

Materials for Key Enabling Technologies

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1. EXECUTIVE SUMMARY

Europe and the entire world face a number of challenges which call for both immediate as well as medium term actions. The European Commission has identified these problems and has suggested focussing, within the upcoming Common Strategic Framework for EU Research and Innovation funding, on initiatives which will strengthen in particular innovation aspects. A number of so-called key enabling technologies which are of paramount importance to achieve the goals for strengthening innovation in Europe have been identified. At the same time it is clear that true innovation is often based on basic research and thus a strong research base has to be maintained and further developed in Europe.

The key enabling technologies (KETs) recommended are: Advanced Materials, Photonics, Nanotechnology, Biotechnology, and Micro-and Nanoelectronics and, as a cross-cutting KET, Advanced Manufacturing Systems. These KETs are not only interlinked but are all based on further progress in materials development. Thus materials science and engineering plays a crucial role.

In addition to these five KETs, E-MRS and MatSEEC have identified the key role of energy. Providing sufficient energy with an acceptable ecological impact in Europe as well as globally is one of society's key challenges which, in view of the threat of climate changes, has to be solved with utmost priority. Efficient energy production, conversion and storage are major objectives for Europe. Europe needs supreme efforts in both basic and applied research of new materials as well as in engineering for a lasting impact on our daily life. By this means the emphasis has to be on sustainable energy sources such as wind energy, energy gained by exploiting tidal forces, photo-thermal conversion and photovoltaics. In order to achieve an efficient conversion of natural resources into electric energy, not only novel

materials and material combinations are needed, but also their structural and electronic properties have to be understood and optimised. As an example, we mention wind turbines, which have to have proper fracture strength and toughness in addition to superior aerodynamic properties. It is suggested that the electric energy produced by these novel techniques should be mainly stored as electrochemical energy. For such storage devices catalytic reactions and thus surface and interface phenomena play a key role. Carbon dioxide is seen as providing new opportunities for the development of an innovative industry capable of large energy storage by replacing carbon fossil fields.

Our daily life is now no longer imaginable without facilities like lap-top computers, mobile phones, smart-phones, etc. However, all these depend on batteries for the delivery of electric energy. Though the most powerful are Li-ion batteries they nevertheless sustain only a certain number of loading cycles before they fail due to thermal expansion during loading. Better electrodes for such batteries are therefore urgently needed. There are good reasons to believe that these improvements will be due to nanotechnology.

Micro- and Nanoelectronics is without any doubt the key enabling technology. Due to the technological and economic importance of electronics, almost all industrial areas depend to an increasing extent on the progress of electronics. Data storage, data transfer and telecommunication are only a few examples. But areas such as control applications in production facilities of automotive and aerospace space industries as well as household appliances, etc. need micro- and nanoelectronics for their functioning too. It is also worth mentioning that with shrinking dimensions of basic elements, quantum mechanical phenomena will play an increasing role, and must be considered when designing future electronic devices.

The field of Photonics is another area, which is considered to become a mainstream technology of the 21st century. Photonic elements, which convert electric signals into light and back into electric signals, are nowadays used e.g. for data transfer over long distances. In the future they will also be used for short distance data transmission e.g. within circuit boards and processors, and will thus in this way increase the data transfer rates within the Terabit/s range. Furthermore, apart from information and communication, photonics will change electric lighting as well due to the increasing use of light emitting diodes. Moreover, photonics has an enormous potential for industrial manufacturing through the use of high power lasers, and will have a strong impact on life and health sciences.

Biotechnology is another rapidly expanding field with great impact on areas such as health-care, where targeted drug delivery is one of the aims, or for daunting analytic tasks like single molecule analysis. This field will benefit from recent advances in nanotechnology such as lab-on-a-chip systems, which can analyse with micro-fluidic methods and sensors consisting, for example, of nanowires by using much less available volumes than conventional techniques. In addition, nanostructured sensors will be a great deal more sensitive than bulk sensors because of their much larger surface/volume ratio.

In the following chapters a detailed analysis of the five KETs and their role in solving the main challenges is presented by starting with an analysis of the present situation and then following up with suggestions and an outlook for the future. Below, we summarise a number of key recommendations:

- In some areas of micro- and nanoelectronics (MNE) Europe is still leading. Among those are power electronics, high frequency devices, and micro and nano-electromechanical systems (MEMS and NEMS). In order to keep and strengthen this position it is of utmost importance that a proper wafer production is available in Europe. All possible efforts must be made to take part in the upcoming transition to a technology based on 450 mm wafers and not to restrict future activities to centres and companies performing design and simulation only.
- Europe is leading in computational materials science worldwide. State-of-the-art multi-scale modelling of the relation between microstructure and properties is needed both for the

- understanding as well as the design of different types of advanced materials. Modern predictive materials modelling will be of key importance for European industry and in this respect the technology transfer to industry needs to be vigorously pursued.
- In the field of advanced materials it will be necessary to strengthen approaches to the rational design and characterisation of advanced materials and their integration into structures and systems. It is therefore imperative to further support the expertise gained in hybrid materials, to integrate concepts of green chemistry and biotechnology in materials design, characterisation and production, and to anticipate and control better the performance of materials during their entire life cycle.
- Due to promising applications in the field of nanotechnology it is mandatory to further develop this technology in areas such as energy, nano-bio applications, healthcare, security, etc in Europe.
- In order to exploit fully the breakthroughs offered by nanotechnology a European open access centre for nanofabrication should be created offering state-of-the-art materials processing and characterisation facilities with strong links to industry.
- Carbon dioxide can be used as a raw material for electrical grid regulation and for the development of a new industry based on its recycling. In order to do this close cooperation between research centres and industries on this issue should be facilitated.

In conclusion, this document also underlines the necessity to strengthen innovation in Europe by creating innovation incubation centres in the form of private-public infrastructures with participation of universities, research centres and industries in several well chosen strategic fields, which are of interest for European industry.

2. THE GLOBAL MARKET AND THE EU POSITION FOR EACH KET

The history of science contains many examples showing how important it is for researchers to have strong will and perseverance in order to achieve the objectives they have set themselves. This is particularly true of materials science in view of the fact that material science and engineering is a multidisciplinary area that strongly interacts with technology. Materials science and engineering is also a well-recognised discipline with its dual grounding in basic science and engineering. As such, it plays a crucial role in many aspects of human activity including interactions with living environments and communication. Materials science develops new-generation energy technologies such as solar cells, as well as providing faster and more reliable means of communication through new electronic, optical, and magnetic materials.

It comes as no surprise then, that the history of materials science is highlighted by existing and often unexpected developments, which were not foreseen, for example, by classical roadmaps.

Following a process that identified the Key Enabling Technologies (KETs) from the European perspective, the European Commission set up a High Level Group that officially started its work on July 13, 2010 focussing on the five KETs which have a high impact in terms of market size and growth potential /refs EC1, EC2/.

- Nanotechnology has a global market estimated at US\$ 147 bn in 2007 with the prediction to grow, in most optimistic assessments, to US\$ 1 or even 3 trillion by 2015. The market share is dominated by the US (40%), followed by Europe (31%).
- Micro- and Nanoelectronics worldwide market was valued at US\$ 261 bn in 2008. Electronic data processing and the telecommunication sector are the largest markets for microelectronics. However, semiconductor components are rapidly penetrating the automotive, medical, industrial or consumer markets. The automotive sector in Europe accounts for a larger proportion of microelectronics sales (19%) than it does in the rest of the world as a whole (8%).

- **Photonics** global market for optoelectronic components was worth US\$ 356 bn in 2008 and is expected to grow at an annual rate of 3.1% up to 2020. The EU has strong positions in many photonics applications such as solid state lightening (*e.g.* LED), solar cells and laser assisted manufacturing.
- Advanced Materials and materials innovations are an important element in practically all manufacturing industries. Markets are expected to offer an additional volume within the EU of € 55 bn over the next 5 to 7 years with considerable potential in the areas of energy (€ 19 bn), environment, health, transport and information and communication technologies (ICT).
- Industrial biotechnology is defined as the application of biotechnology for the industrial processing and production of chemicals, materials and fuels. The global enzyme market was worth about € 2.1 bn in 2008 and Europe is the world leader in key industrial technologies such as enzyme technologies and fermentation.

Materials are present in all five KETs as they underpin their progress either directly or indirectly. In addition, it has been recognised that, "KETs such as new materials for energy production, transportation and storage play an essential role", but have not been explicitly included as a KET/ref EC2/. Energy and materials have a continually and mutually enriching relationship since materials are used to harvest energy or enable energy to be transformed into useful forms /ref MRS1/. For this reason, in this document, "Materials for Energy" are addressed in a separate chapter.

The Electronics Ecos	ystem	2007 → 2010
Electronic End Equip	\$1,580 B → \$1,980 B	
Seminconductors		\$256 B → \$321 B
Seminconductor Equipment		\$43 B → \$48 B
Materials		\$43 B → \$53 B
	Source: SIA	SEMI, an Henderson Ventures, March 2008

FIGURE 2.1:
The Electronics Ecosystem

700 B
180 B
50 B
20 B
10 B

FIGURE 2.2:
The Photonics Ecosystem

3. ADVANCED MATERIALS

Progress achieved in most technologies is closely related to progress in advanced materials. Examples, with different though systematically significant impact on societal needs, are energy related technologies (production, management such as lighting or heat conversion, storage and transformation), health technologies (including biomaterials and substitution devices), industries of the (micro-)electronic sectors, transportation (especially automotive and aeronautic), space, housing and civil engineering, production and construction technologies in general, sport and clothing. This relationship results from the nature of materials science, an inherent interdisciplinary field, coupling fundamental research with engineering, and within which base knowledge is intimately related with technology. It is also the output of progress made in physics, chemistry and engineering, and particularly because of the interactions among these three large sectors.

In the long term, four main directions should be supported because they correspond either to radically novel approaches in advanced materials design or to a societal expectation. These four directions potentially concern all classes of materials and are:

- Research on new advanced materials with novel or improved properties.
- Development of rational approaches in the design of advanced materials or in their integration into structures and systems.
- Inspiration by nature: promotion of eco-design, bioinspiration and the use of natural materials.
- Anticipation and control of the performance of materials during their life cycle, including smart structures allowing for self-sensing and self-healing.

3.1 Research on New Advanced Materials with Novel or Improved Properties

In all industrial sectors, it is necessary to incorporate new functionalities into "classical" materials (e.g. ceramics, metals, textiles, paper, building and construction, etc.) to give them a higher added value. One example is single-crystalline materials with controlled defects. However, beyond such incremental, though necessary, progress, spectacular advances have been reported over recent years on the discovery of materials with new functionalities and/or with a wide spectrum of properties induced by the nanostructuring of matter. Such new families include hybrid materials at the frontier between organic, bio- and inorganic worlds; divided solids with large specific surface areas, including mesoporous materials; novel carbon materials; memory shape materials; metamaterials, etc.

Many of these materials with specific properties condition the tuning and the breakthrough of innovative applications: membranes for separation processes, organic or thin film photovoltaics, functional polymers for flexible electronics, materials and devices for molecular photonics and photostable storage, thermoelectric materials at high and medium temperature, super isolating materials, cores of fuel cells, electrodes for all-solid batteries, molecular footprint materials, barrier polymers for packaging, shock resistant polymers, intermetallics with magnetic, electric, thermal, surface properties. These materials are particularly interesting for their combination of properties: complex metallic alloys, multiferroics, thermochromes, magnetochromes, etc.

In addition to the development of "materials for..." (a specific application), research on entirely new materials should be maintained and further developed. Recent examples are the iron based pnictides to be used as high temperature superconductors, developed in Japan. /ref KAM/.

