkably, silicon is also present in the promising approach of building-up devices based on bottom-up fabrication methods. For example, a silicon NEMS resonator made of a single silicon nanowire grown by CVD methods combines good mechanical properties, ultra high mass sensitivity and additional functionality given by the possibility of exciting flexural modes in two dimensions [58] (Figure 4).

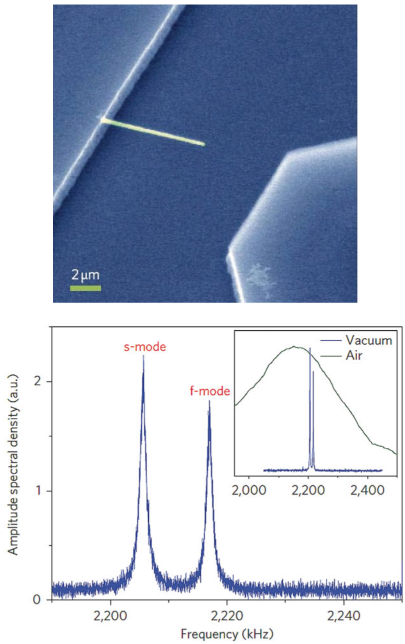


Fig. 4 > NEMS resonator made of a single crystalline silicon nanowire provides good mechanical properties, high resonance frequency and high quality factor, that can be exploited to build-up ultra-high sensitivity mass sensors, including extra functionality due to the existence of several resonance modes. The frequency response of the nanowire can be detected by optical methods [58]./

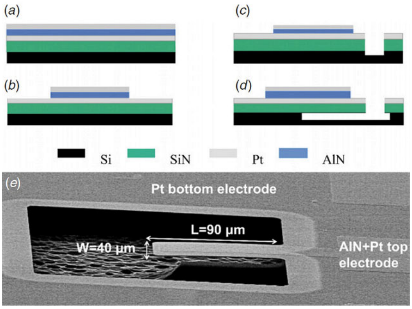


Fig. 5 > Fabrication process and SEM picture of cantilevers with 50 nm thick AlN films that provide ultra-high sensitivity mass sensing with electrical transduction [59]./

In parallel to this majority use of silicon based technology, an increasing attention is being paid to piezoelectric materials due to the possibility of easy implementation of self-transduction (sensing and actuation) [31, 44, 59-60]. Realization of SiN/AlN piezoelectric cantilevers was made (Figure 5). 50 nm thick AlN films presents high piezoelectric coefficient that enables electrical transduction with excellent frequency stability, while SiN provides the good mechanical behaviour, demonstrating an achievable limit of detection of 53 zg/µm^2.

Electron beam lithography is still the most used method to define NEMS devices from an experimental point of view, as it is a simple and proven method, although not convenient for massive fabrication and future industrial application. New prototyping approaches have been recently reported, including the use of focused ion beams [61-65]. However, little progress has been made in finding processes that would allow scaling up the fabrication of NEMS. Some activities include the technology being developed by the so-called *Nanosystems alliance* between Leti and Caltech [66], optical based technologies for fabricating single carbon-nanotube devices [67], and the extension of CMOS technology to integrated NEMS resonators in microelectronic circuits taking advantage of the high resolution provided by DUV optical lithography [68-72] (Figure 6).

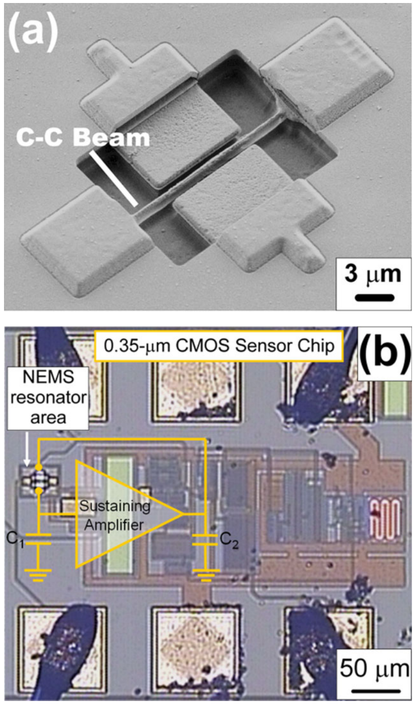


Fig. 6 > Integration of NEMS into CMOS using conventional DUV optical lithography. (a) Shows an SEM image of clamped-clamped metallic beam: the closely located electrodes serve for electrostatic actuation and capacitive detection. The resonator is monolithically integrated into the CMOS circuit shown in (b) for building-up a self-oscillator system [69]./

Besides the top-down fabrication, new approaches have been explored for parallel integration of 1D nanostructures (carbon nanotubes (CNTs), Si NW, ZnO NW) into functional devices. Usually a bottom-up technique is necessary for growing from small amounts of catalysts wire-like nanostructures in a specific chemical and thermal environment. Blank or micrometer-size “forests” of such 1D nanostructures can be easily grown from lithography-defined catalysts. But reaching a position-controlled, single-digit number of wires using parallel fabrication techniques is still a worth-while goal. The localized synthesis can be done by having control either over the thermal environment or over the catalyst position. Blank deposition of the catalyst material combined with localized heating during the growth has been demonstrated [73-81]. Both methods are consistent with horizontal growth on vertical sidewalls, enabling the nanostructures to be positioned between two electrodes.

