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# GENNESYS
## WHITE PAPER

A NEW EUROPEAN PARTNERSHIP
BETWEEN NANOMATERIALS SCIENCE & NANOTECHNOLOGY AND
SYNCHROTRON RADIATION AND NEUTRON FACILITIES

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# GENNESYS

**G**RAND
**E**UROPEAN INITIATIVE ON
**N**ANOSCIENCE AND
NANOTECHNOLOGY

USING

**NE**UTRON- AND
**SY**NCHROTRON RADIATION
**S**OURCES

# TABLE OF CONTENTS

## FOREWORDS

## 3.3. FUNCTIONAL NANOMATERIALS

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Functional materials include all types of chemicals, ranging from organic to inorganic, from metallic to covalent, and from molecular to macromolecular species. In devices, the useful form may be a single crystal, a compound, a thin film or a composite. At the basic level, this offers the possibility of the miniaturisation of a device, with gains in space saving, lower weight, improved heat dissipation, and so forth.

These smart materials are underpinning the technological developments of the 21st century, and play an increasingly important role in the economy and our daily lives, with applications ranging from the automotive, communications and consumer industry to health care. Their functionality can cover a wide range of physical properties, such as piezoelectric, magnetostrictive and semiconducting materials, as well as chemical properties, such as catalysis, absorption, chemical sensing, and electrochemical behaviour. Moreover, these smart materials can adapt, or respond to their environments (see Fig. 3.3.1).

The trend in functional materials is towards increasingly smaller dimensions. The interaction between the multiple structures in the components, with ensuing complexity, e.g. quantum dots or magnetic patterned arrays, demands novel destruction-free and in-situ analytical techniques which, in the future, have to be provided by the European synchrotron radiation and neutron facilities.

Furthermore, simply by reducing the size of a material to the nanometre scale, even when in only one dimension, e.g. in the realisation of an ultrathin layer, its materials properties change. This is due to quantum confinement effects modifying the electronic properties and thus all relevant materials parametres. Technical realisations which exploit this phenomenon are quantum dot lasers, magnetic (GMR) sensors and read-out heads and (since a long time) the ultra-small metal particles in a catalyst. The materials properties of these ultrasmall structures need to be explored, even on the individual basis of a single selected nanoparticle. This can be achieved by using advanced spectroscopic methods, combined with microscopy, which are only available at modern-day synchrotron sources.

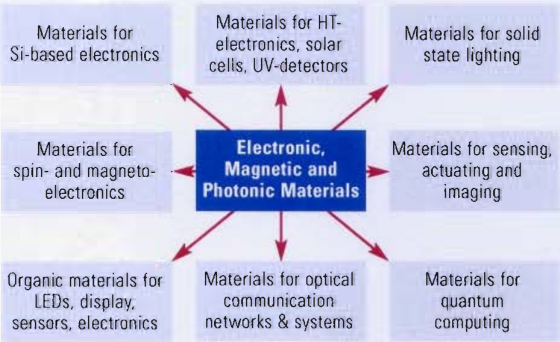


Fig. 3.3.1: Overview of functional nanomaterials.

### Promising applications of nanofunctional materials

The potential uses of nanofunctional materials are:

- **Coatings:** Corrosion and wear-resistant coatings, as well as thermal barrier- and thermal gradient coatings. In future, 'intelligent coatings' will become important e.g. as a response to environmental conditions.
- **Composite materials:** Carbon nanomaterials have a range of special electrical, mechanical and thermal properties. As an additive in polymers, ceramics, metals and textiles, these nanoadditives will improve the matrix material in terms of electrical and thermal conductivity or mechanical strength with low nanomaterial loads.
- **Energy-related materials:** A major goal is an efficient reversible hydrogen storage material. Here, novel microporous materials with an extremely high specific surface area or nanoscale complex hydrides with catalytic nanoclusters may offer the possibility to develop storage materials suitable for mobile applications.
- **Nanoelectronics:** Creation of nanoscale circuits, wires and packaging of semiconductors. The goal of industry is to use these components to manufacture a new class of very small and very powerful electronic devices.
- **Sensors:** Sensors based on nanocrystalline materials offer higher sensitivity and faster response times. These features are already being exploited in metal oxide gas sensors. However, the major problem in gas detection is in selectivity and this is not resolved in a single element sensor. Thus, the future will be in multi-element sensors and the use of neural network methodologies for signal analysis.
- **Catalysts and fuel cells:** Carbon nanomaterials enhance the properties of fuel cells. As catalyst support material for precious metals (e.g. platinum), carbon nanomaterials can help to enhance the power density of fuel cells and help to reduce the amount of platinum.

### 3.3.1. ELECTRONIC AND SEMICONDUCTING NANOMATERIALS

The impact of electronic materials on modern-day society can hardly be overestimated. Electronic technology is embedded in all branches of industry: computing, household appliances, entertainment etc. Especially in the fields of information processing and technology, the drive towards nanoscale electronics is relentless and holds the promise for increasingly smaller and faster devices. Microelectronics is generally recognised as the enabling technology for present and future information systems. However, the craving for information systems with a higher level of capacity is paving the way for the transition from microelectronics to nanoelectronics in the near future. The Semiconductor Industry Association roadmap contains SiGe buffers for strained Si layers and strained Ge from 2005 onwards and silicon on insulator technology from 2003 onwards. By about 2015, these developments in conventional Si-technology will be exhausted due to fundamental physical reasons (quantum effects), as well as material properties (e.g., no reliable oxide barriers can be fabricated with the required thicknesses in the monolayer range). Therefore, alternatives are being intensively studied (see Fig. 3.3.2).

**STATE-OF-THE-ART**

**Si-based electronics**
- Conventional Si-integrated electronics: end of improvements due to mere scaling (Moore's law) in sight (2015)
- SiGe technology: well-developed in Europe, e.g.,
- SiGe buffers for strained Si/Ge heterostructures
- Europe is leading in Silicon on insulator (SOI) technology, e.g. for high-frequency devices

**Si-based electronics**
- New device concepts based on nanostructures developed in research, e.g. quantum dots

**Optoelectronics**
- Europe is behind in optoelectronics, e.g., III-V heterostructures; GaInNAs structures, II-VI HgCdTe ternary systems, ZnCdSSe and ZnSSe devices, and GaAlN for blue and UV emitters (see also the section on photonics)

**Organic semiconductors**
- Materials and devices developed on research level

**FUTURE NEEDS AND CHALLENGES**

**Future potential**
- Continuous improvement of Si/SiGe technology
- High-K dielectrics
- Improving concepts for strained Si/Ge layers beyond virtual SiGe substrates, e.g., using quantum dots as defect-free stressors

**Nanosemiconductor breakthroughs**
- Organic electronic materials, e.g., for flexible displays, organic dielectrics, biosensors
- Materials for powerful storage devices
- New fault-tolerant computer architectures compatible to self-organisation
- Spin electronics
- Quantum computing materials & concepts
- From nanotubes and molecular electronics to organic polymers

**Fabrication challenges**
- Control of growth/self-assembly
- Develop reliable manufacturing processes (Combination of 'top-down' & 'bottom-up' approach)
- Combination of new and existing materials and technologies
- Full integration in single 'system-on-chip' components
- Development of strain simulation for cross-checking experimental results