The aim of this activity is to design and to synthesise or to process new phases and novel atomic architectures to be used as an upstream reservoir which will feed future families of "materials for...". The following recommendations are provided:

- Encourage, maintain and recognise upstream activities on the synthesis of new compounds, complementary to the activities on materials for targeted applications
- Develop adapted processes for the fabrication of such materials
- Bring to the knowledge of industry the original developments in the field of new compounds (to become new materials) which by nature are not yet included in industrial development

3.2 Development of Rational Approaches in the Design of Advanced Materials or in their Integration into Structures and Systems

Materials have long been simply transformed matter which should fulfil a main required function. Future materials and/or material systems should fulfil multi-criteria specifications and therefore they will be multifunctional. Multifunctionality is often obtained from the coexistence within the material of a set of properties which are distributed at different scales. Such evolution of materials research towards an optimised design on demand is a new challenge which cannot be faced by using a blind process. It can only be achieved through:

- (i) detailed insight into the mechanisms which control the properties,
- (ii) *a priori* modelling of the expected properties,
- (iii) the systematic use of the possibilities offered by the combination of different classes of materials,
- (iv) consideration of the potential presented by the variety of forms and architectures of a material, and
- (v) the adjustment of the properties of the interfaces. This new challenge will also require the development of new techniques for materials processing or shaping and for disassembling in order to improve recycling.

Some industries, *e.g.* transportation, require technological breakthroughs; based on equivalent performance, they would allow structures' weight reduction and extension of lifetime in specific operating conditions. In contrast, other sectors like the one of production of energy require devices that can operate in more severe conditions, under complex dynamic loading, under pressure or in vacuum, at high temperature or in cryogenic cooling, in corrosive atmosphere, etc. In these

sectors in particular it is important to favour research in metallurgy taking into account expressed needs in the field of production of electricity by nuclear power.

When advanced materials are to be integrated into devices, such integration should be optimised considering interrogation and detection procedures, manufacturing and processing in given forms, and integration with other materials.

The following recommendations are provided:

- Develop new approaches in materials design
- Develop the use of "numeric material" and confront the approaches developed for different classes of materials
- Develop integration processes/systems for successful and profitable use of the material's functionalities
- Develop instrumentation for materials characterisation: micro- and nanostructure, properties and performance in anticipated operating conditions. Include techniques for the *in situ* characterisation of materials during their processing and the continuation of the development of knowledge and of the use of large equipment (neutrons, synchrotron radiation)
- Reinforce research at the interface among materials chemistry, materials physics and engineering

3.3 Inspiration by Nature: Promotion of Eco-Design, of Bio-Inspiration and of the Use of Natural Materials

This direction corresponds both to radically novel approaches in advanced materials design and to a societal expectation. It promotes inspiration from natural materials and from processes nature uses for their fabrication. Efficiency of such materials, such as bone or wood, is based on their topological and structural organisation (hierarchy) at different scales: nanometre, micrometre and, most often, millimetre. Consequently, the objective is to design and to develop materials or components by modifying architecture, topology and length scales so as to give them the required functionalities.

Environmental constraints (e.g. those requesting clean and secure processes), objectives of sustainable development (e.g. those targeting suppression of over mining of raw materials) and the increase of the cost or of the accessibility of raw materials and their transformation in terms of energy consumption are prevailing conditions in industrial countries and in the EU in particular. It is thus necessary to develop novel axes of research, based on eco-design, which call for renewable resources especially for the production of large diffusion materials, e.g. plastics.

The following recommendations are provided:

- Better integrate the concepts and the objectives of green chemistry and white biotechnology in materials design
- Optimise processes for the fabrication of materials and life cycle of systems
- Build alternatives to materials produced from raw materials with reduced availability
- Integrate a systemic approach in the design of new products, taking into account environmental and societal aspects
- Research processing technologies for large diffusion materials like plastics, compatible with the objectives of sustainable development

3.4 Anticipation and Control of the Performance of Materials during their Life Cycle, including Smart Structures allowing for Self-Sensing and Self-Healing

Society legitimately imposes a high security level for all devices used by mankind. This requires being able to understand and control the behaviour of the materials used during their lifetime. Controlling materials lifetime involves three important aspects:

- Adjustment of a materials' lifetime to its usage. Materials should be designed in such a way that their cost is adapted to the needs and particularly to the lifetime of the device which they are part of. Also the amount of used materials should be mitigated and materials should be recycled according to sustainability and efficiency principles.
- Prediction of the behaviour of the materials in durations which are experimentally inaccessible. This question concerns an increasing number of applications, especially in aeronautics and nuclear energy. It requires developing modelling and simulation tools which are able to provide complementary information to accelerated experiments, when possible.
- Determination of the remaining lifetime (remaining potential) as a function of the aging process experienced by the material during its use. It is convenient here to distinguish between batches of pieces, and systems and structures. In the first case, the evaluation is realised *a priori* by statistical analysis, the distribution width of which should be reduced. In the case of systems and structures it is necessary to dispose of non-destructive control coupled with identification models and precursor events. Precursor events are to be introduced in parts where aging signs are easily identified and quantified as, for example, in intelligent structures.

The following recommendations are provided:

- Observe and detect aging. Develop instrumentation, measurement facilities, probabilistic approaches, stochastic processes of deterioration
- Design smart structures allowing for self-sensing (warning) and self-healing; integrate these concepts together with those of sensors and actuators within the same material

As in the case of the four other KETs, new advanced materials should be processable in the targeted forms. To achieve this, it is mandatory that progress in materials design with regard to more complex and strict specifications should be completed by both new and improved production technologies. Such technologies, incorporated in production lines, should particularly aim at reducing the production costs (e.g. by net shaping); at maintaining and if possible at decreasing the energetic cost; and at minimising the impact on the environment (e.g. by favouring low temperature and solvent-free synthesis). Such new and improved processing technologies may incorporate lasers, plasmas, ultrasounds, supercritical fluids, soft chemistry, spark plasma sintering or surface treatments. Up scaling of these processing technologies for mass production is another important issue in this respect: laboratory scale processing techniques should be designed in view of the pilot scaling.

In some cases, process intensification and security requires down scaling and parallel operation.

The parameters of a fabrication process are numerous and often coupled among them. The investigation of their influence requires extensive experimentation. Modelling, simulation and high throughput (e.g. combinatorial) tools are strong supports for such developments. It should be recalled that development of new synthesis/manufacturing equipment requires considerable funding. This funding necessity should be satisfied as is the case of funding for large facilities for characterisation and testing (synchrotron, neutrons, etc.).

The following recommendations are provided:

- Improve existing, and develop new processing, assembling and transformation technologies adapted to the manufacturing of advanced materials and to their incorporation into systems
- Design laboratory scale processing techniques in view of the pilot scaling
- Integrate processing aspects in materials design and selection
- Ensure development, transfer from academia to industry, and funding of new synthesis/manufacturing equipment

All materials involved in the above items should contribute to **sustainable development**. This will be achieved by applying life-cycle design of end products aimed at reducing environmental impact. In addition to the previously presented requirements, reduced environmental impact is obtained from materials that contain abundant, accessible and less hazardous substances and present high resource productivity and low ecological rucksack.

3.5 Advanced Functional Materials

3.5.1 Prospects of Inorganic Materials for Photonics and Energy

In order to improve already existing and develop new inorganic materials for applications in photonics and nanotechnology, the <u>current research trends</u> in materials science include the following topics:

- Fast processes in oxide nanocrystals
- Materials for holographic recording
- Detection of near-surface electromagnetic fields by optical resonances in atoms
- Optical properties, in particular, luminescence of wide band gap semiconductors
- Materials for electrodes and membranes for high storage capacity batteries and gas sensors
- Glasses for photonics
- Optical fibres and glasses for deep-ultraviolet applications

3.5.2 Prospects of Non-organic Materials for Advanced Multifunctional Microsystems

Both optoelectronic and micro- and nanoelectronic devices are priority in technology development. In order to develop the next generation of multifunctional advanced systems complex knowledge of physical and chemical properties of materials as well as of biological principles is required. The goal is to research relevant optical, electrical and micromechanical properties of materials. The results expected will create fundamental knowledge of the local atomic and electronic structure and its relation to physical and chemical properties of modern multifunctional materials including:

- Possibilities to use surface and interface processes in mono- and multilayer nanostructures for a new generation of surface-active sensors and ultrahard coatings
- Development of light emitters, detectors and visualisation systems on oxyfluoride nanocomposite bases with enhanced quantum efficiency

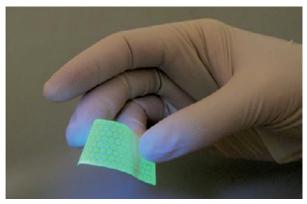


FIGURE 3.5.3.I. Fluorescent organic thin film on flexible substrate. Courtesy of A. Gonzalez-Elipe, Instituto de Ciencia de Materiales de Sevilla, Spain

3.5.3 Materials based on Novel Functional Low Molecular Organic Compounds and Polymers

The goal is to develop novel photoactive organic compounds (oligomers and polymers) and solid state systems for electronics, photonics and optoelectronics. The aim of investigations should be to demonstrate the integration of organic molecules, polymers or nanoparticles into scaleable, functional electronic and photonic devices that are connected to each other and to the outside in a realistic and practical manner. The devices pass information by either a conventional current (electrons) or light (photons). The main research axes include:

- High-density memories
- Molecular diodes
- Organic light emitting diodes (OLED)
- Organic photovoltaic devices (OPV) in low-power format, which will not require expensive fabrication facilities

3.5.4 Metamaterials and Nanostructured Materials

The increasing demands on photonic devices in terms of speed, efficiency and cost/unit ratio require the development of new materials with tailor-made electromagnetic responses. Known as *metamaterials*, these artificial compounds consist of sub-wavelength, in most cases metallic, units arranged on a lattice structure with sub-wavelength pitch. The electromagnetic response of the ensuing material is hence governed by the properties of the unit cell. This enables the development of materials showing electromagnetic properties not found in naturally occurring materials. Prominent examples are metamaterials with a negative refractive index, magnetism at optical frequencies, and a strong plasma response in the low-frequency part of the spectrum.

Emerging application areas span the information technologies (filters, nanoscale optical waveguides, nanosized lasers and detectors), photovoltaics (subwavelength energy concentrators), and biomedicine (imaging and screening).

The first requirement takes into account that most metamaterials consist of intricately shaped metallic sub-units, hence the optical loss is determined by the intrinsic losses of the unit cell. The field of study investigating the optical properties of nanostructured metals is termed *plasmonics*, one of the cornerstones of metamaterials research.

The second requirement acknowledges that thus far most metamaterials have been realised using expensive, slow, top-down nanofabrication techniques (for example electron beam lithography).

Mass production requirements for technological applications will require a switch towards fast, cheap and flexible bottom-up synthesis techniques relying on concepts such as self assembly and organisation, as well as parallel nanolithography schemes (such as nanoimprint lithography).

Another particular challenge lies in the assembly of truly three-dimensional metamaterials. Only then can the flexibility in terms of tailor-made optical properties, expressed via a desired spatial refractive index distribution, show its full potential. This is particularly true for applications exploiting phenomena such as negative refractive index, near-zero-permittivity, and optical cloaking.

Research into three-dimensional assembly techniques is currently still in its infancy, and hence presents a particularly promising opportunity for Europe to take a leading role.

3.5.5 Functional and Multifunctional Oxide Films

Owing to the wide range of functional properties which can be observed in the oxide materials family, thin films of these compounds find numerous applications in a wide range of domains. As a result, the theme "Functional and multifunctional oxide films" is a multidisciplinary theme, since microelectronics, spintronics, materials for energy and biomedical applications can be based on such films.

A typical example of a multifunctional oxide film is the transparent conducting electrodes needed for Si photovoltaic solar cells. In addition, to increase the efficiency of such cells, a conversion layer which can transform a photon in the UV domain (which are not efficiently used in the cell), in the visible or near infrared domain (efficient absorption), should be deposited onto the cell. If a single film (a multifunctional film) can be used as both a

transparent conducting electrode and a conversion layer, this will be a noticeable simplification in the fabrication of Si photovoltaic solar cells.