An alternative method is the localized deposition of the catalyst via parallel techniques such as stencil lithography. The advantage here is the possibility of reaching the single nanostructure limit with high-resolution positioning accuracy [82-83]. Self-limiting deposition of carbon nanotubes from suspension gains control on the number and simultaneously on the orientation of nanostructures positioned between electrodes, allowing for piezoresistive pressure sensors based on single-walled CNTs [84].

The fabrication of suspended nanotube devices was also demonstrated by on-chip stencil lithography that allowed resistless fabrication of electrical contacts to as-grown single-walled CNTs (Figure 7). Contamination issues of wet chemistry are avoided and hysteresis-free CNT FET operation was achieved. Furthermore, shadow masking is compatible with a wide range of contact materials and the contacts are self-aligned to the suspended section of the nanotube [85]. To fully benefit from the tapered contact geometry and the material compatibility, large-scale processes have to substitute the manual movement of the shadow masks. The reduction of charge traps by metallising all oxide surfaces may contribute to drift-stability in the electronic readout of NEMS and cleanliness might help to minimize damping.

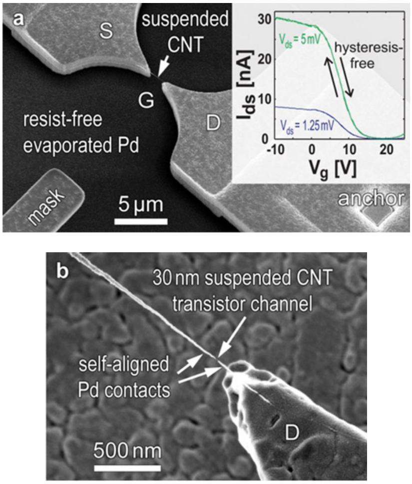


Fig. 7 > Hysteresis-free transistor response of a suspended carbon nanotube contacted by contamination-free shadow masking [85]. (a) SEM image of a nanotube transistor and electrical transfer characteristics. The shadow mask is retracted. (b) Close-up view of the same 30 nm long transistor channel with self-aligned Pd contacts./

In graphene-based NEMS, lithographically fabricated graphene edges are typically nanometre-rough, which can affect the uniformity of characteristics in a set of devices. Cai et al. [86] achieved ultimate dimensional precision by a synthesis technique based on covalent interlinking of precursor monomers. This chemical route provides atomically precise edges and uniform widths of graphene nanoribbons. So far, the surface-assisted synthesis requires metallic substrates hindering device fabrication. Transfer to technologically relevant non-conducting substrates, dedicated etching processes or alternative synthesis surfaces will be needed for NEMS fabrication. The demonstration of junction monomers encourages further investigations to engineer covalently bonded electrical contacts to atomically precise graphene nanoribbons.

Combination of NEMS devices with CMOS circuits provides also a route towards system integration, as it incorporates on-chip the functionalities of signal read-out and amplification. Alternative directions to integration have been proposed in order to reduce the parasitic signals in capacitive detection [87-88]. In addition, many efforts are directed towards combination with diverse devices and structures: integration of field effect transistor for electrical read-out [89-90], integration of a Schotky diode for optical detection [91], integration of waveguides [92-93] and integration of nanofluidic channels [94]. In this latter approach, the degradation of the performance that experience mechanical resonators when operated in solution due to the viscose drag is overcome by defining a suspended nanochannel (Figure 8). Using this approach, the best mass resolution in solution using NEMS sensing 27 ag has been demonstrated. A step further in the use of NEMS for system integration is the proposal of using piezoelectric NEMS resonators for extracting signals from biosensors [95]

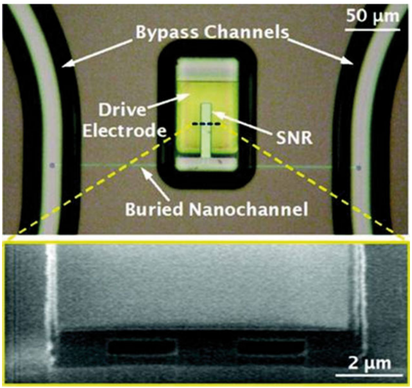


Fig. 8 > Suspended nanochannels used for the realization of NEMS mass sensors, providing a mass resolution below 30 ag [94]./

5. Electronics

NEMS devices may play a role in future electronics both in the analogue and digital areas. For several years they have been proposed as basic building blocks for telecommunication systems by replacing components that cannot be integrated using conventional technologies. More recently, application of NEMS in information processing is gaining more attention, mainly because their lower power consumption and harder resistance to harsh environments compared to pure electronic processing in miniaturized systems. Application of NEMS for developing high efficiency telecommunication systems is being addressed by several groups [43, 67-68, 70-71, 96-104]. NEMS resonators are called to replace quartz crystals in the field of the RF communications due to their capability to be fabricated with standard IC process, the higher frequencies they can achieve and the small area they require.

The primary building blocks for any telecommunication system are oscillators. Self-sustaining oscillator with feedback can be implemented by employing a NEMS resonator as the frequency determining element for the feedback oscillator. Such NEMS oscillators are active systems that are self-regenerative; thus are distinct from the more readily available NEMS resonators, which are passive devices and require external signal sources to provide periodic stimuli and driving forces to sustain the desirable stable oscillations. Therefore the NEMS oscillators clearly could have important potential for a number of emerging applications. An important drawback when reducing the dimensions of NEMS is the resulting increase of the motional resistance, especially for the use of capacitive detection. In this case, piezoresistive sensing is viewed as a promising alternative [104]. Some other relevant examples of the use of NEMS for telecommunications are the mechanical implementation of filters [70] and frequency convertors [96].

NEMS switches also present great potential for application in other areas, like logic computation [105] and memories [48, 106].