**Characterisation challenges**
- Organic dielectrics
- Self-assembled systems
- Sensitivity down to monolayers
- Characterisation of defects, e.g., grain boundaries, dislocations
- Surfaces and interfaces
- Complex alloys

**FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRONS SOURCES**

**Synchrotron radiation**
- Non-destructive investigation of heterostructures and buried nanostructures.

**Characterisation of defects, surfaces & interfaces**
- Use of highly focused nanobeams (< 20 nm) for simultaneous real and reciprocal space resolution
- In-situ studies during growth

**In-situ studies during device operation**
- Exploitation of fully coherent x-ray beams for the direct reconstruction of real space properties and to study time-correlation properties (in-situ growth, diffusion, self-organisation, degradation)
- Combination of diffraction, imaging, and spectroscopy of nanostructures.
- Dedicated beamlines for series and failure analysis for industrial development

**Neutrons**
- (Needs further evaluation after the availability of intense pulsed neutron beams)

Fig. 3.3.2: Opportunities and challenges for synchrotron radiation and neutrons in future research for nanosemiconductors.

The spectrum includes thin films and super lattices, atomically corrugated surfaces, nanosized atomic clusters, assemblies of molecular materials, and quantum dots. The pursuit of new methods for preparation, synthesis, characterisation, and detailed examination and prediction of the properties of nanomaterials constitutes nanoscience and nanotechnology. Special technological benefits from nanoscience demand the exploitation of novel properties at the nanoscale to functionalities for industrial application. While, for instance, defects in conventional two-dimensional layers are a decisive obstacle for conventional Si technology, with self-assembled nanostructures, defect-free strained SiGe and strained Si can be fabricated. Hence there is a clear need to control the growth of self-assembled nanostructures, and to combine this new "bottom-up" approach with the conventional lithographic structure definition ("top-down"). Apart from the challenge to create new or better materials and ever smaller structures, it might become necessary to invent new fault tolerant computer architectures, which are compatible with fluctuations in self-organised materials.

The Si-Ge technology is well-developed in Europe. In the field of optoelectronics, however, Japan and US companies are leading. This includes the development of III-V heterostructures employed in optical fibre communication systems, Ga-In-N-As structures for the production of laser diodes, II-VI Hg-Cd-Te ternary systems for very long wavelength devices, and compounds such as Zn-Cd-S-Se and Zn-S-Se and Ga-Al-N for visible and UV-light emitters.

### Specific challenges for synchrotron radiation and neutron facilities

In future Si-technology, synchrotron radiation and neutron facilities must contribute to solve urgent material problems, in particular with a view to:
- The study of defects in conventional Si layers;
- The growth of defect-free strained SiGe and strained Si;
- The determination of inhomogeneous strain fields;
- The determination of inhomogeneous chemical composition profiles;
- The study of self-organised semiconductor nanostructures (quantum wires and dots).

In the development of advanced materials, several research needs have been identified:

- Use of Ge instead of Si: this transition will require extensive characterisation work, including the characterisation of the composition and the roughness at the interface with Ge;
- Design of foams of organic dielectrics as low-K oxides: urgent need for *in-situ* characterisation techniques;
- Development of Ga-N/Al-Ga-N piezomaterial: systematic destruction-free investigations of strain and dislocations;
- Tailored growth of self-assembled monolayers: systematic investigations of structure, coverage, heterogeneity and steric hindrance;
- Development of plastic electronic materials: microscopic study of the effect of grain boundaries.

### 3.3.2. PHOTONIC NANOMATERIALS

One of the most important discoveries in modern optics is the fact that the optical properties of matter are not invariant but controllable. Three methods for their efficient control are known:

(1) Dielectric and metallic nanostructures such as photonic crystals and microcavities.

(2) Composite nanostructures, metamaterials, with components whose sizes are smaller than the optical wavelength.

(3) Quantum confinement of electrons and holes in nanostructures such as quantum dots and quantum wells.

All these technologies are achieved by the self-organisation of nanomaterials and nanofabrication.

Photonic technologies enabled high-speed broad-band telecommunication, and revolutionised displays (flat panel displays). Solid state lasers and light-emitting diodes have replaced other light sources, enabling novel optical solutions from car displays to endoscopic surgery. Compared to the US and Japan, Europe is behind in optoelectronic and photonic applications, and a large effort will be required to close this gap. Severe obstacles have to be overcome in the near future in order to further the photonic field and make it market competitive.

A similar breakthrough is expected for short-distance data exchange, e.g. between CPU's and graphics adapters or storage networks, or within local networks. Here, cost- effectiveness will be the decisive factor. So far, no light sources, modulators and detectors can be fabricated at reasonable costs and with the desired degree of integration with electronic devices. It is unclear at the moment, whether hybrid solutions (which are cost-intensive due to packaging effort) or solutions integrated on-chip will (ultimately) be the optimum solution.

The following main fields of development can be foreseen (see also Fig. 3.3.3 and 3.3.4):

- III-V materials: GaN (405 nm) high density optical storage;
  - GaAs/AlGaAsP (660 nm) coupling to plastic optical fibres;
  - GaAs/AlGaAs/GaInP (800-1000) pumping rare earth laser;
  - InGaAsP (1310 nm) coupling to silica fibers;
  - nP/InGaAs (1550 nm) coupling to silica fibers;
- Organic materials: highly flexible, cheap in production, low thermal budget compatible with CMOS, hybrid integration to CMOS possible;
- Integration of photonic circuits (driven by telecommunication systems). Up to 10 GBit/s hybrid integration sufficient, for >40 GBit/s monolithic devices required;

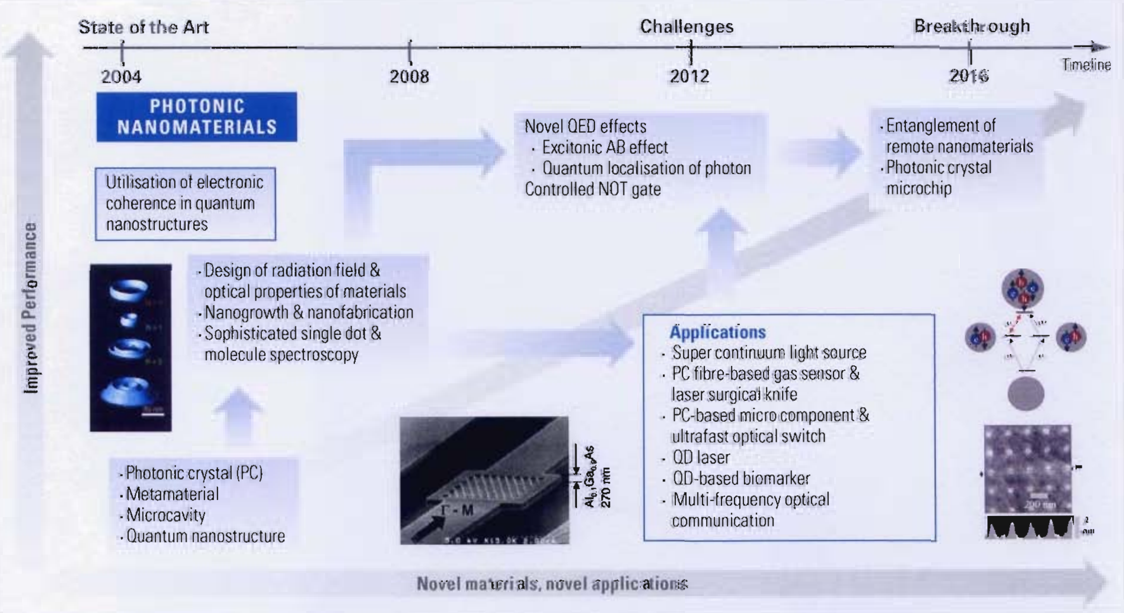


Fig. 3.3.3: Roadmap highlighting the future research on photonic nanomaterials research.