Depending upon the crystalline structure and the nature of the oxygen-cation bonding (ionic or covalent character), very different kinds of oxide materials can be obtained. For example, wide band gap insulating materials, well suited for optical applications, in which collective phenomena involving electric dipole interactions can yield ferroelectricity. The electronic properties of oxide compounds go from metallic conductivity to superconductivity with of course the well known transparent semiconducting oxides. Unpaired spins in these oxide compounds results in ferromagnetism or ferrimagnetism. Moreover, metal-insulator transitions can be observed depending on temperature, pressure or magnetic field, increasing thus the interest in the oxide films. Taking into account that some of the compounds of this family are biocompatible and show mechanical properties well suited for applications in the domain of the life sciences, it is easy to understand the historical interest in oxide materials.

It should be noted that numerous reviews can be found giving the state-of-the-art concerning oxide films, their growth, composition, morphology, structure, microstructure and physical properties and their potential applications in many domains. In particular, the MRS Bulletin /ref MRS2/ in the papers on "Wither Oxide Electronics" gave an extensive overview of this specific domain and presented some expected perspectives which have to be taken into account. For example, oxide heterostructures offer the possibility to generate new electronic phases at interfaces and new electronic systems with properties that cannot be achieved in the bulk. These phenomena, which can lead to the formation of conductive and even superconductive interfaces, may be at the origin of new applications.

Various approaches can be envisaged for the formation of multifunctional oxide films including:

- the combinatorial approach which is mainly based on the use of multitarget systems. In this way it is possible to form oxide films with a broad range of compositions
- the doping of the oxide matrix by elements to induce some functional properties. For example, rare earth doping of a oxide matrix, (i.e. in which the rare earth dopants can be easily substituted to cationic elements) finds applications in optoelectronics, while doping of semiconducting oxides by transition metal elements can lead to ferromagnetism at elevated temperatures for spintronics applications
- the formation of nanocomposite films, the formation of films constituted by the random stacking of oxide nanoparticles, is a key point for applications in the field of nanoscience and nanotechnologies

4. MATERIALS FOR ENERGY

Providing sufficient energy in Europe and globally with an acceptable ecological impact is one of the key challenges faced today by society, and in view of threatening climate changes, an extremely urgent one. There are many issues with no easy answers, but there are also many promising solutions and ideas already available in a in a more or less advanced state of research.

It is accepted that such a global challenge calls for better coordination. This is especially true in the European context where virtually no raw material is sufficiently abundant to cover all needs. Furthermore, Europe needs to decrease CO₂ emissions according to the Kyoto agreement.

The energy issue should be addressed in all of its aspects, starting from production to transformation and transport by taking into account new and renewable methods with low environmental impact. Finally, the end use of energy is to be seriously considered as quite a substantial part of energy request is due to industrial and domestic users, both in appliances and electronics, where a significant waste of resources occur.

Advances in materials science have been key enablers for improving energy efficiency in all aspects above and in many different areas such as harnessing of solar energy (solar cells), transport (automotive industry and e-mobility) energy efficient buildings, etc.

In this chapter, the main challenges and possible solutions from the materials' perspective are presented in three main areas:

- energy production from renewable sources
- energy storage and distribution/transportation
- more efficient energy consumption

It is to be noted that the division above is arbitrary or even incorrect to some extent, since energy cannot be produced or consumed, but only transformed from one state into another. However, for the purpose of structuring this document, this commonly used terminology will be employed. We also restrict ourselves mainly to electrical energy, which is only part of the global energy cycle.

4.1 Energy Sources and Production

Energy production from renewable sources has a wide range of possibilities. *Photovoltaics*, *wind* and *tidal power* are already increasingly used, and, in some cases have exceeded even optimistic expectations: *e.g.* in 2009 in the countries of the European Union the share among the *new* installations for electric power production was as follows: Wind (39%, 10 GW), Natural Gas (26%, 6.6 GW), Photovoltaics (16%, 4.2 GW), Coal (9%, 2.4 GW) and Biomass (2.2%, 0.6 GW). All these new installations depend on the use advanced materials for energy conversion.

Further increase of efficiency remains, however, the main issue. The use of *biomass* is a further asset in the energy portfolio, but also needs to be considered in the correct perspective: the energy that can be harvested per area and per year is only about 1/40 of photovoltaics efficiency. Thus the main question is how to best exploit otherwise wasted potential, for instance by using biogas from landfill sites.

Thermoelectrics so far have a comparatively low efficiency as well, but have a considerable potential in the use of waste heat that cannot be used otherwise. Even at moderate efficiencies, the total efficiencies of, e.g., combustion engines can be increased considerably by converting waste heat into electricity.

Nuclear Power (using fission as well as fusion processes) cannot be considered as a renewable energy source, and has a big and unsolved problem which is nuclear waste. Materials development is required at different levels and in particular to limit the negative ecological impacts.

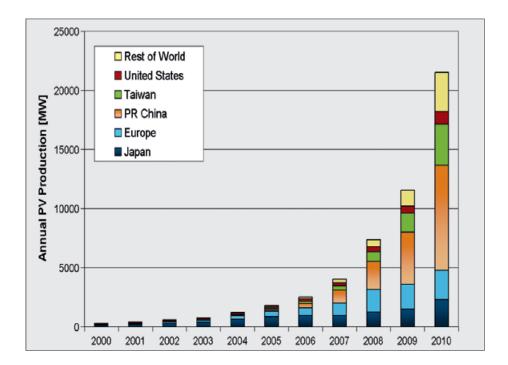


FIGURE 4.1.1.1.

World PV Cell/Module
Production from 1990
to 2010
(data source: Navigant
[Min 2010,a], PV News
[Pvn 2010] and own analysis)

4.1.1 Solar Energy

The use of solar energy can be seen as the safeguard of the energetic basis for mankind. Under steady conditions our sun provides more energy to the Earth within one hour than mankind consumes within one year. The photovoltaic (PV) industry is predominantly based on silicon which is the second most abundant element in the Earth's crust and, because of microelectronics, the most extensively investigated material. The prospective research topics concern the efficiency of solar cells, their long term stability as well as the cost-effective production of silicon. For countries with low solar irradiation it is very important to exploit the entire spectral range making compound semiconductors a viable option, especially in layered structures and in concentrator solar cells. Each kWh gained from solar energy saves about 1 kg of carbon dioxide!

There are two routes for solar energy generation: solar thermal and solar photovoltaics. In the solar thermal approach, the sun's radiation is converted to heat that is either used directly, for instance, for passive water heating, or indirectly concentrated, known more commonly as concentrating solar power (CSP). In solar photovoltaics, semiconductors are used to convert solar radiation into electric energy, which can be either used locally in autonomous systems or connected to central power grids using dc-ac converters. Photovoltaics is a semiconductor market and will provide a best in class renewable energy.

At present European industry is leading in photovoltaic materials, equipment and technologies. The success of photovoltaics as a large-scale, renewable energy source relies on the capability of lowering the cost and increasing the energy conversion efficiency of solar cells. In order to attain both goals new materials and processes need to be developed for future PV devices. It is widely accepted that future activities in this field will focus on the possible impact of nanotechnology and hybrid systems based on organic/inorganic coupling, for innovative PV systems.

In the field of solar photovoltaics, the range of materials used is limited to a few elements and compounds like silicon (wafer based and thin films), GaAs and its derivatives, CdTe, a few chalcopyrites (CuInGa(SSe)₂) and some dye and organic compounds. Calculations of the electronic bandstructure of most of these materials were performed already in the 1970's and with the help of these a wide range of compound materials was identified as suitable candidates for solar cells. However, the systematic synthesis, investigation and characterisation have not been carried out for all of the potential materials.

Investigation of the fundamental material research aspects was often neglected due to the fact that these have a time-scale beyond the short term needs of industry. In fact, new materials synthesis and characterisation takes a significant amount of time and it is not guaranteed that these materials can be manufactured in a cost effective way. Therefore, the risk associated with research on new materials is high. On the other hand, not taking this route is even more risky since the result

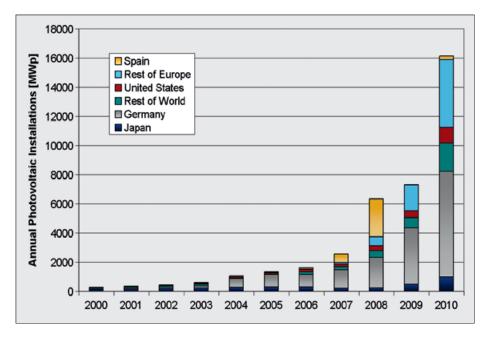


FIGURE 4.1.1.2

Annual Photovoltaic
Installations from 2000
to 2010
(data source: EPIA [Epi 2010],
Eurobserver [Sys 2010] and own
analysis)

may be to run into a potential roadblock for PVs in the future if the commonly used materials are no longer available at economic prices.

The impact of nanotechnology has already been emphasised: it offers the possibility to harvest the full solar spectrum by quantum related phenomena such as Multiple Exciton Generation (MEG), the use of Intermediate Band (IB) materials, or the tailoring of the solar cell absorption through size tuning of nanostructures embedded in the active device area. Despite the fact that for some of the ideas it has been possible to show a proof of concept, their implementation within a large-scale, mature technology requires extensive scientific investigations and technological development.

Looking at the overall picture, it is important to note that silicon is still the dominating material with more than 85% of the total market for PV panels. This suggests that for the next 10–20 years significant research activities will be focussed on the use of siliconbased or silicon-compatible thin film structures. These materials include, of course, nanodots, nanowires, nanotubes and other kinds of nanostructures able to improve the direct conversion of photons into electrical charges.

Moreover, while in the past most attention has been dedicated to the active part of solar cells (the region where photons are absorbed and create electronen—hole pairs), the new concepts of PV devices evidence the critical role of all parts forming a solar cell: anti-reflecting coating, transparent conductive oxides (TCOs), metallic contacts, interfaces and substrates. Therefore, for example, the deposition of TCO is also a critical issue for the next generation solar cells.

The PV industry has demonstrated its capability to lower the costs of PV systems in terms of cost per

Watt-peak (Wp) systematically over the last few decades following a learning curve with a learning experience in the order of 20%. This means that for every doubling of cumulative production, the cost decreases by 20%. However, it is of fundamental importance to realise that increased efficiencies contribute to cost reductions not only on module level – where most of the materials research is currently carried out – but also on the balance of system level.

Further large scale implementation of PV modules will also require *intelligent modules* in order to minimise losses attributed to partial shading or power fluctuations. To realise such intelligent modules, smarter control strategies and alternative power electronics topologies that dynamically optimise the yearly electricity production of these modules have to be developed and integrated. There is also need to control parameters (such as the conversion factor of DC/DC converters) in real time. Additionally, monitoring devices (such as distributed temperature sensing) would enable the plant-level controller to optimise the energy yield - ultimately we might be able to make trade-offs between lifetime and maximising power here and now. Technology wise, this implies that additional power electronic circuits and sensors need to be placed in and around the module. Materials research is urgently needed to realise such components.

Future grid-connected PV systems will be subject to more stringent regulatory requirements for the delivery of "ancillary services" to support the electricity grid when reserve and reactive power injection (for voltage support) has to be delivered. As the electricity grid has to deal with positive as well as negative balances, this involves the "shaving" of peak production and tempo-





FIGURE 4.1.1.3

Monocrystalline
Si Solar cells
Source: First Solar
Manufacturing GmbH,
Frankfurt (Oder)

FIGURE 4.1.1.4

Thin-film solar module

Source: Conergy SolarModule

GmbH & Co. KG, Frankfurt

(Oder)

rarily boosting power output. Lowering the output is easily achieved by moving away from the Maximum Power Point (MPP), but when storage is available, the energy conversion can be kept at maximum level and the output difference stored for later recovery.