Main advantages are not only the expected lower power consumption [107], but also the possibility for operation at high temperatures [54]. The feasibility of building-up several computational and memory blocks by using only passive components and mechanical switches has been recently demonstrated [108]. Although NEMS-based switches cannot compete with MOSFETs in terms of switching speed, they can provide alternative paths for reduction power consumption of electronic circuits, with possibilities for high density integration [109]. A paradigmatic example is the realization of the analogous of a semiconductor transistor by means of a three-terminal NEMS switch [110]. NEMS switches provide zero leakage current, almost infinite sharp on/off transitions and a square hysteresis window.

6. Nonlinear MEMS/NEMS applications

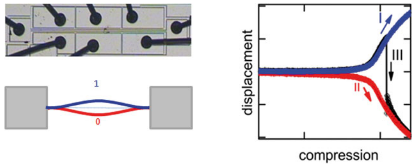
Mechanical sensors and actuators usually act as linear transducers. It is worthwhile having a look at the behaviour of mechanical resonators several 10s of microns in size to learn and adapt to sub-micron scale, where possible. At large amplitudes nonlinear effects dominate the response and reduce the range over which mechanical resonators can be applied as linear transducers. Nonlinear effects can be balanced in order to restore a linear response [88, 111-113]. On the other hand, there is a growing interest in MEMS/NEMS operating in the nonlinear regime. Characteristic phenomena were observed in the nonlinear regime, including multi-stability, hysteresis, and chaotic motion [14, 19, 114-115]. Several new applications based upon nonlinear MEMS/NEMS have been demonstrated. This is an important range in sensor applications, and to enhance it several concepts have been proposed.

Figure 9 summarizes four nonlinearities in doubly clamped beams or wires and singly clamped cantilevers that are 10s of micrometer in size. Euler buckling, Duffing nonlinerarity, geometric nonlinearity and parametric instability. Perhaps the best-known instability in mechanics is Euler buckling (Figure 9 a) and makes use of a buckled bistable beam that does not require energy to remain in a bistable state. This enables applications in micromechanical relays, switches and non-volatile memory [106, 116-118]. Other nonlinearity in doubly clamped resonators is due to the displacement-induced tension, Duffing nonlinearity (Figure 9 b). Here two vibration amplitudes can be stable at the same driving conditions and fast transitions between the states can be induced by applying short excitation pulse. The distinct jumps in this bistable response can be used to resolve closely spaced resonators in arrays [113, 119-120]. Strongly driven cantilevers exhibit a similar response, a geometric nonlinearity, as is shown in Figure 9 c. Since the cantilever is singly-clamped, it can move without extending leading to parametric instability [19, 88, 121]. Besides driving a resonator with a force, it can also be driven by periodically changing one of its parameters, for example the spring constant. When this parametric drive exceeds a threshold, oscillations occur and two phases of the resonator are stable [122], see Figure 9 d. A small change in the driving signal alters the symmetry of the system, and can be detected very accurately by measuring the probability of the resonator being in either phase [123]. Small signals can also be detected by dynamically changing the coupling between two parametric oscillators [18].

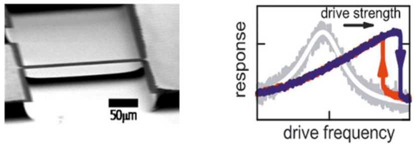
A bistable mechanical resonator can be used to represent digital information and several groups have demonstrated mechanical memory elements. Elementary mechanical computing algorithms have been implemented by coupling resonators in a tuneable way [30, 124]. The coupling can also be formed by properties intrinsic to the resonator. In this case, no connections are needed as the algorithm is executed in a single resonator. This concept was demonstrated by exciting a parametric resonator at multiple frequencies, where each excitation signal represents a logic input, and the resulting motion is the output (Figure 10) [125].

The high Q-factor of mechanical systems compared to electronic circuits, and the low 'on' / high 'off' resistance of MEMS/ NEMS switches could provide a key to low-dissipation signal processors, and it is believed that mechanics holds a promise of low-power computing in the distant future [126-127]. Mechanical computing is also applicable in harsh conditions where electronics fail, e.g. at high-temperatures or in high-radiation environments (oil industry, space and defence).

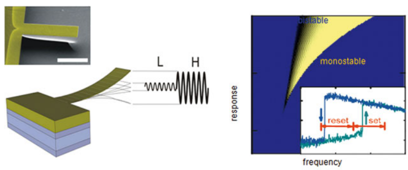
In a bistable MEMS/NEMS, otherwise detrimental noise can be employed to amplify the response to weak signals. This counter-intuitive process where noise enables the detection of weak signals is called stochastic resonance, and has been demonstrated in doubly-clamped beams at high noise levels [128-131]. Noise-induced switching between stable states of a nonlinear oscillator can also improve the figure of merit in energy harvesting applications [132]. By matching the energy barrier to the noise intensity, the noisy displacements of a bistable piezoelectric power generator are amplified and this results in an increased output voltage, when compared to energy harvesting with a linear transducer. Implementing this scheme in nonlinear MEMS/NEMS could lead to efficient power generators for stand-alone devices.



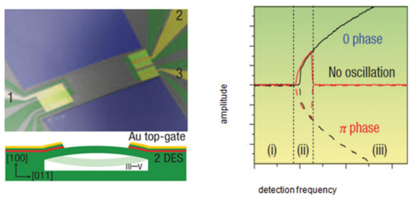
(a) **Euler buckling:** A doublyclamped beam buckles when the compressive stress exceeds a critical limit. The post-buckled state, up(1) or down(0), represents one bit of information [106, 116-118].