- Integration of photonic and electronic components, driven by interconnects: intra-building (also automotive and aerospace), intra-backplane (servers, eventually PCs), intra-chip.

In the search for new applications, new material developments based specifically on nanomaterials are required. In principle, two routes are followed, however, so far, these have been only at the basic research level: (i) the production of colloidal nanocrystals with specially designed optical properties, which have then to be incorporated in a lithographically produced device; (ii) the use of epitaxial methods and self-organisation, to directly introduce nanostructures into devices. In the latter approach, very similar prospects and hindrances are met to the ones in nanoelectronics. In turn, major challenges in material design and material characterisation, requiring novel characterisation solutions, will be encountered. These solutions will have to be developed and provided by the synchrotron radiation and neutron facilities. In particular, the interface structure in heterosystems, defects, and chemical composition and strain distribution within and around nanostructures should be considered important issues (see Fig. 3.3.5).

Particular targets areas for future research exploiting synchrotron radiation and neutron facilities are (see also the following roadmaps: Fig. 3.3.3 and Fig. 3.3.4, and Fig. 3.3.5 for a schematic diagramme):

**Manipulation of optical properties of nanomaterials**

- Development of materials with arbitrary optical properties by sub-wavelength structures.
- Antireflection effect of surface nanostructures, and structural colour originating from periodic structures.
- Nanostructured optical materials ("metamaterials") with arbitrary refractive index, permittivity, or permeability.

**Nanooptical circuits**

- The current optical circuits based on planar waveguides are very large compared with the optical wavelength due to the weak light confinement. To dissolve the scale mismatch with the electronic circuits and to realise electronic-photonic integrated circuits, wavelength-sized optical circuits based on photonic crystal waveguides or plasmonic waveguides is of great importance.

**Non-linear optical devices**

- Non-linear optical devices, which control light with light, are required for all-optical logic devices and for ultimate ultrafast optical communication. In addition to the synthesis of optical materials with large non-linearity, the development of optical cavities based on photonic crystals or plasmonics is required for obtaining large electric fields.

**Nanostructures for ultrasensitive chemical analysis**

- Giant electric field enhancement in photonic crystals or plasmonic crystals is expected to bring us novel methodologies of ultrasensitive chemical analysis. Research on biochips or establishment of environment analysis processes, which enable us high speed detection of arbitrary molecules in a small volume with very low concentration, is vitally important.

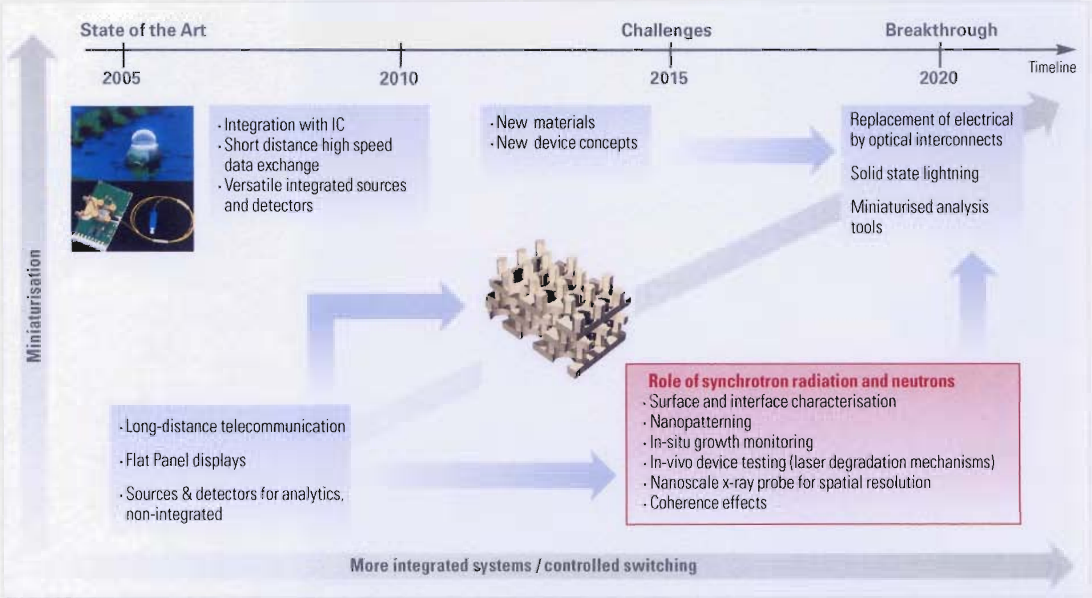


Fig. 3.3.4: Roadmap on the contribution of synchrotron radiation and neutrons towards functional photonic nanomaterials research

**Exploitation of the quantum nature of photons**

- Quantum nature of photons would be brought into use. Entangled photons are indispensable for quantum computation and quantum cryptography. In particular, realisation of strong light-matter interaction, e.g., based on the combination of quantum dots and photonic crystal cavities, is of prime importance. Single photon sources, which generate non-classical light, would also be utilised as a new class of light sources.

### 3.3.3. NANOMATERIALS FOR NANOMAGNETISM AND SPINTRONICS

The discovery of the interlayer exchange coupling in magnetic superlattices in 1986 and the giant magnetoresistance (GMR) effect in 1988 can be considered as the starting points of what is known today as nanomagnetism. The next developments will be the introduction of antiferromagnetically coupled layers in hard disks (AFC disks) and the change from in-plane or longitudinal recording to out-of-plane or perpendicular recording media.