Such a storage function may be centralised or distributed – possibly a micro-storage for short term needs will be introduced at the module level in close conjunction to DC/DC converters. These storage components could consist of improved supercapacitors with low leakage and innovative thin-film battery approaches.

To realise such innovative approaches needs further development of the respective power components and storage technologies as solar modules increase in temperature during operation which is not favourable for the lifetime of current power electronics and storage technologies.

4.1.2 Biomass

Biomass is a renewable energy resource derived from waste. Biomass comes from both human and natural activities and uses by-products from the timber industry, agricultural crops, raw material from forests, household wastes, and wood. Like wind, solar and other forms of renewable energy, biomass produces lower amounts of CO₂ emission than its fossil fuel counterparts. Therefore, the main driver for the deployment of biomass in Europe is the need to reduce carbon dioxide emissions and ensure a secure energy source.

Biomass can be converted into methane and various types of biofuels and used in numerous applications. Synthetic natural gas is, for instance, already being used to produce biodiesel, bio-oil, and biofuel. The conversion of biomass to bioenergy involves materials and catalysts in many processes. For example, in the conversion of wood to methane, wood gasification may be performed in a fluidised bed with abrasion resistant and catalytically active materials, where the resulting

raw producer gas is cleaned from sulphur species by an absorber material and finally converted over a methanation catalyst.

Research has to be focused on the investigation and further development of the materials involved in biomass conversion with the following characteristics:

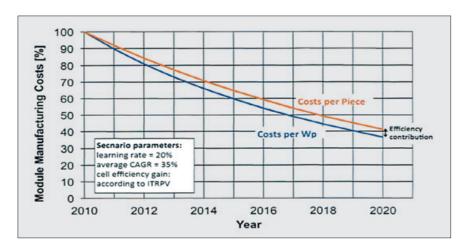
- Materials that keep their high initial catalytic activity even in highly contaminant-loaded hot gas streams
- Materials that are not affected by the high temperatures in these conversion processes
- Abrasion resistant materials when used as fluidised bed material
- Materials that are cheap and easily processable as well as being sufficiently resistant to corrosion. This could either be achieved by careful tests of known alloys or by new materials developed for this particular application. New coatings, which prevent the attack of corrosive inorganics at the underlying metal surface could also provide a solution

4.1.3 Thermo-Electric Energy

Thermoelectric generators enable the direct conversion of heat to electricity, but at present they are only used in a few niche applications such as supplying the energy for spacecraft and satellites, in Peltiercoolers in laboratory instrumentation or for medical applications. The efficiency of thermoelectric devices depends on a figure of merit Z which increases with electrical conductivity and temperature and quadratically with the Seebeck coefficient but decreases with thermal conductivity. Previously thermoelectric materials in their bulk form were based mainly on compounds containing heavy elements like bismuth telluride or selenide, or lead compounds, but also on bulk SiGe alloys. To reduce thermal conductivity by enhancing phonon scattering, more advanced bulk materials were based on partially filled structures like skutterides (e.g. those based on alloys of CoSb₃) /refs ADM, THB/ have pioneered the

FIGURE 4.1.1.5

Module manufacturing costs
based on an empirical learning
curve with a learning rate of 20 %
(Source: Semi Europe: www.ITRPV.net)



use of quantum confinement phenomena in quantum wells, in quantum wires and quantum dots to enhance the Seebeck coefficient, a field which receives a lot of attention particularly in the Us. The new advanced thermoelectric *bulk* materials contain nanoscale inclusions /ref ADM/ with typical dimensions of the order of 10 nm, for an efficient reduction of the thermal conductivity, without affecting the electrical conductivity too much, and an increase of the Seebeck coefficient. In particular the production of cost-effective nanocomposites with randomly distributed nanoparticles has turned out to be essential for future wider-spread use. Whereas the commercial market for thermoelectric devices so far is rather small at present this could grow with improved materials.

Apart from various semiconducting alloys and compounds with metallic or semimetallic inclusions, metal oxides have been identified as promising thermoelectric materials. They are chemically stable even at very high temperatures of ~1200 K. Research in this field has already produced most encouraging results.

4.1.4 Nuclear Energy

Nuclear power currently accounts for about 20% of worldwide electricity production and the demand is steadily increasing. As a consequence the demand per production unit increases and the enhanced yields result in the fact that materials used as structural components or as fuel must operate under extreme conditions. In addition, the waste stockpile increases and ecological solutions are required.

Throughout the last 20 years, Europe has been a leader in nuclear materials science in strong cooperation with American, Asian and other countries. The studied materials are component materials for future generation units such as advanced fission/fusion systems, and structural materials for thermal reactor units.

Fuel materials including the fuel matrix and targets for transmutation have to be considered taking into account their operation as well as the waste materials for disposal.

A common topic for future nuclear power systems is the trend towards high operation temperatures and high burn-up. An additional key challenge for the successful development of materials for fission and fusion systems is the harsh neutron irradiation environment.

A combination of *multiscale modelling* and *advanced experimental test techniques* need to be used investigate and to resolve issues related to the different types of materials used:

- Component materials for advanced fission/fusion systems
- Component materials for thermal reactor units
- Fuel materials, fuel matrix and targets for transmutation
- Waste form materials for disposal

Research of new materials including metals, carbides, nitrides, oxides utilised as alloys, solid solutions or composites should focus on higher stability or better mechanical performance.

Characterisation of these materials is carried out using advanced techniques; ex-situ studies on irradiated material and at elevated temperatures are required and are performed with accelerators and in piles in reactors. Characterisation should be performed in-situ by non-invasive techniques (by for example using inert windows for observation and analysis via video, Raman, DRS, XAFS, PIXE, etc).

The final goal is to develop advanced materials as component for fusion and generation IV (GENIV) fission systems; highly reliable materials for structural parts of thermal reactors with excellent behaviour inpile; economical fuel materials and targets for transmutation; and ecological waste form materials for

geological disposal. R&D efforts should therefore be directed into making the use of nuclear materials more sustainable, safe, economical and ecological.

4.2 Energy Storage and Distribution

Several of the energy sources mentioned above are not available constantly and in a predictable manner, and hydro- and nuclear power plants cannot react quickly enough to short-term fluctuations in energy demand. Therefore energy storage is a key requirement and in this context three major technological solutions are considered.

In the first place, batteries might play a role provided that *high-capacity batteries* are available. These are needed for electric vehicles, and can be used for decentralised storage. The challenge is to achieve the required capacities within the time-frame defined by industrial needs. Anyhow, battery development will be very important for local energy storage at a smaller scale. Similarly *super capacitors* will mainly be used for fast energy storage/delivery at a small scale.

A very promising technology, but so far not fully developed, is *energy storage in the chemical form*, using electrical energy to produce methane, ethanol, or other synthetic fuels essentially from $\rm CO_2$ and $\rm H_2O$. The fuels produced in this way have a very high energy density, are easy to store and transport, and can easily be converted back to electricity or other energy forms using conventional as well as novel techniques. This technology can also contribute to a reduction of $\rm CO_2$ emissions from conventional caloric power plants.

A key issue in the distribution of energy is the development of better grids ("smart grids").

4.2.1 Li-Ion Batteries

The challenges for Li-ion battery systems are very high, due to the rapidly increasing requirements for high performance energy storage systems. Studies suggest an increase of the market volume for batteries based on Li-ion technology of 77 B € in 2025. In general batteries store chemical energy and, on demand, convert it directly into electrical energy to power a variety of transportable applications such as cellular phones, laptops or other portable electric devices. These applications require compact, lightweight, and low cost storage systems. Requirements for materials used for energy storage systems in electric vehicles are deliverance of high currents for fast charging/discharging, high energy density, long cycle life, safety and low cost.

Current rechargeable lithium ion cells suffer from safety problems, low energy density, complicated battery designs, toxicity issues (cobalt), and limited resources of raw materials.

The development of next-generation lithium batteries requires the investigation of high-performance materials and the exploitation of new systems. The most promising research directions are:

- In the near future novel carbon varieties including nanostructures, lithium alloys, and improved silicon structures are promising candidates for the anode. For cathodes, high voltage materials (~ 5V) such as Ni-Mn-Co oxides show high promise and are a "hot" research topic. With improvement in the performance of new electrode materials, the demands on the electrolyte are also increasing These might be met by polymer electrolytes and ionic liquids. Beyond the chemical issues, nanoscaling and -structuring will play an important role in the future of batteries technology.
- In the longer term, the design and development of systems such as Li-sulphur and Li-oxygen (air) batteries should be envisaged. It expected that these systems can exceed the energy density of "conventional" Li-ion batteries by roughly tenfold.
- Other systems, e.g. Zn-air or organic batteries are promising and have to be considered on the long term, despite the fact that at the moment the replacement of the Li-ion technology by other cell chemistries is not yet foreseen.

Other future research directions are the development and fabrication of thin film Li-ion batteries which can be used to power added functionalities in devices such as credit cards.

4.2.2 Supercapacitors

In recent years supercapacitors (SCS) have found their market niche for several applications and the corresponding world market is expected to increase to US\$ 900 M for large devices (> 300 Farad) by 2015. If small capacitors (those found in cameras, mobile phones) are included, the market is estimated to be well above US\$ 2 B

Supercapacitors have proven long cycle life (> 500 000 full Depth of Discharge (DOD) cycles) with high efficiency and high power. However, in many applications the relatively low energy of SCs is a major issue.

As a consequence the main research and development goal for the next generation of SCs is the increase of stored energy. In order to achieve this goal two approaches are being followed:

- Novel electrode and electrolyte materials which allow for an increased cell voltage
- Hybrid designs by utilising battery and capacitor materials

4.3 Carbon Dioxide as a Raw Material and a Future Chemical Fuel for a Sustainable Energy Industry

4.3.1 General Objectives

The continuous increase of the concentration of CO₂ in the atmosphere, and the related consequences, have pushed the European Parliament and the European Commission to launch a programme for CO₂ sequestration in the ground (more details can be found in many reports, including STOA (IP/A/STOA/FWC-2005-28/SC20 and 2008-01; PE 416.243). According to the European SET plan, by 2020 20% of European emission should be captured and stored. It has to be noted that the world total emission of CO₂ will reach 30 gigatons in 2010.

In order to achieve the plan's objectives, industrial units are planned, with a unit price of approx $\varepsilon_{1.2}$ bn for an adsorption capacity of 5 millions tonnes per year. In the future, several hundred will be needed to make a significant impact. The three foreseen essential steps are: collect the CO_2 as close as possible to the source, transfer it by pipeline to adequate locations and pump it in the soil.

We propose to consider CO₂ as a <u>raw material</u> which can be recycled as a <u>chemical fuel</u>, which can be used as an energy source, thus generating a <u>completely new industry</u> in Europe.

4.3.2 How does this Process work?

In the first step CO_2 has to be collected. Work is starting at an industrial scale to establish the efficiency, the cost and the risks of these processes using amine, ammonia or zeolites for the adsorption step. The <u>raw material</u> $\underline{CO_2}$ (as gas or liquid) has to be chemically reduced by hydrogen to make a synthetic fuel (*synfuel*).

Industrial pilot plants for carbon dioxide capture for thermal power stations, at smaller capacity between 10 to 200 MW, are working today (BASF, TOTAL, ALSTOM, Dow Chemical, IFP, RWE, BP, Power Pass Corp, etc.).

The details of the different reactions have already been considered in two workshops (2008/Paris and 2009/Strasbourg) and a symposium at the E-MRS Fall Meeting in Warsaw in September 2010. During

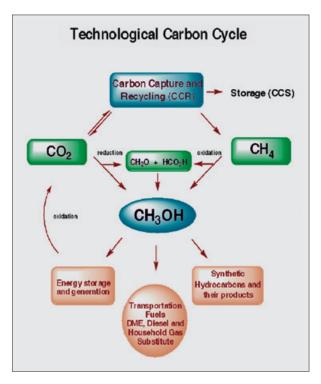


FIGURE 4.3.2.1. **Technological Carbon Cycle** (Courtesy of George Olah).

the Energy Conference organised in Fall 2009 in Stockholm under the Swedish Presidency, Prof. George Olah, Nobel Laureate in Chemistry confirmed our model (see Figure 4.3.2.1 below from his presentation). The efficiency of the whole process, *i.e.* the economics, will depend largely on the quality of the catalysts and progress using nano-catalysts have been shown very recently, as well as the splitting of H₂O by solar photons.