(b) **Duffing nonlinearity:** In doubly-clamped beams and strings, the displacementinduced tension results in bistability. At the same drive conditions, vibrations with a high and a low amplitude are stable [19, 133].



(c) **Geometric nonlinearity:** In cantilever beams vibrating at large amplitudes, by the geometric nonlinearity the resonance frequency becomes dependent on the amplitude. The amplitude of a strongly driven cantilever is bistable [88, 120-121].



(d) **Parametric instability:** A parametric oscillator is driven by modulating the spring constant at twice the resonance frequency [122-123]. Information can be encoded in the oscillator phase: $\Phi=0$ (0) or $\Phi=\pi$ (1) are stable.

Fig. 9 > Nonlinearities in microresonators: the designs and responses of doubly-clamped beams, wires and singly-clamped cantilevers./

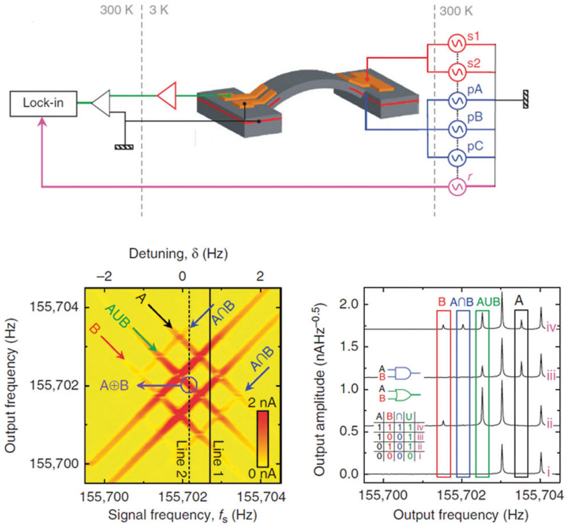


Fig. 10 > Multi-bit logic in a doubly-clamped resonator. (a) Setup and resonator with integrated piezoelectric transducers for direct and parametric driving and on-chip motion detection. The response is measured close to the resonance frequency f0 by directly driving the resonator at $f_s+\delta$, while parametrically exciting it at $f_{pA}= 2f_0+\Delta$ and $f_{pB}= 2f0-\Delta$. (b) Mixing between the parametric and direct drive results in splitting of the mode, where higher order mixing frequencies occur when $\Delta\neq 0$. When the parametric driving signals are considered as logic inputs, where A (B) denotes the presence of the parametric excitation at f_{pA} (f_{pB}), logic functions can be implemented. Depending on the drive frequency (horizontal axis) and the detection frequency (vertical axis), the resonator functions as an AND (∩), OR (∪), and XOR (⊕) gate. (c) shows cross-sections of (b), to demonstrate the resonator logic response when the parametric signals are switched on and off. In these experiments Δ=0.5 Hz. More complex logic functions are possible by generating more mixing frequencies by driving the resonator at multiple frequencies./

7. Carbon based NEMS

Despite most NEMS devices being based on silicon technology, during the last years carbon-based NEMS devices have been gaining more and more interest, mostly because of their high Young modulus and small diameter. The carbon-based mechanical resonators have large tunable frequencies and exhibit large amplitudes. Due to their low mass, they operate in a different regime from their silicon-based counterparts, as evidenced by the very strong nonlinear response. Moreover, they generally exhibit an extremely high sensitivity to external stimuli, making them interesting candidates for various sensing applications for fundamental studies as well as applications. As discussed above, fabrication processes for carbon nanotube based and graphene based NEMS resonators are now well established for prototyping and demonstration activities. From an applied point of view, the challenge is to fabricate devices suitable for large-scale applications that operate at room temperature. Future research is still necessary to elucidate which of the two carbon forms, carbon nanotubes or (few layer) graphene, due to its larger area, is easier to contact and to fabricate on an industry-scale [134].

An example of a suspended carbon nanotube device is shown in Figure 11. These bottom-up devices are expected not to suffer from excessive damping, as their surface can be defect-free at the atomic scale. Combined with their low mass the expected low damping makes them ideal building blocks. Moreover, because of their small sizes carbon-based resonators typically have frequencies in the MHz to GHz range. All these properties (low mass, high Q, large frequencies) are advantageous for sensing applications and the study of quantum properties of resonating objects [135]. For example, when cooled to dilution refrigerator temperatures, carbon-based resonators can be in the quantum mechanical ground-state while exhibiting relatively large amplitude zero-point fluctuations.

Position detectors of carbon-based bottom-up NEMS, however, are not yet as sophisticated as those for the larger top-down silicon-based counterparts. Consequently, neither non-driven motion at cryogenic temperatures (either Brownian or zero-point motion), nor active cooling have been reported for carbon-based NEMS. Nevertheless impressive progress in understanding the electromechanical properties of bottom-up resonators has been made in recent years using so-called self-detecting schemes. In these schemes, the nanotube or graphene resonator both acts as the actuator and detector of its own motion.

Various device geometries with carbon-based materials exist. The motion of singly-clamped carbon nanotubes has been visualized in scanning [136] and transmission electron microscopes [137]. Another method to detect motion of singly-clamped carbon resonators is based on field emission of electrons from a vibrating tip [138]. When a large voltage is applied between a multi-walled carbon nanotube and an observation screen, it lights up at the position where electrons accelerated by the electric field are impinging. The vibration amplitude is enlarged by applying a RF driving signal, and the spot blurring becomes even more pronounced on resonance. Furthermore, the electric field also pulls on the nanotube, thereby increasing the resonance frequency. The method has also been used to build a nanotube radio [139] and a mass sensor approaching and achieving atomic resolution [140].