**STATE-OF-THE-ART**

**PHOTONIC NANOMATERIALS**
**Photonic crystals (PC)**
Artificial opal
Colloid crystal
Photonic crystal slab
Photonic crystal fiber
Diamond structure
Simple cubic structure
**Metamaterials**
Plasmonic nanostructure
Negative index material
Chiral structure
Random and fractal structures
**Microcavities**
Microsphere
Microdisc
Micropillar
Micropyramid
Photonic crystal cavity
**Quantum nanostructures**
Quantum well
Quantum dot (QD)
Quantum ring

**Measurements**
Near field scanning optical microscope (SNOM)
Single dot spectroscopy

**Unusual phenomena**
Photonic bandgap
Modified Planck's law
Purcell effect
Smith – Purcell radiation
Classical localisation of photon
Small group velocity
Enhancement of:
- non-linear optical processes
- stimulated emission
- optical bistability

Waveguides with sharp bends
Super continuum generation
Super prism
Super lens
Negative refraction
Surface enhanced Raman Scattering
Quantum confinement of exciton & biexciton
Rabi oscillation
Strong coupling
Rabi splitting

**FUTURE NEEDS AND CHALLENGES**

**MAIN RESEARCH ACTIVITIES**
**Fabrication**
Sophisticated lithography:
- Electron beam
- Focused ion beam
- Ultraviolet & X-ray

Controlled self-organisation:
- STM assisted positioning of QD
- Vertically coupled QDs
- Anodic oxidation
- Semiconductor nano"molecules"
- Quantum double rings
- Remote fabrication in SEM

**Characterisation**
Further development of:
- Probe microscopes
- Single dot spectroscopy
- Single molecule spectroscopy
- Single photon spectroscopy
- Photon correlation
- Fourier spectroscopy
- Ultrafast spectroscopy

**Cavity QED**
- Development of high-Q PC cavity
- QD – PC coupled structure
- Quantum gate operation

**Applications**
Super continuum light source
PC fibre-based:
- Gas sensor
- Laser surgical knife

PC-based:
- Optical microcircuit
- Optical microcomponent
- Ultra-fast optical switch

QD laser:
- QD-based biomarker
- Multi-frequency optical communication

**Novel phenomena**
Quantum localisation of photon
Optical detection of single spin
Single molecule Raman scattering
Single photon propagation in PC
Entanglement of remote QDs
Excitonic Aharanov – Bohm effect
Controlled NOT gate

**FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRONS SOURCES**

**SYNCHROTRON RADIATION**
- Material characterisation: defects, interfaces, especially for monolithic integration
- Organic materials development: stability in time-resolved studies, dependence of stability on structure
- In-situ growth monitoring to understand growth phenomena and improve growth techniques
- In-situ device testing, change of properties and degradation of devices during operation, needs non-destructive technique

**NEUTRONS**
- Systematic neutron studies of electron-phonon interactions to reveal the dephasing mechanism in quantum nanostructures
- Quantum "optics" of neutrons

Fig. 3.3.5: Opportunities for synchrotron radiation and neutron techniques in the field of photonic nanomaterials.

The ever increasing need to store and process data has fuelled applied and fundamental research in probing the temporal and spatial limits of magnetic switching. Exploring the magnetisation in MRAM-bits by applied magnetic field pulses is a very active research field involving real-time studies of synchrotron based time-resolved spectromicroscopy. Novel switching phenomena based on angular momentum transfer from a spin polarised electrical current are beginning to be explored. A completely new field is being developed where information transfer is no longer based on charge transport leading to heat dissipation problems especially in nanosized structures. Instead, AC spin currents spin transfer phenomena across – and spin accumulation at – interfaces, play an increasingly important role in many spintronics applications for nanoscale objects.

Key future needs for advanced analytical techniques are (see Fig. 3.3.6):

- The determination of coupling angles and domain structures in magnetic heterostructures and superlattices;
- The precise measurement of magnetisation profile in dilute magnetic semiconductors;
- The real-time measurement of magnetisation reversal and domain formation in exchange-biased systems;
- The microscopic understanding of proximity effects in spring magnets.

A fundamental understanding of the microscopy of the magnetic state of nanomagnets is needed to discover new phenomena. To this end, it is of critical importance to characterise and elucidate the physical and chemical factors that control the magnetic properties of nanoassemblies.

**The need for synchrotron radiation and neutron facilities for future research and development of nanomagnetic materials**

Synchrotron radiation and neutrons provide a unique analytical access to magnetic systems; they have been vital for the present understanding of magnetism, in particular in complex, small and low-dimensional systems (see Fig. 3.3.7). In nanomagnetism, it is essential that synchrotron radiation and neutrons will offer clever new analytical solutions for the study of: i) smaller scale objects, ii) on a shorter timescale and, iii) with higher precision.

A major impact of synchrotron radiation and neutrons is expected from:

- Time-resolved experiments on magnetic nanostructures down to pico- and/or femtoseconds resolution;
- Ultrahigh resolution studies of the electronic structure, giving new insight into coupling phenomena and revealing the electronic origin of the anisotropy of magnetic materials;
- Stroboscopic spectroscopy and nanodiffraction experiments using pump-probe type excitations (temperature, magnetic field);
- Monitoring of interfacial diffusion and reactions at interfaces of metal and organic multilayers on the nanoscale;
- Systematic studies of spin-structures and spin-fluctuations in artificial superlattices and laterally patterned arrays.

### 3.3.4. SUPERCONDUCTORS

The discovery of oxide high-temperature superconductors (HTCS) in 1986 has given the field a major new stimulus. However, HTCS present a multitude of materials problems at the atomic or nanometre

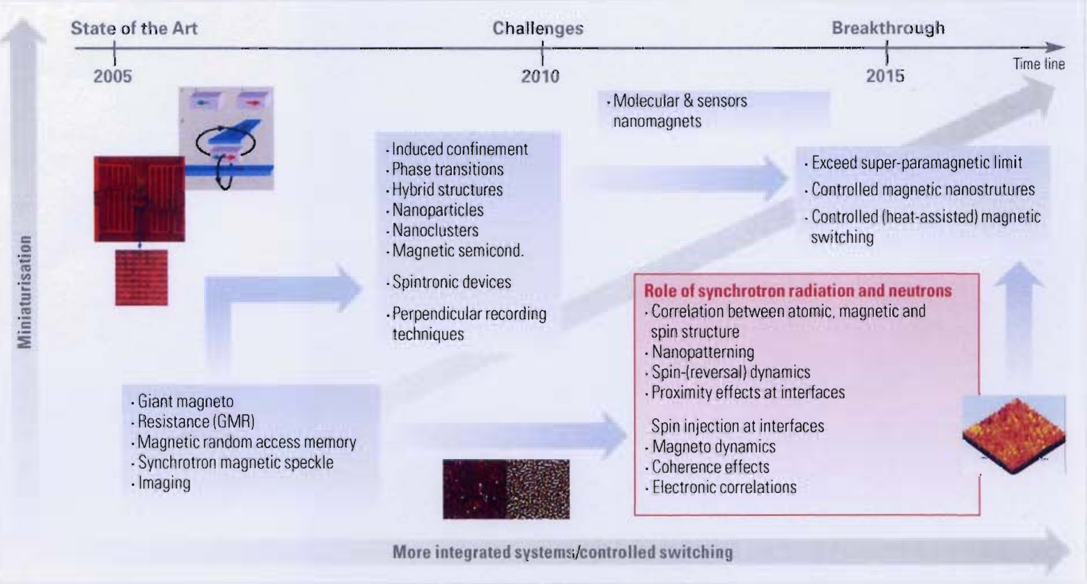


Fig. 3.3.6: Roadmap on the contribution of synchrotron radiation and neutrons towards functional magnetic nanomaterials research.