These technical proposals have received strong support from J.E. Stiglitz (Nobel Prize in Economy 2001) who declared recently "should the world endeavour to have carbon emissions paid at their real price... (it is essential) to promote incentives for innovations and investment in all techniques, companies, (and) home equipments which are more energy efficient".

4.3.3 Applications

As a large spectrum of applications of chemical fuels is possible, we restrict ourselves here to the <u>chemical</u> storage of excess electricity.

European authorities have decided that by 2020 a larger fraction of our electricity should be generated by renewable energies, photovoltaic, wind, and ocean. (Project 20-20-20). However, these are nonconstant sources of energy over time and it will become more and more difficult to stabilise the grid (e.g. the incident in Germany during 2009). Storage of elec-

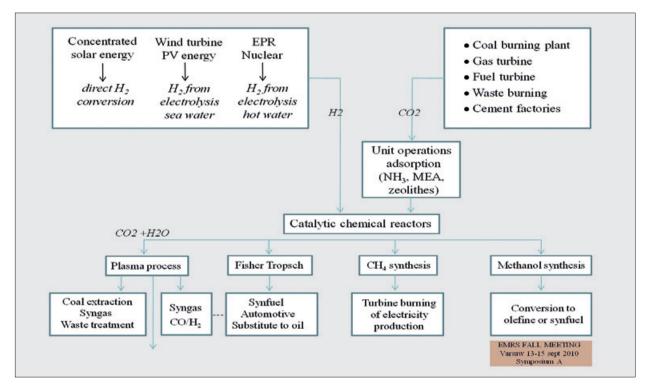


FIGURE 4.3.3.1. CO2 recycling

tricity is therefore a necessity; however, this is not possible directly: batteries will be insufficient as will be pumped-storage hydro-electric installations.

Large power plants, especially <u>nuclear reactors</u>, are not very flexible as a result of which the electricity price in Europe changes in the same day from about 5 cents to more than 1.0 \in per kW/h. Low cost electricity can be used to dissociate the water molecule H_2O and to generate the hydrogen H_2 needed for CO_2 reduction (it would even be possible to combine photovoltaic and nuclear in a same plant, one part of the electricity coming in the daytime from PV and from the large plant overnight). This chemical transformation of CO_2 into methane (CH_4) or methanol (CH_3OH) or synfuel will establish the capability to store electricity through a chemical process.

Even if not considered here in detail, it is obvious that these chemical fuels can become the energy carrier for <u>transportation</u>. The thermal engines in cars cannot be replaced in the short term at large scale either by fuel cells, or by batteries, because both the technological and economical developments are not mature for large energy storage. But an evolution of the engines will make possible the use of the fuels generated by CO₂ recycling as proposed in Figure 4.3.3.1.

4.3.4 Key Steps for a Development based on CO₂ Valorisation

- <u>The development of e H₂ production:</u> efficiency from electrolysis of sea water is one of the most ambitious goals and is dependent on catalysis research for new electrodes. Today, hydrogen is mainly produced from methane derived from fossil fuels large oil fields or shale gas.
- Secondly, catalytic materials are the key step: for the redox recycling of CO₂, strong scientific research network is needed for high efficiency stable catalytic materials in order to develop exothermic catalytic reactors with high efficiency conversion rate.

For large chemical plants the cost of the catalyst is one of the main factors that contribute to the cost of the process. Therefore, this key step needs to be developed by taking into account the efficiency and the selectivity of the catalyst including the support, the new kinds of spinels or perowskites which are able to replace expensive metals such Pt, Rh, Pa or rare earths such as Pr, Nd, Pm. Nanostructures may also become of great importance.

• <u>Develop economical and technical research on the engineering of the grid</u> control in a mixed flux of conventional and renewable energy supply. At the same time, new fields of scientific research can be explored. One of these is the direct splitting of H_2O by solar photons. It should however be noted that already today

there are overseas laboratory scale instruments, and large scale facilities are under construction.

• <u>Carbon dioxide as a raw material for electrical network</u> regulation

Taking into account this proposal, we can imagine a strong connection between the traditional electrical network and its regulation/control by including a large amount of renewable energy systems such as photovoltaic panels, wind turbine, biomass combustion, or thermal solar turbine. We have to remember that the goal is to reach 20% to 30% renewable capacity in the next ten years.

The flow sheet below provides an overview (Figure 4.3.4.1).

4.3.5 World Wide Equipment under Construction

From the most recent publications, one can observe the starting up of industrial and some pilot plants. Energy storage from the chemical reactions of carbon dioxide and hydrogen allow transformation from a gas phase to a liquid phase.

From the publications we can highlight the pilot plant developed by Professor K. Hashimoto to propose

energy storage from photovoltaic panels via carbon dioxide reduction by hydrogen produced by an electrolysis plant. The key steps are electrolysis and CO_2 reduction.

4.3.6 Safety and Sustainability of the Process

The chemicals and materials involved in the whole process are CO_2 , H_2O , H_2 , CH_4 and CH_3OH , all chemicals which are largely in use today. Of the metallic catalysts, those with nano-structures have to be handled like other metallic nanoparticles, as used in cosmetics or even medicine (MRI).

The large development of new catalysts is one of the key aspects of these processes. Most of the catalysts are formed from amorphous Ni-Zr and Ni-Zr-rare earth element alloys. Ni/(Zr-Sm)Ox catalysts are the main powder used for mass production but in order to avoid dependence on rare earths, new catalysts using Ni supported by tetragonal ZrO2 and others using Ni-Zr-Ca or Ni-Zr-Mg supported on tetragonal ZrO2 stabilised by Ca₂+ or Mg₂+ have been developed. These new nanostructured materials with large surface area and strong stability to the carbon dioxide impurities permit an increase in efficiency of the process and a decrease in cost.

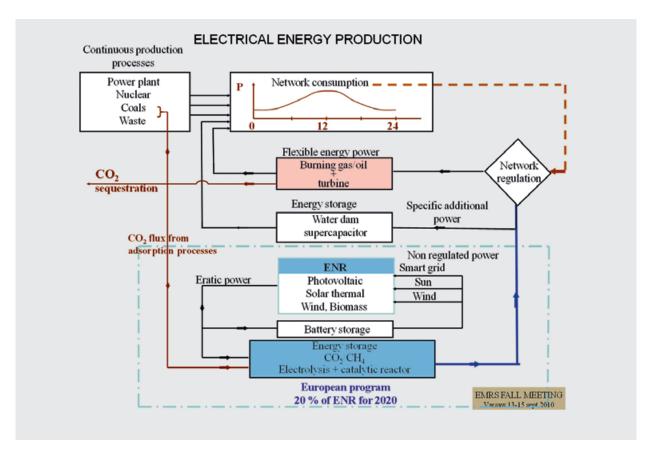


FIGURE 4.3.4.1. Electrical Energy Production

At the same time materials like perowskites or stabilised zirconia support, with a high thermal conductivity in order to control the selectivity of the process, have to be chosen. Today the recycling of catalysis materials allows the environmental impact of byproducts to be controlled and land fill pollution to be eliminated.

4.3.7 Economical Impact

The whole process will generate large industries installed in close vicinity to the generation sources of CO₂ with a substantial creation of jobs. These jobs cannot be delocalised due to the cost of CO₂ transport.

The first ambitious European project is starting in Germany, called CO₂-Reaction using Regenerative Energies and Catalytic Technologies (CO₂RRECT). The partners envisage a system in which surplus electricity from solar cells and wind turbines is stored as hydrogen generated via water electrolysis technology supplied by Siemens. The hydrogen can then react with CO₂ to form building blocks and other chemicals (see www.CEN-ONLINE.ORG, 9 sept 13.2010). This project allows the production at the same time of chemical products and synfuel depending on the catalysis and the economical aspect of each product.

4.3.8 Conclusion

Energy production by decarbonised processes is a major objective of the European Economic Program but it needs strong research in new materials in the large field of catalysis. Sustainable development in the field requires the creation of specific catalytic supports with large area and nanostructured active species for specific adsorption sites and high energy activation in order to increase the final energy balance of the process.

Renewable energy systems are increasing more quickly than expected but the discontinuous production of energy of these techniques needs energy storage for electrical network regulation and control.

Hydrogen from large electrolysis plants can work in connection with renewable energy systems, coal or nuclear plants and can be used as an intermediate for chemical energy storage through CO₂ in liquid product, as synfuel, or methane for electrical network regulation.

Carbon dioxide appears to provide strong opportunities for the development of a new industry of large energy storage to replace carbon fossil fuels. This strategy can be described through this roadmap taking into account the development of each step: the CCS carbon dioxide industrial plants being needed to store the carbon dioxide. This includes:

- The large development of renewable energy systems and plants (including photovoltaic, wind turbines, biogas, etc.)
- The electrolysis of sea water at large scale in order to optimise the cost of hydrogen production which is the main cost of the synfuel production
- New industrial plants for carbon dioxide reduction in alignment with the best economical options: synfuel or methane for energy regulation and some specific chemical products such as urea for agricultural fertilising

4.4 Energy Conversion

One of the most promising technologies for the conversion of chemical energy into electrical energy are *fuel cells*. Several concepts are currently being investigated, but intense research is still required to make the technology fit for industrial applications. Concerning the direct use of electrical energy, the efficiency of devices and appliances is an important issue, to actually reduce energy consumption, and developments in microand nanoelectronic have an important role to play as detailed in the corresponding chapter.

4.4.1 Fuel Cells

The world commercial market for fuel cells, including revenues associated with prototyping and test marketing activities, as well as actual product sales is expected to triple to US\$1.9 bn by 2013 and then almost triple again to US\$ 5.1 bn in 2018. Market gains will be stimulated by ongoing technological advances, helping to drive costs down to competitive levels in a growing number of applications, and supported by improved economies of scale as fuel cell manufacturers ramp up production. In industrialised areas such as the US and Europe, efforts to reduce dependence on imported oil and address environmental concerns will also contribute to fuel cell commercialisation activity and sales growth over the coming decade. Product sales will increase substantially in China and other developing countries, but the US, Europe, Japan, Canada and South Korea will account for over four-fifths of all commercial demand in 2018 /ref MAR/. Commercial demand for fuel cell systems, which totalled 17,800 units in 2008, will expand exponentially until 2013, when unit sales will reach 1.3 million, and then climb another sevenfold to 9.95 million units in 2018. Although market gains are projected to be strong for most applications, virtually all of this increase will be attributable to an explosion in demand for portable fuel cell systems,

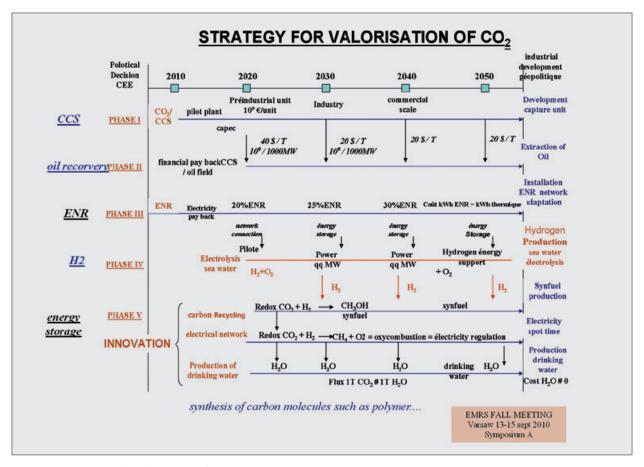


FIGURE 4.3.8.1. Strategy for valorisation of CO₂
Sources: /EMRS/, /SCI/, /SC2/, /SC3/, /CEJ/, /CSS/, /CHW/, /SC4/, /PAT/, /APC/

which is expected to account for 98 percent of all unit sales in 2018.