For doubly-clamped resonator geometries, it is also advantageous to use the suspended device ***itself*** as a detector of motion. Using current rectification and frequency mixing, information about the driven motion of the suspended nanotube and graphene has been obtained. Sazonova ***et al.*** [36] were the first to apply frequency mixing to suspended carbon nanotube resonators. They observed multiple gate-tunable resonances with Q-factors on the order of 100 at room temperature. Subsequently the bending mode vibrations of a carbon nanotube were also identified [141]. Nowadays the technique has been employed by many groups, not only restricted to carbon nanotubes, but also to suspended doubly-clamped graphene sheets [37]. Furthermore, several variations to the original mixing scheme have been implemented, including frequency [142] and amplitude modulations [143].

At low temperatures, Coulomb blockade can be used to drastically enhance the displacement sensitivity. For example, the change in equilibrium position of a suspended nanotube quantum dot after adding a single electron easily surpasses the zero-point motion. A strong coupling results between mechanical motion and the charge on the nanotube, leading to frequency shifts and changes in damping as a function of gate voltage [10, 144]. The readout using current rectification is employed instead of frequency mixing [10, 145]. While the nanotube motion is actuated by a RF signal on a nearby antenna, the detected signal is at DC (Figure 11, page 48). The key to understand this is the notion that nanotube motion effectively translates into an oscillating gate voltage, leading to changes in the DC current, which are the largest on resonance.

The technique is of special interest as it allows for the motion detection with small currents, enabling the observation of ultra-high Q-factors, exceeding 100,000 at mK temperatures [145]. Furthermore, the experiments show that the dynamic range is small, i.e., carbon-based resonators are easily driven into the nonlinear regime as illustrated in Figure 12 (page 48). This can be understood from the small tube diameters or the extremely thin membrane-like shape of the graphene flakes: with increasing driving power the amplitude of flexural motion rapidly grows to their characteristic sizes inducing sizable tension in the resonator. In addition,

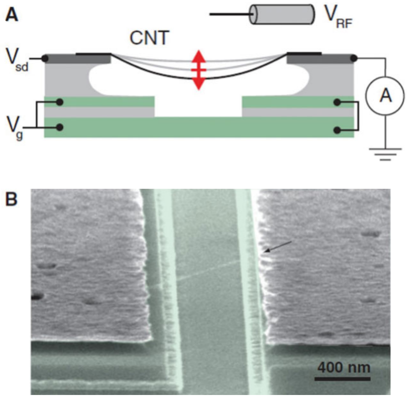


Fig. 11 > a) A high Q mechanical resonator layout with suspended carbon nanotube; A suspended carbon nanotube is excited into mechanical motion by applying an ac voltage to a nearby antenna b) SEM image of a suspended carbon nanotube clamped between two metal electrodes. A bottom gate can be used to tune the frequency of the resonator, b) [10, 145]./

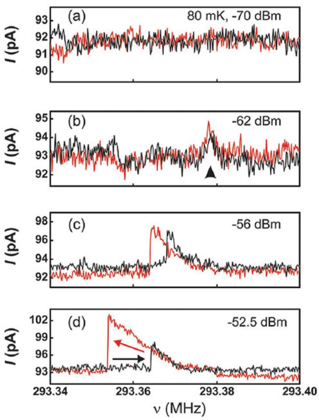


Fig. 12 > Evolution of the resonance peak with increasing driving power (a-d) at a temperature of 80 mK [10]. Black (red) traces are upward (downward) frequency sweeps. At low powers, the peak is not visible, but upon increasing power, a resonance peak with Q=128627 appears. As the power is increased further, the line shape of the resonance resembles the one of a Duffing oscillator exhibiting hysteresis between the upward and downward sweep [145]./

nonlinear damping effects have recently been reported using mixing techniques in nanotube and graphene resonators [146]. Finally, electron tunneling and mechanical motion are found to be strongly coupled [144-145] resulting in single-electron tuning oscillations of the mechanical frequency and in energy transfer to the electrons causing additional mechanical damping.

8. Towards functional bio-NEMS

High-frequency NEMS are attracting more and more interest as a new class of sensors and actuators for potential applications to single (bio)molecule sensing [53, 147]. For NEMS to be considered as a viable alternative to their actual biosensing macro counterparts, they have to simultaneously meet three major requirements: high mass responsivity (MR), low minimum detectable mass (MDM) and low response time (RT).

Without any doubt, as emphasized by theoretical studies [148-149], the two first specifications (MR and MDM) can be successfully addressed by NEMS devices. Such predictions have been already validated in case of virus sensing [150], enumeration of DNA molecules [151] or even single molecule nano-mechanical mass spectrometry [53]. Hopelessly, nanometer scale sensors have been proved, still in theory [152-153], to be inadequate to practical RT scales which, if confirmed as such, could definitely impede the NEMS' route towards realistic biosensing applications. To prevent this from happening, one possible trade-off strategy would consist in taking advantage from considering a single NEMS device not alone, but as part of a functional array of similar devices [154]. This paradigm allows, while preserving the benefits of high MR and low MDM of a single device, to use the considerably higher capture area of the NEMS array, because the RT reaches practical relevance. However, in that case, the non-reactive areas of the chip containing multiple sensors functionalized with a single type of probe molecule must be adequately coated with an anti-fouling film in order to lower the probability of adsorption of target molecules anywhere else than on sensitive areas and hence to permit ultra-low concentration detection.