## STATE-OF-THE-ART

**Magnetic materials and properties**

Magnetic semiconductors
Magnetic vortices
Quantum transport
Confinement structures:
- Clusters (size, interdistance)
- Nanopillars & nanoarrays
- Nanowires
- Nanocontacts
- Molecular nanomagnets

Complex heterostructures
New spintronics systems
Manipulation of spins
Organic spintronics

**Synthesis**

Self-assembled growth
Nanoscale lithography
Upgraded cluster techniques
Computer simulation

**Industrial application**

Electronics:
- MRAM
- Magnetic recording
- Device switching

Spin – FET, Spin – LED
Biomedicine:
- Drug delivery
- MRI

## FUTURE NEEDS AND CHALLENGES

**Nanomagnetism**

Magnetic phenomena:
- Phase transitions in confinement (Dimensional crossover)
- Anisotropy
- Domain wall propagation
- Magnetic roughness
- Exchange bias
- Magnetisation switching
- Spin transfer and dissipation

**Nanomagnetic materials**

Hybrid structures:
- FM/Semiconductor
- FM/Insulator/FM
- FM/Superconductor

Nanoparticles & clusters
Magnetic semiconductors:
- Magnetic tunnel junctions
- Spin dependent transport

**Advanced characterisation**

Enhanced microscopic understanding of:
- Nanostructure and magnetism
- Spindynamic in nanoconfinement
- Effect of impurities
- Magnetic polarisation of embedded atoms
- Local contribution of spin and orbit to magnetic moment

**Industrial application**

New spintronic devices

## FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRONS SOURCES

**Exploration of new nanomagnetic materials**

Characterisation of:
- Superlattices and interfaces
- Nanoscale phenomena
- Hierarchical materials
- Magnetic semiconductor
- Magnetic viruses
- Dynamic effects (down to fsec timescale)

**Development of new instrumentation and techniques**

Complimentary instrumentations integration
Synchrotron radiation, neutrons and other techniques (MOKE, MFM, SNOM, SEMPA)

- Specular reflectivity/off-specular scattering
- New beamline SR PEEM /XMCD
- Micro- and nanodiffraction (time-resolved)
- Magnetic nanospectroscopy (soft x-rays; also time-resolved)
- Lens-less imaging (time-resolved)
- Pump-probe experiments (at neutron spallation sources and FEL's)

Fig. 3.3.7: Roadmap: Opportunities for synchrotron radiation and neutron techniques in the field of nanomagnetic materials.

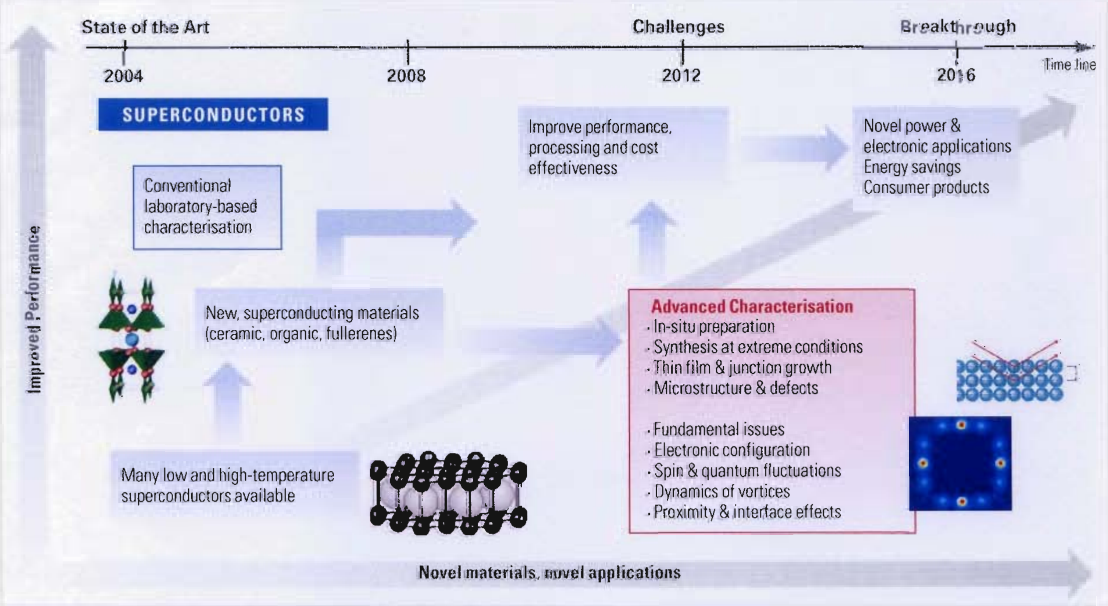


Fig. 3.3.8: Roadmap on the contribution of synchrotron radiation and neutrons towards superconductor nanomaterials research.

**STATE-OF-THE-ART**

**New superconductors**
HTC:
- Cuprates (YBCO & BSCCO)

LTC :
- $MgB_2$
- Intercalated bucky-balls
- Heavy fermions
- Ruthenates
- Boron-doped diamond

**Advanced synthesis**
Nb-Ti, Nb- Sn, Nb-Al
BSCCO-2212/BSCCO-2223
YBCO-coated conductors
Single crystals growth
High-quality thin films
Nanoscale materials

**Superconducting devices**
Multiple-barrier heterostructures
Planar multiple-barriers
Nanoscale heterostructures
SFS & SFNF'S junctions

**Applications**
Power cables:
- Accelerators; MRI, motors, generators, condensers, transformers,etc.

Electronics:
- Filters
- Josephson devices (SQUIDS)

**FUTURE NEEDS AND CHALLENGES**

**MAIN RESEARCH ACTIVITIES**

**Materials-related issues**
Search for new superconductors
New synthesis & doping techniques
Defects and microstructure
Nanomaterials
Nanomanufacturing

**Fundamental science issues**
Electronic structure & quasi particle dynamics:
Magnetism and spin fluctuations
Quantum fluctuations
Strong correlations
Vortices
Single vortex physics
Multi-vortex physics
Proximity and interface effects
Non-equilibrium effects
Spin injection

**Nanostructured superconductors**
New phenomena & processes
Tunnel-junctions
Nanowire networks
Heterostructures & superlattices
Nanoclusters

**Advanced synthesis & doping techniques with in-situ control**
Thin film growth
Synthesis at extreme conditions
Bulk samples, single crystals, thin films
Atomic-layer engineering
Combinatorial materials science
High-throughput screening
Field-effect & photo-doping

**Advanced characterisation of properties**
Chemical & structural composition
Ultrathin films
Hybrid structures
Magic nanoclusters
Nanowires
"Stripe"- order formation
Spin fluctuations
Electron-phonon interaction

**FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRONS SOURCES**

**Fundamental aspects**
- Exploration of the HTC coupling mechanism
- Systematic neutron studies of electron-phonon interaction
- Soft x-ray spectroscopy and x-ray diffraction to explore the coexistence of magnetism and SC (ARPES, XES, RIXS, HREELS, XAFS, ITS)
- Exploration of quantum fluctuations with neutron and x-ray spectroscopy
- Systematic exploration of thin superconducting films and interface phenomena using grazing incidence diffraction and spectroscopy

**Novel materials**
- Dedicated x-ray and neutron beam lines for high throughput studies of novel SC materials
- Dedicated x-ray and neutron beam lines for combinatorial materials science

Fig. 3.3.9: Opportunities for synchrotron radiation and neutron techniques in the field of superconducting nanomaterials.

scale which have to be solved in order to optimise them for practical use. Most of today's superconducting devices are still based on conventional superconductors. Present applications involve solenoids, ranging from small magnets for academic research to huge systems for large laboratory facilities (accelerators). The biggest actual market is for superconducting magnets used in medical diagnosis, in particular Magnetic Resonance Imaging (MRI).