Demand in fuel cells for portable electronics will be spurred by users' frustration over the shortcomings of batteries as a power source for high-drain electronic devices. Declining product costs should contribute to make fuel cells – which have the potential to offer much longer run times than batteries – an affordable source of portable power.

4.4.1.1 Polymer Electrolyte Fuel Cells

Polymer Electrolyte Membrane Fuel Cells (PEFCs), also called Proton Exchange Membrane (PEM) fuel cells, in particular the ones applied as stacks in automobiles, use hydrogen fuel and oxygen from the air to produce electricity. Hydrogen fuel is channeled through flow fields to the anode of the fuel cell, while oxygen (e.g. from the air) is channeled to the cathode of the cell. At the anode side a catalyst (e.g. Pt) splits hydrogen into electrons and protons which pass through the PEM to the cathode, while the electrons travel along an external circuit. The electrons and protons recombine with oxygen at the cathode to form water which flows out of the cell. All of these basic components of a fuel cell — membrane,

catalyst, and electrodes with flow fields – should be further improved. One of the most important materials in a PEFC is the polymer membrane, which is proton (H^+) /hydroxyl (OH^-) ion conducting.

Proton-exchange membrane fuel cells (PEFCs) are currently the most widely used technology and their dominant market position will be strengthened over the coming decade. PEFCs operate at relatively low temperatures (allowing them to be fabricated in multiple sizes and shapes), offer quick start-up (a major advantage in both backup power and vehicular settings) and can operate over a wide range of power outputs. As a result, more organisations are actively working to develop and market PEFC systems than any other single fuel cell chemistry. However, demand for direct methanol fuel cells (DMFCs) will rise at a faster rate. DMFCs are a variant of conventional PEFC technology that can extract hydrogen from methanol without the need for a reformer, making them highly suitable for powering small electronic devices.

A goal for mid- and long-term research is the development of new and cheaper *membranes* with increased conductivity, which should be independent from the water content. Another requirement is

an improved understanding of the stability criteria in fuel cells.

The *catalyst* material is extremely important in a PEFC and presently mainly platinum is being used. New, cheaper (more active and stable) materials, *e.g.* alloys, should be developed. A better understanding of the catalytic activity of Pt and alloys is also required. As an example, it remains unexplained why a polycrystalline Pt surface has an activity 10 times higher than a Pt nano-particle.

Research should also address the development of new methods for producing *nanostructured surfaces* and improve *platinum support materials*, by for example providing more stable support materials, better carbon materials, and new binder materials.

The understanding of the *electrode structure* including porosity, mass transport and its effects on the performance of the fuel cell is crucial.

All of the above-mentioned topics are related to materials. As an example, bipolar plates are made of conductive materials in fuel cell stacks with gas flow fields which serve as the anode on one side and as the cathode on the other. Metals require better methods for structuring and coatings for low resistance and less corrosion. New concepts of cell circuitry (high voltage vs. high current) are also related to the materials used in these devices and their properties.

For the particular application of PEFC in <u>fuel cell</u> <u>cars</u> additional specific requirements exist and include the following need for materials research:

- For the hydrogen tank liner highly hydrogen-gasimpermeable polymeric materials are needed
- High strength, low cost, fibres for tank containment should become available together with cheap production routes for carbon fibres
- For bipolar plates corrosion resistant, gas impermeable, heat and electric conductive materials with a fast and low cost production route should be developed, avoiding any post-treatment such as coating
- For the interconnect between flow field and catalyst in the fuel cell, highly porous materials with tunable structures (permeability, tortusoity, thickness) will be required. At the same time these materials should be resistant to corrosion, mechanically stable, and possess good thermal and electrical conductivity

4.4.1.2 Solid Oxide Fuel Cells

Solid oxide fuel cells (SOFCs) have in principle the same components as PEFC, *i.e.* two electrodes, a fuel delivery system and membrane, but in this case the membrane is a ceramic material, *e.g.* an oxide, and the fuel cell is operated at higher temperatures (800–1200 °C). SOFCs are traditionally foreseen for stationary applications. They are technically feasible today,

although still too expensive. Sales of high-temperature solid-oxide fuel cells will also grow at an above average pace because of their ability to use multiple fuels and their high energy efficiency, which can exceed 80% if excess generated heat is recaptured for co-generation purposes.

An important aspect is the issue of degradation in the interconnect of an SOFC stack which electrically and physically connects the anode of one fuel cell to the cathode of the adjacent fuel cell. These interconnects can be made of ceramic or metallic materials.

Research needs to be performed on degradation, which is the main cause for failure in SOFCs. In addition, the need to replace the stacks often increases costs and hinders the commercialisation of SOFCs.

Future SOFC research should also be directed towards small to medium size SOFC systems for portable and stationary systems operating at low temperatures, *i.e.* 350–550 °C. It is known that small scale SOFC systems, so-called micro-SOFC systems, could replace state-of-the-art batteries, because they are small, lightweight, and deliver high power.

Finally, research is required in order to merge SOFC and high temperature ceramic technology with microelectromechanical systems (MEMS) technology from the Si industry.

5. NANOTECHNOLOGY

The Key Enabling Technologies, photonics, biotechnology, advanced materials, micro and nanoelectronics and nanotechnology, are all interlinked. Importantly, in all five areas the general Materials Science and Engineering approach is a guiding principle – *i.e.* processing-structure-property relationships. In nanotechnology this guiding principle still applies but now the behaviour is critically dependent on scale so that the structure at the nanoscale provides properties not necessarily observed in bulk materials.

This means that materials at the nanoscale require highly specialised and sometimes new sets of tools for fabrication and for property measurement. This concerns all other KETs. In the area of photonics for example, plasmonic structures are necessarily at a nanoscale and by definition, nanoelectronics will require processing of, for example, magnetic structures or multiferroic structures for memory devices or for communications devices. Biosensing is an area where nanostructured metals can provide surface enhanced properties useful for Raman detection of critical bio-markers. Other examples include nano-structured electrodes for batteries, nanoscale thermoelectrics for autonomous microsensors, nanostructures, surfaces for catalysis, etc.

Numerous challenges are raised by the nano-world: consideration of physical and physicochemical phenomena from quantum physics, characterisation and modelling not only at the design stage but through to the integration of the fabrication processes. This integration should ensure a multi-scale coupling/fit and should be considered at an early stage; i.e. from the design of the material or of the system. At the application level, complementary scientific challenges concern the emergence of the fields of intelligence, of cognition, of biology and of energy (including information and treatment in micro and nano-objects and systems); the design and the characterisation of micro and nano-biosystems at the scale of the living cell; and the generation and management of autonomous energy provision within such systems.

5.1 Materials and Fabrication

The ability to control, manipulate and design materials at the nanometre scale (10⁻⁹ m) will be one of the major technology drivers of the 21st century /ref WB/.

Fabrication falls into two basic technologies. Nanostructures made by "top down" methods (e.g. vacuum deposition methods such as pulsed laser deposition/sputtering/e-beam evaporation, molecular beam epitaxy often involving epitaxial growth of thin films on single crystal substrates) and nanostructures made by "bottom-up" methods whereby chemistry dominates through solution processing or by using surface energy considerations to achieve self-assembly.

5.1.1 Top-down

Progress in microelectronics is characterised by the continuous decrease of the dimensions of the components as for example:

- Multisegmented nanorods for display applications
- Using molecular thin films as precursors for the fabrication of nanostructured oxide thin films
- Nanocrystalline metals as well as nanocrystalline/ amorphous composites for high-strength structures

5.1.2 Bottom-up

New tools have been developed allowing for the observation and the manipulation of nanometric objects, in addition to synthetic routes based on chemistry and on self-assembling. From nanometric objects to the construction of structures and the creation of advanced materials with novel properties and combination of properties.

5.1.3 Nanotechnology for Energy

One of the "Grand Challenges" that constitutes a truly global challenge is that of energy. Sustainable and clean energy security is essential for continued industrial and economic development within the EU. Processes that are non-sustainable, or that contribute to pollution in any form, are simply unrealistic in the long term. Hence there is an overwhelming requirement for new developments in both materials science and in new nanostructures for energy. Some of the key technologies are:

- Fabrication of nanorods and wires by templated electrodeposition
- Nanostructured magnetocaloric/electrocaloric materials for energy efficient refrigeration
- Nanostructured oxides for catalytic decomposition of water
- 3-D templating approaches for materials for sensing, energy and plasmonics
- Quantum-dots on high area inorganic nanomaterials for photovoltaics
- Fundamental principles of electrochemical charge transport; potential application in catalyst or solar cell optimisation
- Developing nano-anntenae (dipole-whiskers) for optical rectenna (energy harvesting) devices
- Nanostructured thermoelectric compounds for energy harvesting
- Nanostructured energetic materials for combustion applications
- Nanotechnology for electronics applications

In recent years the European presence in the area of electronics and semiconductor fabrication has faced global competition but this also presents a considerable opportunity to address new materials and new fabrication processes for electronics. Processes that are far simpler to carry out experimentally and indeed industrially include bottom-up processes described above, polymer nanolithography, soft lithography, embossing, ink-jet printing, that have been developed order to produce structures at very low cost.

In the area of electronics the EU has the ability to make a significant impact in:

- Application to interfaces relevant to organic optoelectronic/spintronic devices
- Artificial spin ice honeycomb structures and planar nanostructured ferromagnets
- Quantum well narrow gap nanostructured Hall and MR sensors for imaging
- Metallic nanostructures for nanoscale light manipulation

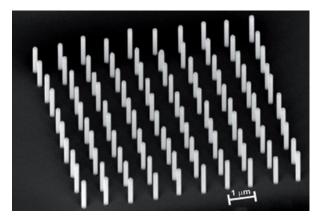


FIGURE 5.1.2.1. (left) **InAs Nanorods** Courtesy of IBM Research, Zurich

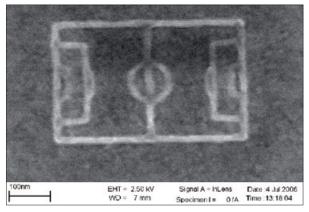


FIGURE 5.1.2.2. "The smallest pitch of the world"
The structure is realised with Allresist PMMA-Resist
(a product of the company Allresist GmbH). Line width of the goal
line is 8 nm. With it Allresist GmbH was the winner of a competition
for the smallest pitch of the world on the occasion of the World Cup
2006 in Germany. @Allresist GmbH, Strausberg, Germany.