To address the production of massively parallel arrays of NEMS for bio-recognition applications, one has to be able to perform uniform, reliable bio-functionalisation of nanoscale devices at a large scale (the array's level), while being able to obtain an anti-fouling surface everywhere else. For this to become reality, a major challenge is the functionalisation of closely packed nanostructures in such a way that biological receptors are precisely located solely onto the active biosensing areas, thus preventing the waste of biological matter and enabling the subsequent biological blocking of the passive parts of the chip. So far, the issue of the freestanding nanostructures functionalisation has been seldom addressed because of the absence of generic tools or techniques allowing large-scale molecular delivery at the nanoscale. One way to circumvent this difficulty would be to perform the functionalisation step before completing the fabrication of the NEMS. This strategy can typically be used in a top-down NEMS fabrication process by protecting the biological layer during the subsequent NEMS fabrication steps, that consists in placing the functionalized nanostructures at specific locations on a substrate and releasing them [155] The main limitation of this strategy is the trade-off between the choice of the post-functionalisation processing steps and the resilience of the chosen biological receptors to such technological constraints, which for most of them are biologically unfriendly.

9. Energy harvesting

The impact of NEMS technology in the energy harvesting field, i.e. a discipline aiming at converting wasted ambient energy into useful electrical energy to power ultralow consumption ICT devices, is still incipient. A notable level of maturity has been achieved in this field by MEMS applications, where energy is extracted from ambient vibrations. Several mechanical to electrical transduction methods have been applied so far, but piezoelectric has demonstrated to be the preferred solution because of the increasing integrability of piezomaterials and, especially, due to the simplicity of the associated power management circuitry. Although most of the technologies and concepts that have been demonstrated to be feasible at the micro-scale using MEMS are not improved when dimensions are reduced at NEMS scale, the combination of piezoelectric and nanowire technologies becomes relevant. A very recent study [156] theoretically demonstrated the giant piezoelectricity of ZnO and GaN nanowires, which is due to the effect that charge redistribution on the free surfaces produce the local polarization. This effect, which has been theoretically reported previously [157], demonstrates that it is more efficient to fill a certain volume with a compact array of nanowires than to use a bulk thin film piezoelectric substrate, a clear enhancement produced by nanometre scale downscaling. An exhaustive study of the potential performance of piezoelectric nanostructures for mechanical energy harvesting is provided by C. Sun et al. [158]. In this paper, the authors compare rectangular and hexagonal nanowires and 2-D vertical thin films (nanofins), as well as different piezomaterials such as ZnO, $BaTiO_3$, and conclude that the power density ideally obtainable by filling the whole volume is in the range of 10^3-10^4 W/cm^3.

This previous concept is in fact experimentally exploited in many different ways to implement energy nanoconverters or energy nanoharvesters based on arrays of piezoelectric nanowires. One specific nano piezotronic technology is based on combining the piezoelectric properties of ZnO nanowires or fine-wires (its micro scale version) with the rectifying characteristics of the Schottky barrier, formed between the ZnO (semiconductor) and a metal. Most recent work demonstrate biomechanical to electrical conversion using a single wire generator, which is able to produce output voltages around 0.1 V from human finger tapping or from the body movement of a hamster [159], or even from breathing and heartbeat of a rat [160], which demonstrate the potential applicability of NEMS on self-powering implanted nanodevices. High-output power nanogenerators have been also obtained by a rational assembling of ZnO nanowires in a 2-D array. The obtained nanogenerators are able to power real devices as a LED [161] or an LCD [162]. Power densities of 11 mW/cm^3 are experimentally demonstrated and by multilayer integration 1.1 W/cm^3 are predicted.

Still in the field of biomechanical energy harvesting, a very recent study solves the performance trade-off between piezoelectric coefficient and stretchability [163]. Typically, organic piezoelectric materials like PVDF (Polyvinylidene fluoride) are flexible, but show weak piezoelectricity and inorganic ceramic materials as PZT, ZnO or $BaTiO_3$ have piezoelectric coefficients one order of magnitude higher, but are brittle. PZT ribbons buckled by the attachment on a pre-stretched PDMS substrate display simultaneously high piezoelectricity and integrity under stretching and flexing operations [163]. Also the embedding of PZT nanofibers into a PDMS substrate is used to generate peaks of voltage and power around 1.6 V and 30 nW from external vibrations, respectively [164]. But not always organic means low piezoelectricity. The method to directly write PVDF nanofibers with energy conversion efficiencies one order of magnitude higher than those of thin films was developed [165]. The method, based on near-field electrospinning allows the mechanical stretching, polling and positioning of the nanofibers. Finally, a very smart example of inorganic piezoelectric into organic polymer embedding is of ZnO nanowires embedded into a PVC substrate [166]. The collective stretching of the nanowires produced by the temperature induced polymer shape-change allows achieving power densities around 20 nW/cm^3 at 65°C by means of a non-conventional thermoelectric effect.

Solutions to unsolved challenges, such as a real co-design of the NEMS energy transducers and the power management circuitry or the introduction of unexplored materials to span the sensitivity to new energy sources, will define the future research tendencies in this field. As an example, suspended graphene nanoribbons have demonstrated to efficiently harvest the energy from thermal fluctuations due to the mechanical bistability induced by a controlled compressive stress [167].