### Breakthroughs

Breakthroughs in the field of superconductors are intimately related to progress in materials research. The technical performance of HTCS is often superior but production and material costs are still too high. The preparation of bulk superconductors presents particular material problems that are intimately linked to their functionality. In thin-film HTCS, there are many examples of how non-thermodynamic compounds can be stabilised through epitaxy with substrate or buffer layers. Of particular interest in the search for new materials is the phase spread method, where composition gradients in thin films are intentionally introduced. Structural characterisation of such layers during growth requires in-situ technologies with a high level of sensitivity and reliability. These technologies can be provided by the synchrotron radiation and neutron facilities (see Fig. 3.3.8).

**Role of synchrotron radiation and neutron facilities**

See Fig. 3.3.9. Developments in spectroscopy and electron microscopy (e.g. new detectors) and different scattering techniques (X-ray and neutrons) at the nanoscale will in parallel ensure our ability to study structure and bonding and, ultimately, obtain an atomic level relation between structure and function. As the limits of performance are pushed, the figures of merit of nanostructured superconductors (junctions, wires, clusters, etc.) need to be optimised. Then knowledge about the (sub-)microscopic nature of the structures and how they evolve is crucial. This requires detailed high-resolution characterisation of the microstructure of the devices and a high level of correlation between structure, property and fabrication parametres.

The prime analytical technologies are:

- Angle Resolved Photoemission (ARPES)

  For the future, many developments can be expected in ARPES. With higher resolution, it will become possible to explore if one can: (i) get mean free paths for the low energy excitations comparable to those measured in transport, (ii) resolve the spin charge separated components to the point where we can look at the temperature dependence of each separated component.

- Neutron scattering

  Neutron scattering has played a central role in cuprate studies, yielding many spectacular successes including the anti-ferromagnetic parent state and its destruction by hole-doping, the observation of 'stripes,' and universal spin excitation structure. Neutron scattering studies of the cuprate and other exotic superconductors will play a central role in the future of the field.

- Resonant X-ray Scattering (RXS)

  RXS investigations (elastic and inelastic) will become increasingly important for the study of electronic ordering near buried interfaces in materials that have been nanopatterned. Improved scattered energy analysis will also allow for detailed study of 'fluctuating' order, and the use of high magnetic fields will allow the study of field induced charge ordering in vortices.

### 3.3.5. CARBON NANOMATERIALS

The discoveries of fullerenes in 1985 and of carbon nanotubes in 1991 opened a completely different perspective from that of carbon materials based on flat graphite-like hexagonal layers. Carbon nanotubes have particularly attracted the attention of many scientists in the wide fields of science and technology as an important component in the realisation of nanotechnology. The synthesis of carbon nanotubes can be accomplished in a wide variety of methods that involve the catalytic decomposition of a carbon sample containing gas or solid. Some of the most common techniques are chemical vapour deposition, arc-discharge, and laser vaporisation synthesis. Nanostructured films with controlled architectures are desirable for many applications in optics, electronics, biology, medicine, and energy/chemical conver-

**STATE-OF-THE-ART**

**Carbon nanomaterials**

Model system:
- Basic science
- Nanotechnology

Building blocks:
- Integrated devices
- Nanoelectronics
- Nanoelectromechanics
- Nanooptics
- Nanofluids

**Fullerenes**

Endohedral systems
Polymerised phases (1-2-3 D)
Structural perfection
Adsorption & storage possibilities

Carbon nanotubes & peapods:
- Ideal model as 1D-solid
- High structural perfection
- Unique structure & chemical stability

Interesting physical properties:
- Metallic
- Semiconducting
- Magnetic
- Superconducting

**FUTURE PROSPECTS**

**Carbon nanotubes**
**Research activities**

Controlled growth & production:
- Nanotubes with defined length, diameter and helicity
- Optimise chemical doping
- Upgrade self-assembly
- Separate metallic/semiconductor structures

Fundamental properties:
- Confinement-related effects
- Electrical, magnetic, optical, mechanical and thermal
- Correlation between atomic structure and electronic properties
- Inter-tube coupling

**Potential applications**

Composite materials
Adsorption & storage devices
Electrical & mechanical systems
Battery electrodes
Field emitters
Chemical sensors
Catalysis
Field – effect – transistors
Printing – memories – logics

**FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRON SOURCES**

**New synthesis & doping techniques**

In-situ analysis to achieve:
- Controlled growth and hybrid structures
- Production of high quality & quantity
- Synthesis in extreme environments
- Upgrade purification & separation
- Optimisation of self-assembly
- Optimisation of chemical doping of peapods
- Fabrication of high-strength fibres
- Nanofluid structures

**Novel properties**

Advanced characterisation of:
- Chemical & structural composition
- Nanotube-polymer composites
- Transfer processes
- Interactions metal-nanotube, molecule-nanotube
- Electron excitation dynamics
- Architecture of integrated nanotubes devices
- Nanotube-based opto-electronic devices

**Particular challenges**

Single molecule diffraction and spectroscopy:
- Tailoring of nanobeams
- Controlling radiation damage (x-rays)
- Time-resolved diffraction and spectroscopy experiments
- Inelastic neutron spectroscopy for thermal excitations in CNT arrays

Fig. 3.3.10: Opportunities for synchrotron radiation and neutron characterisation methods for research on carbon nanomaterials.

sions. Low-temperature, aqueous chemical routes have been widely investigated for the synthesis of continuous films, and arrays of oriented nanorods and nanotubes.

The amazing mechanical and electronic properties of the nanotubes stem from their quasi one-dimensional structures and the graphite-like arrangement of the carbon atoms in the shells. Thus, the nanotubes have high Young's modulus and tensile strength, which makes them preferable for composite materials with improved mechanical properties. The nanotubes can be metallic or semiconducting, depending on their structural parametres. However, with our present knowledge of the nanotube growth process, a control of these parametres has not yet been accomplished. This eventually will open the ways for application of the nanotubes as central elements in electronic devices, including field-effect transistors (FET), single-electron transistors and rectifying diodes (see Fig. 3.3.10 and 3.3.11).

### 3.3.6. DIELECTRIC NANOMATERIALS FOR FUTURE Si-BASED MICRO- AND NANOELECTRONICS

Advanced dielectric materials are a prerequisite for the improvement of future Si-based micro- and nanoelectronic circuitries so as to achieve improved performance, and higher functionality, which has been developed mainly for today's Si-based micro-electronic circuitries. Today, the semiconductor industry is paving the way for the transition from micro- to nanoelectronics. This, in turn, will allow for the further improvement of the performance of Si-based IC's. In accordance with the International Technology Roadmap for Semiconductors (ITRS), the development of new dielectric materials will be IC manufacturers' primary goal in making the production of Si-based nanoelectronic devices feasible. In this race for capitalizing on research breakthroughs, synchrotron radiation and modern neutron sources have a large potential to keep the "time to market – periods" of the technology short and European IC manufacturers competitive.