- Multilayers with nanophotonic functionality
- Nanostructured metals for metamaterials applications: structure and processing
- Conductance of single molecules for application in nanoelectronics and electrochemical nanoscience
- Nanostructured phononic materials for sound and thermal management
- Phase change materials are so far used as rewritable optical storage media (e.g. in DVD-RW (rewritable) and blue-ray RW's). In this class of materials in addition to changes of the optical properties, the electrical conductivity can change by orders of magnitude and this property offers a potential for the use of phase change materials as non-volatile electronic storage media

5.1.4 Nano-Bio Applications

The extraordinary rise in the area of nano-bio is driven by the need for healthcare at low cost and this means both early diagnosis and then effective treatment. Nanotechnology has a crucial role to play here both in sensing and in targeted delivery. There is a requirement to develop chemistry at the nanometric scale: building entities from various functional bricks. Examples include:

- Allowing chemical compatibility with host medium (lures)
- Detection of specific media or environment (sensors)
- Ability to act in the medium (programmed or programmable delivery drugs, molecules, or probing substances for imaging). The aim is to establish the basis for numerous advanced techniques of diagnostic or delivery. This could also apply to the biotechnology KET
- Solid-state nanopores for single biomolecule sensing
- Charge transport in confined space
- Medical applications of stochastic sensing
- Enhancement of nano-traceability through studies at the micro- and nano-scale, at the frontier with biology (biochips, unique cells and molecules) resulting in the detection and the neutralisation of micro-organisms and pesticides. Impact is expected on environment, water, food analysis and security

5.1.5 Nanocomposites

Advanced functional materials are an integral part of modern technology. Current and future research is focused on a range of thin film and nanostructured materials for electronic, optical and magnetic applications. <u>Systems</u> which show promise both from ease of processing and resulting function are:

- Polymer composites with platelike nanoparticles (layered silicates), obtained by mixing solutions, emulsions and melts of different polymers with suspensions and powders of nanoparticles
- Polymer composites with submicro- and nanoparticles

The goals of the investigations are:

- Acquisition of the interrelationships between structure and properties of the investigated systems
- Development of the principles of the purposeful structural design
- Smart control of the exploitation properties of the composites by use of MFC (Macro Fibre Composite) and PZT (Lead-Zirconate-Titanate)

The expected results are:

- Design principles and technological methods of the nanocomposites and functional materials
- Recyclable polymer nanocomposites with enhanced stress-strain, barrier, adhesion, rheological and other properties for broad range applications
- Nanocomposites with innovative sensor and actuator properties
- Scientifically justified methods for the smart control of the construction properties
- Composite materials consisting of MFC piezomaterials

5.2 Characterisation

At the nanoscale we currently have the ability to explore the potential of use a wide range of advanced characterisation techniques including scanning tunneling electron transmission microscopy (STEM) associated with a range of spectroscopies, for example electron energy loss spectroscopy and Electron Energy-Loss Near Edge Structure. New surface probe techniques offer fresh insights into the properties of materials at the nanoscale. Not only is there a pressing requirement to employ state-of-the-art characterisation tools, there is also a need for the development of new tools to interrogate the physical, chemical, and electrical properties of materials at the nanoscale. In particular there is currently an absence of agreed techniques to examine directly the electrical properties of materials at the nanoscale so for example accurate measurement of capacitance, microwave loss tangent and polarisation become a challenge in nanostructured thin films. In addition at plasmonic frequencies the properties of metals and in particular losses are crucial.

The following aspects should be addressed:

- Characterisation of chemistry, structure and bonding at interfaces on the atomic scale
- Developing the study of organic/organic soft heterointerfaces and hard/soft heterointerfaces using cross sectional microscopy)
- In-situ experimentation to study mechanical and physical properties on the nanoscale
- Development of correlative and multiscale approaches to characterisation to relate nanoscale properties to macroscopic devices
- Developing optical methods using tagging (fluorescent nanoparticles) or multiphotonic spectroscopy. The aim is to visualise and investigate cells, neuron networks and could also apply to the Biotechnology KET
- Investigation of fundamental properties and of growth mechanisms allowing for progress to be made in the design and the use of new nano-systems and nanostructured materials

5.3 Theory and Simulation

Underpinning all these is the requirement for materials theory and simulation and in Europe we possess world-leading strengths. A key requirement here is the integration of several modelling techniques in order to cover a wide range of length scales from atomic structure to finite element modelling of large scale materials structures and processes.

There are several techniques available for theory and simulation of materials at the nanoscale and these techniques are required to guide the fabrication, synthesis, auto-organisation and auto-assembly of nanometric objects and systems. Topics to be investigated include:

- Electronic excitations caused by irradiation damage of metals, including channelling. Frictional damping of atomic motion caused by electronic excitations during irradiation damage
- The dynamics of dislocations under shock-loading
- The atomic structures of grain boundaries in elemental systems such as silicon and ferromagnetic iron, and in multi-component oxides investigated by novel algorithms
- Merging atomistic and continuum approaches to facilitate predictive models

5.4 Summary and Recommendations

Nanotechnology pervades all area of Materials Science and Engineering (MSE). Industrial acceptance and implementation of nanotechnology is demonstrated by the global market estimated in 2007 to be US\$147Bn and predicted to rise to around US\$1Trillion in 2015.

The science and engineering at these length scales requires quite different approaches compared with classical physics. Different and hence "classical" engineering must be modified to encompass length scales at the nano level. But this brings enormous opportunity in new materials, in materials processing for novel properties and for entirely new device concepts.

The applications of nanomaterials and nanostructures are indeed all pervasive and impact on the key "Grand Challenge" areas – Energy, Healthcare and Security.

A key paradigm must be the ability to make materials and nanostructures and the ability to measure their properties accurately. This may appear obvious but measurements, for example, of the high frequency electrical properties of nanometre dimension thin films on substrates is not a trivial task yet is crucial for our understanding and development of new materials and devices. The main recommendations are:

- Ensure that EU research has access to the best materials processing capability
- Ensure that EU research has access to the best possible characterisation facilities
- Ensure that we achieve the capability to understand unequivocally what the characterisation methods are informing us
- In order to achieve the above we need first class theory and simulation (modelling) of materials and structures including atomistic simulation, molecular simulation and the integration of these in multi-scale modelling schemes. Europe is world-leading and we must ensure that we maintain this position

6. MATERIALS FOR MICRO-, NANOELECTRONICS AND SILICON PHOTONICS

6.1 Micro- and Nanoelectronics

The semiconductor industry has been a key contributor to European economic growth and prosperity, and an important enabler of European success in the communications, consumer electronics, industrial machinery, and automotive industries. The semiconductor industry will also provide solutions for important issues in our society and serve as the foundation for progress in energy conservation, renewable energy, transportation, telecommunications, biotechnology, medicine, and many other fields. Semiconductors are critical to European industry and welfare, and must be prioritised to keep European industry competitive. Currently, there are more transistors per laptop than people on the earth and Europe needs advanced semiconductor manufacturing for competitive production for the digital revolution.

The EU and some of its member states recognise the strategic and economic value of the semiconductor industry and proactively support the sector by initiating R&D programmes such as the EU framework programmes and Eurêka, with specific funding lines for semiconductor-related R&D (SEA, ENIAC, JESSI, MEDEA OF CATRENE). /ref SEMI/ Europe has a leading position in the application of microelectronics *e.g.* in the telecommunication, automation, automotive, health and energy industries.

Micro- and nanoelectronics is a broad field, which comprises materials science, technology (wafer, chip production etc.), circuit design and system design. In addition, materials science links the other three fields because both circuit design and system design are based, among other things, on the performance of active and passive devices, which, apart from the structuring, is extremely dependent on the materials they are made of.

Micro- and nanoelectronics means the multifunctional integration of electronic devices where the main objectives in time have been to further increase the:

- Packing density (devices/area)
- Complexity (functions/chip; analog vs. digital, etc.)

- Multi-functionality (variety of devices, diodes, transistors, LEDs, etc)
- Signal processing rate (information/unit time)

In order to provide a reference document of requirements, potential solutions, and their timing for the semiconductor industry, technology roadmaps have been provided since the 70s. The US Semiconductor Industry Association (SIA) has produced the National Technology Roadmap for Semiconductors (NTRS), which in 1999 became the International Technology Roadmap for Semiconductors (ITRS) /ref ITR/. The most frequently cited trend is in integration level, which is usually expressed as *Moore's law* (1965).

In the years beyond 2010, the line width of conventional Integrated Circuit (ICs) will approach natural limits and new approaches have to be found by combining, for example, miniaturisation (*More Moore*) with diversification (*More than Moore*). By merging for instance system-on-chip (SoC) with system-in-package (SiP) solutions may be found beyond Complementary Metal Oxide Semiconductor (CMOS) technology.

Though roadmaps are needed in order to force industry thinking ahead, it soon turned out that the



FIGURE 6.1.1

Major Centres for Nanoelectronics in Europe
Sources: /ESF/, /SEM2/

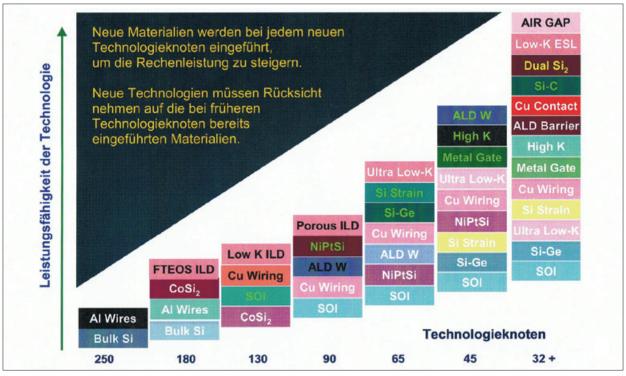


FIGURE 6.1.2. Increasing number of materials employed in consecutive technology nodes

Source: Global Foundries, Dresden, Germany

trustworthiness and reliability of roadmaps is very time limited. Looking ahead more than 8-10 years always turned out to be difficult if not impossible. A typical example is the 1975 IC Technology Roadmap. According to this roadmap, CMOS Technology should have ended in 1982 and been taken over by Silicon-on-Insulator (SOI) technology. As another example, GaAs should have replaced silicon technology in 1984 and E-beam/ X-ray lithography substitute optical lithography at about the same time. None of these predictions have been realised: 25 years later, CMOS is still a dominant technology and in spite of the performance advantages of III-V compound semiconductors, the market share of ICs fabricated with III-V compound semiconductors has up to now always been smaller than 5% of all manufactured ICs. Why?

The answer is: economics. Market shares are in most cases determined by the performance/cost ratio and not by performance alone. This implies that the objectives of a key enabling technology are accompanied by requirements of the market, which includes lowest possible prices by minimising costs. This implies, with regard to micro- and nanoelectronics, the improvement of yield due to an effective wafer processing technology. In addition, being first on the market is of paramount importance.

Whenever future applications of nano-science in electronics are considered, one should be aware of reference points such as the implications of parallel

processing and long term projections in silicon based production technologies for 2016 and room temperature devices which are:

- Dynamic memories with 64 GB storage capacities
- Minimum feature sizes of ≤ 22 nm
- Microprocessor chips with 60 billion transistors
- Operation frequency of 28 GHz
- Minimum device gate length of 9 nm
- System-on-chip manufactured on 450 mm Si wafers operated at 0.4 volts supply voltage
- Experts are convinced that Moore's law and growth of semiconductor industry will continue at least for the next 10–20 years

<u>Research areas</u>, which are presently considered as most interesting for the impact of material science on IC technology are:

- CMOS with high-mobility channel materials or combination of high mobility III-V n-MOS and (strained) germanium p-MOS integrated on silicon substrates for improved CMOS performance
- Silicon-based THz devices in combination with other high-mobility materials
- Electronic photonics or silicon photonics
- Organic electronic devices
- Nanotubes
- Electric field effect in atomically thin carbon films (graphene)
- Milli-Volt switch (Milli-Volt powering should be

regarded as a goal for future digital circuits)

- Sensor networks
- Biochips

An important impact of materials science on IC Technology and Engineering is *interdisciplinarity*. Cooperation of materials scientists with other research areas such as medicine, biology, biomedicine, chemistry and mechanics has opened up completely new markets. Though these applications are still considered as niche, they may develop into considerably larger share in the market in the future.

6.1.1 "More of Moore"

Since the beginning of the microelectronic era, the number of new materials involved in IC fabrication has steadily increased to keep the pace imposed by the Moore's law. Indeed, downscaling together with performance improvement of both devices and interconnection networks would have been impossible without integration of many functional materials with enhanced properties. From the 1960s the number of new forms of materials so far introduced in the CMOS architectures exceeds 20.