10. Summary and outlook

The progress in the field of NEMS has continued at good pace during the last years. The area of NEMS is entering into a more mature stage, addressing real applications in the areas of sensing, telecommunications, information processing and energy harvesting. A step forward is made for better understanding of nonlinear behaviour contributing to sensing and logic applications. The easy access to the nonlinear regime and the defect-free material properties make NEMS also excellent tools to study nonlinear dynamics in a more general context. Signal detection and sensitivity limits together with NEMS integration into complex systems at larger scale are continuously enhanced. Incorporation of new materials improves device performance in terms of sensitivity, working range and efficiency.

While device concepts and fundamental knowledge of the properties of NEMS structures are very much advanced, a fabrication technology that would fulfil the requirements for high dimensional precision, material compatibility and high throughput is still the limiting factor for commercial applications. In consequence, more effort in developing suitable fabrication methods adapted to industry is advisable to guarantee the future success of the field.

The field of nonlinear NEMS is emerging, and new phenomena are discovered which will be applicable in ultrasensitive detectors, mechanical signal processors and efficient energy harvesters. Weak signals can be amplified by making beneficial use of environmental noise, by employing processes like stochastic resonance. At weak driving devices may be optimized as to achieve nonlinear characteristics to reduce the electrical power consumed by the strongly vibrating NEMS. To this end, it is essential to understand the dissipation mechanisms in NEMS resonators. Modelling nonlinear NEMS requires numerical methods, which can be computationally intensive even for simple beam structures. More complex structures with multiple degrees of freedom can be hard to impossible to model quantitatively. Tight fabrication tolerances are required in order to predict and/or reproduce the dynamic behaviour in the nonlinear regime within a workable tolerance window. In order to employ noise-enhanced detection schemes, the barrier between the stable states of the bistable NEMS should be reduced. New ways to couple nonlinear NEMS in an efficient and adjustable way will further expand the NEMS toolbox. It allows the construction of extremely complicated dynamic systems, with many new concepts being discovered at present, and still a wide horizon to be explored.

Carbon-based mechanics is a relatively new research field, but the push for refining detection schemes and integrating carbon-based materials into silicon technology will undoubtedly lead to the construction of better sensors, which may eventually be quantum-limited. A bright future thus seems to being lying ahead for these miniature devices. From a fundamental physics point of view, challenges lie in improving detection schemes so that thermal motion at low temperatures and eventually zero-point motion can be detected. From a fundamental physics point of view, challenges lie in improving detection schemes so that thermal motion at low temperatures and eventually zero-point motion can be detected. The carbon-based resonators also provide a unique system to study the nonlinear properties of mechanical resonators especially in the quantum regime. Furthermore, it is presently still unknown what the limiting factor is in the intrinsic damping of carbon-based resonators. This is a more general issue in NEMS as damping in silicon resonators is also not understood in detail.

In the field of energy harvesting, the challenges to be faced are related not only to the efficient conversion, but also to the management and storage of the harvested energy at the nanoscale. Novel concepts and devices based on NEMS technology and oriented to the management/storage of the energy in a pure mechanical form would improve the energy efficiency of the overall harvesting process, since no conversions from the mechanical to the electrical domain would be needed. And finally, cchallenges making use of NEMS arrays in the biosensing realm can be thus foreseen both at the front-end for differential functionalisation of closely packed sensors and at the back-end, for the integration of actuation and sensing capabilities at nanodevice arrays levels.

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Conducting metallic nanowires for flexible transparent electrodes

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Nanomaterial; Nanowires; Transparent Electrodes; Silver

1. Introduction

Transparent electrodes are widely used in technologies like LED displays, photovoltaics, touch screens, etc. The fabrication of high quality transparent electrodes is not simple since excellent performances are expected for both optical transparency and electrical conductivity.[1] The current industrial technologies mainly rely on vacuum processes and TCOs (Transparent Conductive Oxides) such as ITO (Indium tin oxide) and FTO (Fluorine doped tin oxide) films. The as-made ITO transparent electrodes suffer from some limitations like costly fabrication process and risky price of indium. Moreover, a major issue comes from the brittleness of such materials since they are highly prone to cracking on flexible substrates. This last point is actually a significant drawback because many commercial devices are expected to be highly bendable in a near future. The market of conductive films for flexible electronics is forecasted to be more than 3 US$ billion in less than 10 years, which is obviously a striking figure.[2] Thus there is real need to find new low-cost, large area, high performance, solution-processable materials to fabricate these electrodes. Some significant work has recently been carried out using organic polymers, carbon nanotubes, graphene or metal grids for fabricating transparent electrodes with good performances. [3, 4] However up to now the overall performances are not satisfactory for a large panel of applications.

Recently, extensive efforts have been performed to develop transparent electrodes based on conducting nanowires. The idea is to create one-dimensional nanomaterials with very high aspect ratio and excellent electrical conductivity that could be deposited as a percolative random network. Thanks to percolation (which implies very low contact resistances between contacting nanowires), it should possible to obtain thin films with high electrical conductivity, and high transparency since nanowires would be scarcely deposited on a surface, leaving plenty of space for light to go through. The efficiency is expected to be comparable to those of TCOs, plus bendability property.

2. Synthesis of metallic nanowires

Up to now, the most studied metal is silver. This can be attributed to its very high electrical conductivity (63×10^6 $S.m^{-1}$), and to the rather simple batch process to make large amounts of nano-objects. The solvothermal route is convenient for making solutions of silver nanowires which can be directly used by various deposition techniques.[5] The diameters of the nanowires are generally in the range 40-70 nm, and the lengths between 2 and 20 µm. The solutions of silver nanowires are stable for weeks.