**Future researchs needs and analytical challenges**

See Fig. 3.3.12. The research and technology areas of high priority to achieve an in-time transfer of basic research results on dielectric nanomaterials into Si-based micro- and nanoelectronic technologies are:

- To optimise dielectric film preparation and processing techniques
  - · Film deposition techniques with atomic control for research and industrial needs;
- Adaptability of "state-of-the-art" machinery to integrate dielectric nanomaterials in Si-based nanoelectronic devices.
- To develop characterisation methods for dielectric nanomaterials
  - · Techniques with high spatial and energy resolution,
  - · High sensitivity for defect engineering,
  - · On-line diagnostic capability etc.
- To study materials science of dielectric nanomaterials
  - · to tailor dielectrics on the nanoscale;
  - · to evaluate emerging materials concepts for device applications;
  - · to study the fundamental/ theoretical understanding of nanodielectrics.

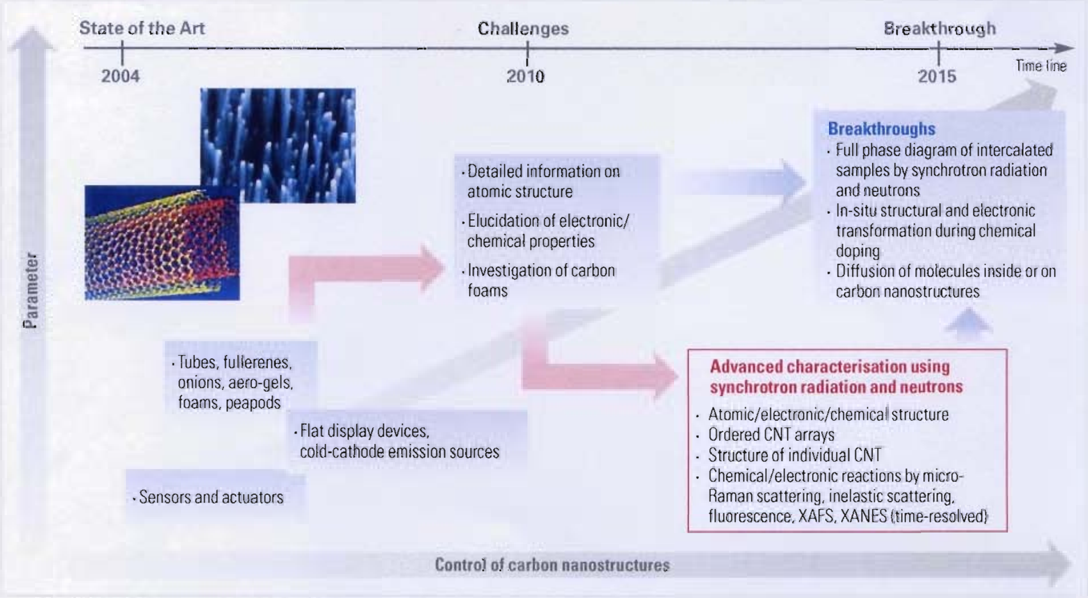


Fig. 3.3.11: Roadmap for future research on functional carbon nanomaterials.

**Future role of synchrotron radiation and neutron facilities**

Synchrotron radiation and neutron facilities are of key relevance in the successful development of advanced dielectrics for Si-based micro- and nanoelectronic IC's. In order for Europe to keep a world-wide competitive position in the nanoelectronics technology; the European Commission must promote the innovation of this important sector of nanomaterials development and encourage a new partnership between university/industry and the synchrotron radiation and neutron facilities. The synchrotron radiation and neutron facilities in turn must provide brilliant beams in the energy ranges of interest; detectors with fast electronics and high dynamic range for nanoscience studies.

The specific needs for the development of advanced dielectrics are:

- High spatial resolution diffraction and spectroscopy beam lines for micro- and nanobeam studies;
- Dedicated beamlines for non-destructive depth profiling of thin films with highest sensitivity to defects;
- Experimental set-ups for high resolution spectroscopy and diffraction studies.
- To reduce "time to market" periods for new nanodielectrics in Si-based micro- and nanoelectronics, the infrastructure of the large scientific test facilities should be adapted and upgraded to the requirements of the IC-industries, this requires:
- Improved beam time access and use by technology-oriented allocation procedures, user–friendly control and data handling software;
- Synchrotron radiation and neutron beamlines with new level of automatisation and standardisation.

### 3.3.7. CONCLUSIONS AND RECOMMENDATIONS

The properties of synchrotron radiation and neutrons present enormous potential for research and the promotion of innovation in the large field of functional nanomaterials:

**SCIENCE**

- Studying fundamental mechanisms at the atomic level
- Unraveling the complexity in novel materials
- Tuning of functionality

**INNOVATION**

- Tailoring devices
- Processing
- Fabrication

This will imply that the synchrotron radiation and neutron centres will naturally become a focus for the nanomaterials research and technology in Europe. The competitive scientific and industrial interests will push the existing infrastructure capabilities such that it will provide:

**Cross-fertilisation**

- More intense collaboration between various research communities and industries;
- Technology and knowledge-transfer through multi-disciplinary research & development.

**Infrastructure**

- Real time, in-situ experiments – down to sub-picoseconds;
- Nanoscale focus of experiments – spatial resolution better down to 10 nanometres;
- Atom-selective spectroscopy – ability to resolve microscopic environments;
- Surface and interface sensitive diffraction and spectroscopy experiments – Essential for the study of the all important interfaces of composites;
- New imaging, tomography and microscopy techniques;
- Soft (destruction-free) probes for organic and biological nanomaterials.

**Public Awareness**

- Make facilities attractive to young scientists, non-specialists, commercial/industrial clients;
- Provide more/better training programmes. University "road-shows".

**Scientific Breakthroughs**

- Clarify how electronic, optic, magnetic properties depend on atomic structure (superconductors, carbon nanotubes, magnetic materials, 3D atomic structure usually cannot be determined by other techniques);
- Identify the bottlenecks in material and device design (by defect characterisation, in-situ and in-vivo characterisation, measurement of otherwise inaccessible material properties in the material volume);
- Develop "local diffraction probes" by nanobeams, to combine and correlate spatially resolved diffraction and imaging results with other locally resolving methods like microscopy, micro-photoluminescence (this will in the near future only be possible at synchrotron radiation sources);
- Investigation of buried interfaces in composite materials, which are most of the functional materials discussed. This can only be achieved with synchrotron radiation and neutron scattering. Nanotechnology aims also to imitate natural materials, which are to large extent composite materials, where the interface properties dominate or entirely determine the material properties!

The impact of synchrotron radiation and neutron on the development of new functional nanomaterials is given in the following diagramme (see Fig. 3.3.13).

**Overall Guidelines**

Several specific measures and recommendations for the future use of synchrotron radiation and neutrons can be formulated, corresponding to different timing periods to both policy makers and facilities.

In the short term:

- Upgrade existing sample environment: low temperatures, high magnetic fields and pressures, availability of in-situ growth chambers;
- Install secondary lab-based characterisation techniques for simultaneous measurements;
- Improve detector technology: 2D-detectors, He 'hemispherical' detectors, faster read-out, better dynamic range etc.