3. Fabrication of electrodes

Various techniques can be used to fabricate transparent electrodes including spin-coating, airbrush spray, drop casting and others. Different substrates can be used, most often glass or transparent plastics are preferred. Eventually, random networks of nanowires can be transferred by PDMS stamps, laminated or embedded in polymers to afford conductive transparent materials

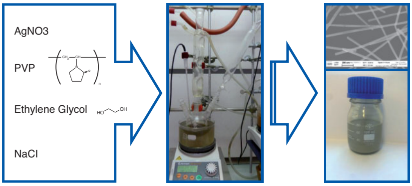

Fig. 1 > Synthesis of silver nanowires.

with lower roughness.[6-8] Typically, sheet resistances lower than few tens of ohm.sq^{-1} are obtained at 90% transparency in the visible spectrum, down to less than 1 ohm. sq^{-1} at ~60% transmission.

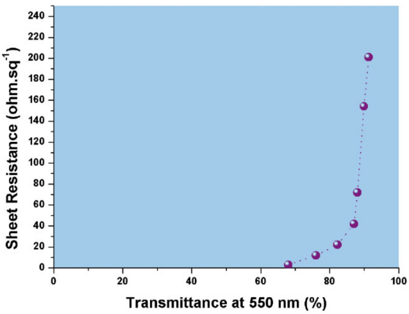

Fig. 2 > Sheet resistance as a function of the transmittance for Ag NWs based electrodes.

The electrical conduction through the network of nanowires can be described by percolation theory. Several figures of merit have been proposed to characterize and compare this technique with other nanomaterials based electrodes.[9] The results are very promising notably with regard to emerging technologies based on carbon nanotubes or graphene. Further improvement appears still possible for instance by enhancing the form factor of the individual building blocks.

One of the main advantages to use such nanomaterials is related to the fact that high flexibility can be achieved. Many bendings at low radius of curvature can be realized without alteration of the sheet resistance, which is clearly not the case for TCOs deposited on plastics.

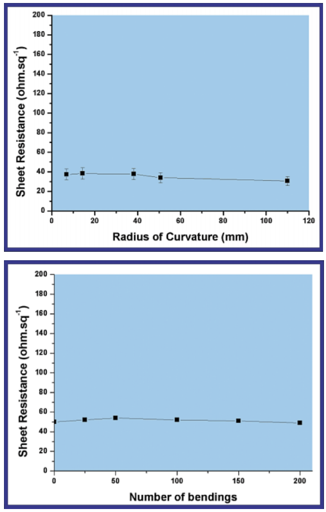

Fig. 3 > Sheet resistance as a function of a) radius curvature and b) number of flexion for Ag NWs based electrodes on PEN.

4. Application to functional devices

Beyond intrinsic performances of the electrodes, a major challenge comes from their integration in functional devices. Some recent works have shown that silver nanowires can be good candidate for various applications, keeping in mind that for multilayered structures, surface roughness of the electrode should be minimized in order to avoid potential shorts. Indeed, the nanowires are rather long (few microns or tens of microns) and can protrude to form local spikes. The smoothing of electrodes can be achieved by different processes like lamination, dry transfer technique, or nanowires can be embedded in polymers to solve this issue. Several functional devices have been prepared using silver nanowire based electrodes with interesting comparison to conventional TCO electrodes. Some recent reports on light emitting devices demonstrate the great potential of this technology.[10] For instance, Pei at al. have shown that flexible silver nanowire electrodes on a crosslinked transparent polyacrylate substrate are suitable for the fabrication of flexible polymer light emitting diodes.[11]

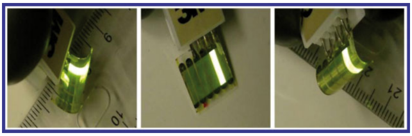

Fig. 4 > Source: Ref 10

Solar cells are currently amongst the most studied devices. Some recent works have shown that silver nanowires can be good candidate for this application, in particular for organic solar cells.[7, 12] For instance, Peumans et al. proposed to use composite transparent electrodes fabricated via lamination of silver nanowires into the polymer poly-(4,3-ethylene dioxythiophene) :poly(styrenesulfonate) (PEDOT:PSS).[8] Integration of this composite into P3HT:PCBM organic photovoltaic cells was realized. It was observed that the performances were the same to those using ITO (Indium Tin Oxide) on glass (open circuit voltage 0.615 V, short circuit current density 10.4 mA cm^{-2}, fill factor 0.65 and power conversion efficiency 4.2%). Good results were also obtained on PET (polyethylene terephthalate), indicating that this system is compatible with flexible substrates like plastics.

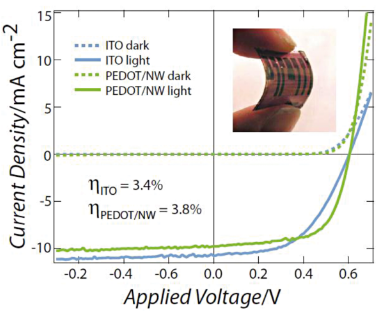

Fig. 5 > Source: Ref 8

5. Conclusion

One-dimensional conducting nanomaterials and particularly metallic nanowires appear as promising building blocks for the development of innovative flexible transparent electrodes. Their synthesis is rather simple and their integration into functional devices has been demonstrated.

It is interesting to note that it is possible to take advantage of the intrinsic properties of the metallic nanowires (high conductivity, low dimension, flexibility) to fabricate macroscopic materials with improved performances. This is a nice example that shows how nanomaterials can provide new alternatives to well established processes, and even lead to further improvement by introducing properties expected for future market products.

6. References

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