## DIELECTRIC NANOMATERIALS FOR FUTURE Si-BASED MICRO- AND NANOELECTRICS

### FUTURE APPLICATIONS

**LOGIC DEVICES**

Silicon-on-Insulator (SOI)

Low-k Interlayer Dieelectrics

High-k Gate dielectrics

Ferroelectric Gate dielectrics

**MEMORY DEVICES**

**High-k materials**
Dynamic Random Access Memories (DRAM) and Flashcells
**Ferroelectric materials**
Ferroelectric Random Access Memories (FRAM)
**Various dielectrics**
1)Tunnel oxides for Magnetic Random Access Memories (MRAM)
2) Phase Change Random Access memories (PCRAM)
3) Holographic data storage, etc.

**MEMORY DEVICES**

**Wireless communication**
1) Dielectrics for Meta-Insulator-Meta (MIM) capacitors
2) Surface Acoustic Wave (SWA)-Filters
**Data transmission**
Microwave Communication Systems
Neuroelectronic Interfacing
**Diagnostic Devices**
Lab-on Chip solutions
**Sensors**
Electronic Noses
Pyroelectric IR-Detectors
Tactile sensors

### RESEARCH AND DEVELOPMENT NEEDS

**PREPARATION**

**Deposition**
atomic scale control
(mass flow, oxygen pressure etc.)

**Research**
flexibility for materials screening

**Industry**
highmass flow for production

**Processing**
top-down and bottom-up approaches

**CHARACTERISATION**

**Dielectric Techniques**
leakage, dielectric constant and loss, defects and interface states

**Materials Science Techniques**
high sensitivity
non-invasive character
high spatial resolution
high energy resolution
on-line diagnostics

**MATERIALS**

**Experimental**
materials manipulation n the nanoscale
(global and local approaches etc.)
materials for new device concepts and physics
(oxide electronics, spintronics, orbitronics etc.)

**Theory**
growth kinetics,
thermodynamics,
electric properties etc.

### CHALLENGES FOR SYNCHROTRON RADIATION AND NEUTRON FACILITIES

**SENSITIVITY**

**Machine**
adequate brilliance in the different energy ranges

**Detectors**
fast electronics of high dynamic range

**RESOLUTION**

**Spatial resolution**
beamline optics for micro- and nanobeam studies

experimental techniques for non-destructive depth profiling

**Energy resolution**
experimental set-ups for high-resolution spectroscopy and diffraction studies

**VARIOUS**

**Beamtime access**
technological-oriented evaluation procedure

quick access upon demand for successful proposals

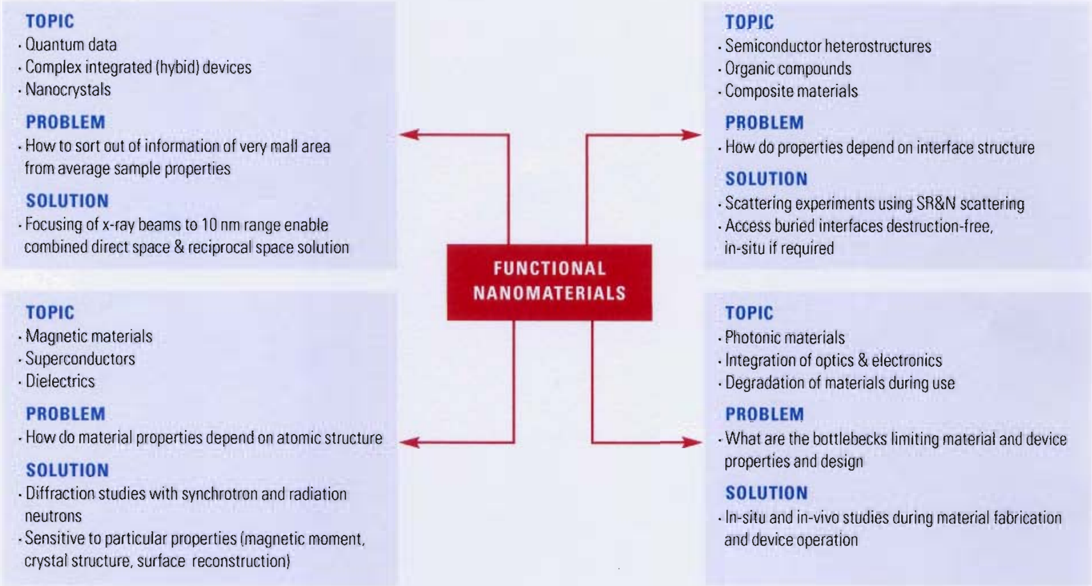
**User Friendliness**
ISO-certified beamlines
control and data handling software

Fig. 3.12: Dielectric nanomaterials for future Si-based micro- and nanoelectronics – challenges for synchrotron radiation and neutron facilities.

- Develop hybrid scattering experimental techniques;
- Explore the potential of combined neutron and synchrotron beam lines (not absolutely necessary – the samples can also be transferred but this should be facilitated);
- Stimulate the interaction between modelling methods to the experimental measurements, with a longer term view of using the predictive capabilities to direct experiments in nanomaterials sciences;
- Increase attractiveness for non-specialist users (for instance by providing user-friendly sample environment and automatic data analysis procedures) and to create a fast access lane for exceptional exploratory test experiments;
- Users would welcome faster turn-around times between submission of project proposals and actual experiments at the synchrotron radiation and neutron facilities. The long delay between submission of proposals, uncertainty of approval and eventual allocation of beam time makes the incorporation of synchrotron radiation and neutron experiments into any research project unattractive. Nevertheless, there are provisions for industrial projects at any synchrotron source to get speedy access and turnaround. Basic research projects just need to be of sufficiently high scientific quality.

As a long-term project, there should be a considerable investment in the infrastructure: new dedicated beam lines and detector development, creation of 'Centres of Excellence' in specific nanoresearch fields, user-support facilities.

Most of the leading industrial research is already carried out outside of Europe and it may be expected that the European neutron drought will undoubtedly lead to a similar situation for academic research. Europe has to present all the effort needed to allow it to maintain its position as a global leader in the development of novel LINAC-based x-ray and neutron sources.



**TOPIC**
- Quantum data
- Complex integrated (hybid) devices
- Nanocrystals

**PROBLEM**
- How to sort out of information of very mall area from average sample properties

**SOLUTION**
- Focusing of x-ray beams to 10 nm range enable combined direct space & reciprocal space solution

**TOPIC**
- Semiconductor heterostructures
- Organic compounds
- Composite materials

**PROBLEM**
- How do properties depend on interface structure

**SOLUTION**
- Scattering experiments using SR&N scattering
- Access buried interfaces destruction-free, in-situ if required

**FUNCTIONAL NANOMATERIALS**

**TOPIC**
- Magnetic materials
- Superconductors
- Dielectrics

**PROBLEM**
- How do material properties depend on atomic structure

**SOLUTION**
- Diffraction studies with synchrotron and radiation neutrons
- Sensitive to particular properties (magnetic moment, crystal structure, surface reconstruction)

**TOPIC**
- Photonic materials
- Integration of optics & electronics
- Degradation of materials during use

**PROBLEM**
- What are the bottlebecks limiting material and device properties and design

**SOLUTION**
- In-situ and in-vivo studies during material fabrication and device operation

Fig. 3.3.13: Schematic overview for the needs of synchrotron radiation and neutrons.