The challenges in terms of <u>materials research</u> in the "More of Moore" approach can be divided into two categories:

- The first one is *nano-materials integration and process* compatibility, i.e. how to introduce a given material with sub-micrometre dimensions in a given architecture, with the proper characteristics, without destroying the performance of already fabricated materials. These requirements are more and more stringent along with the increase in complexity of multi-layered architectures. For example new ultra-low k dielectrics of sufficient stiffness and compatibility with the multi-level backend process are still needed to fulfil the roadmap specifications in terms of inter-connexion delays required for the next generation nodes. At the same time, the fabrication of low leakage and low defect high k dielectrics for the next generation CMOS gates is still an issue under investigation.
- The second one is the *physical limits of the Metal-Oxide-Semiconductor (MOS) transistor* which calls for new concepts of active devices. From now onwards, research in the future will concentrate mostly on the integration of post-CMOS architectures with either nano-dots, nano-wires or carbon nanotubes to maintain the pace in the miniaturisation of logic and memory devices without degrading the characteristics such as the on/off current ratio.

In addition, critical mechanisms such as carrier or heat transport in low dimensional nanostructures become very different from those at higher dimensions, so that new models for nano-materials are needed to simulate the devices correctly. Predictive models will require a more precise knowledge of nanostructures' parameters such as grain size, defects, surface and interface composition and chemistry of the materials.

Following years of discussion, research and development on the new Si wafer diameter of 450 mm has started. The objective behind the transition to 450 mm is similar to the transition from 200 mm to 300 mm: to raise productivity and to lower costs by an increased wafer surface (factor of 2.25), to process more chips per process pass, supported by a paradigm shift in manufacturing.

The research and development activities affect all areas of semiconductor manufacturing, ranging from wafer substrate, process equipment and metrology, to manufacturing science. While first manufacturing facilities are not expected before 2018, these research topics provide obvious chances for Europe to participate and lead 450 mm developments with proven strengths in substrate material, manufacturing equipment and measurement devices.

Preparatory work in Europe has already started with initial research on silicon-based materials, standards, automation and early prototypes of process and metrology equipment. It is now time for Europe to enter deeper into the worldwide 450 mm community with coordinated R&D efforts to maintain and extend its strength as first-class supplier for semiconductor manufacturing for 450 mm wafers. As a final benefit, the knowledge gained in 450 mm automation and process efficiency is expected to be fed back into next generation 200/300 mm manufacturing, thereby enhancing productivity for the already established 200 mm and 300 mm manufacturing facilities in Europe. Important aspects and advances are expected to result in improved process and equipment control, green and increased energy efficiency and equipment modularity approaching "plug and play" capabilities.

6.1.2 "More than Moore"

As the limit of Moore's law for conventional 2D devices gets closer, a new paradigm for downscaling using vertical multi-chip architectures recently appeared as an alternative route to keep the pace of system integration. In this regard, the "More than Moore" approach making use of heterogeneous 3D stacked architectures,

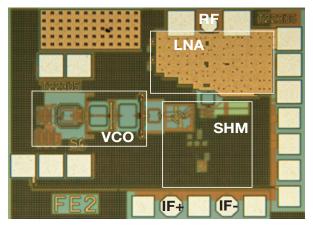


FIGURE 6.1.3. 122 GHz Receiver in SiGe Bicmos
Source: IHP, Frankfurt (Oder), Germany (IEEE journal of solid-state circuits, Vol. 45, No. 9, September 2010, pages 1644-1656 and IEEE
BCTM 12.2, 978-1-4244-4896-8/05/\$25.00 © 2008 IEEE, pages 182 -185)

calls for even stronger efforts to maintain a continuous improvement of **device performances** in terms of speed and power consumption. This trend motivates research on the integration of new materials such as thick conductors for coils and vertical inter-connects, magnetic oxides for passive devices and thick dielectrics for electromagnetic isolation.

6.1.3 Packing Density

Access to a leading and effective wafer production process is paramount for micro- and nanoelectronics in order to fulfil the requirements of the market. Unfortunately, wafer production in Europe has declined considerably during the last few years. One of the reasons for the decline has been labour costs. However, due to the high degree of automation of wafer production, salaries are no longer a convincing argument for having the CMOS production placed in Asia. Instead, capital costs are now stated as the main issue for choosing the venue of fabrication.

Provided the necessary funding is made available at the European level two options can be envisaged:

- The first is to invest in the most leading wafer fabrication technology with respect to scaling and wafer size.
- The second option is to invest in 300 mm wafer production with feature sizes of 100 nm (or even larger) and focus on diversification.

Though the first option would have a positive effect on European semiconductor companies, it is nevertheless a very expensive one. Furthermore, conventional ICs are approaching natural limits and More Moore (miniaturisation) will eventually generate additional concerns due to the high stand-by power (leakage current) and the fact that devices are already now power-constrained.

Taking into account that the interest in diversification (More than Moore) by combining silicon technology with other materials such as germanium, III-V compounds or graphene, has recently increased considerably, it is worthwhile considering the second option. Combining these materials with silicon technology will have considerable effects on conventional wafer production not only due to a significantly more complicated technology but also with respect to equipment. It is therefore expected that the most leading wafer fabrication facilities will have to adapt to cope with these new technologies. These multi-material technologies are for the moment restricted to niche applications. However, it is expected that these technologies will soon produce global breakthroughs in new areas of application such as medicine, agriculture, biology, etc. Since investment in such wafer technologies at an early stage of development is much less expensive than the leading wafer production, it could be advisable investing in minor silicon wafer production facilities with different materials.

Independent of whether the *More Moore* or *More than Moore* approaches prevail, it is of paramount importance that wafer production in Europe is ensured for the benefit of both industry and the research institutions. European funding in this field would have a much larger impact if research in micro- and nanoelectronics at universities and research centres is supported by the presence of wafer production at the European level.

6.1.4 Complexity

As already mentioned, interest in increasing the number of functions per chip has increased considerably. Aspects and technologies considered as most promising for improving the complexity of ICs are:

- Architecture
- Operational principles
- Micro-Electro-Mechanical Systems (мемs)
- Electronic photonics (including waveguides and silicon photonics)
- Sensors
- Spintronics

Regarding *architecture*, there is a trend in going from planar gate to double gate (fin-fet)/trigate and further to wrap gate allowing for ultimate scalability. A major concern is the integration of nano-materials and process compatibility *i.e.* how to combine a hybrid material with sub-micrometre dimensions with a given

architecture while at the same time keeping the desired characteristics performance of already fabricated materials. These requirements are more and more stringent and go along with the increased complexity of multilayered architectures.

The fabrication of low leakage and low defect high k dielectrics for next generation CMOS gates is still an open issue with different possible options.

When considering *operational principles*, one should realise that, as an example, Metal Oxide Semiconductor Field effect Transitors (MOSFETS) are limited by so called inverse sub-threshold slopes, which cannot exceed 60 mV/decade. To achieve steeper slope devices, the presently most promising candidates are Tunnel FETS (TFETS). However, Si-based TFET devices are limited by the drive current. Non-Si alternatives such as III-V hetero-structures based on small bandgap materials like InSb are considered as interesting alternatives. But steep slopes over several decades have yet not been demonstrated.

These few examples show that more intensive research is needed to improve the operational principles of IC devices.

Sensors are needed for many applications. Microand nanoelectronic sensing principles make use of virtually any imaginable physical property of semiconductor material (electronic, electro-magnetic, mechanical, photonic, piezo-electric etc.) and translate it to electric quantities (current, voltage, power). Smart sensors containing digital signal processing and communication interfaces will permeate our life in the future with increasing intensity at home, in the car, in the working environment and on (and in) our body. They will be integrated in appliances, textiles, and production lines and will communicate wirelessly with one another, implying that for an effective application of sensors the complete exploitation of interconnectivity is crucial. In order to make these applications feasible, a combination of technologies will be necessary.

Taking into account the complexity of the involved technologies and the economic potential it is paramount that sensors are considered as one of the most urgent research areas.

Conventional electronic devices rely on the transport of electrical charge carriers in a semiconductor such as silicon. Several attempts have been made to exploit the 'spin' of the electron rather than its charge to create a new generation of *spintronic* devices which will be smaller, more versatile and more robust than those currently making up silicon chips and circuit elements. Spin orientation of conduction electrons survives for a relatively long time, which makes spintronic devices particularly attractive for memory storage and magnetic sensors applications. Some researchers are convinced

that spintronic devices may even be used for quantum computing where electron spin would represent a bit (called qubit) of information.

Future applications of spintronic devices will include spin-based transistors having advantages over MOSFET devices such as steeper sub-threshold slope. Considering that the potential market of spintronic circuits is believed to be worth hundreds of billions of dollars a year, this area should be regarded as one of the most promising in micro- and nanoelectronics.

Due to their importance in the European context, silicon photonics and MEMS technologies are described separately in the following sections of the document.

6.1.5 Multifunctionality

Presently, several approaches are considered as most promising for improving the multifunctionality of devices in micro- and nanoelectronics and these are:

- Silicon based THz devices
- CMOS with high mobility channel materials or combination of high mobility III-V nMOS and (strained) germanium pMOS integrated on silicon substrates for improved CMOS performance
- Silicon photonics and heterogeneously (III-V/Si) integrated photonics
- Electric field effect in atomically thin carbon films (graphene)
- Biochips
- Power electronics

High-speed silicon-based hetero bipolar transis*tors* (HBTs) with f_{max} up to 0.5 *THz* have been developed and produced in Europe for more than a decade. Recently a 2.0 ps world record gate delay for SiGe HBTs has been announced by IHP (Frankfurt/Oder) in competition with world-leading companies like Intel and IBM/ref IEDM/. Approaching the THz region allows the realisation of cost effective solutions for applications in areas such as security (airport control), production checks (quality control), astronomy and science (THZ spectroscopy), biometry and biomedicine (identification of health problems, THz tomography), short-range wireless communication and data transmission as well as military applications. It is therefore no surprise that the interest in such devices and circuits is overwhelming in spite of the fact that they are still covering niche applications. However, as mentioned earlier, due to the multidisciplinarity it is expected that at least some of these application may develop into products with large market shares.

The example of silicon based THz devices shows once again that investments in private wafer produc-

tion specialised in niche areas such as THz devices and circuits may be reasonable ventures for strengthening the competitiveness of European companies. Though the speed limit of silicon-based THz devices is expected to be around 1 THz, further improvements of the silicon technology is expected due to the heterogeneous incorporation of other materials such as III-V compounds and germanium. The heterogeneous incorporation of other materials is not only of interest for THz devices but will also be of great importance for other devices such as the *CMOS technology*.

GaN-based semiconductors, for example, are wide bandgap materials that feature a higher breakdownvoltage (threshold) than conventional semiconductor materials, such as silicon or GaAs. By using different channel materials, MOS transistors with very diverse properties can be produced, which allow for design circuits with unpredicted assets. Nitride semiconductor power transistors on a silicon substrate, for example, show improved control and suppression of electrical currents when powered off. Using different materials also allows changing the structure of the devices. For example, by tailoring the layer beneath the gate electrode improves controllability of threshold voltage that intercepts electrical currents, to enable low-power losses, high speed switching, and high-temperature operations.

CMOS with different channel materials integrated on silicon substrates will improve CMOS performance considerably and is therefore considered as one of the most interesting developments in the near future.

Biochips are currently not made from semiconductor materials but from plastics or glass. Fluidic channels, electrodes, pumps and receptor molecules can be integrated in these substrates. Typical biochips have sensor functions, such as the detection of DNA, RNA, proteins, antibodies, etc. Semiconductor biochips are still under research. The most well-known semiconductor biochips are probably implantable integrated circuits for electrical excitation or readout of neurons (e. g. "retina implant"). Since integrated electronics on plastics or glass are not readily available, conventional biochips have no integrated signal processing electronics. On the other hand, semiconductor biochips have a huge potential for medical and even consumer applications due to their high integration level, miniaturisation, and low cost. This implies that medical costs could be dramatically reduced for well-known analytic methods and expensive analysis methods could be made available to everybody (e.g. DNA analysis). Furthermore, analysis of single cells can be performed with unprecedented accuracy, and mobile and patient-operated analysis, as well as tele-medical applications, will enable better health care and prophylaxis.

In conclusion, biochips based on micro-and nanoelectronic circuitry will be of great interest for medical applications in the future.

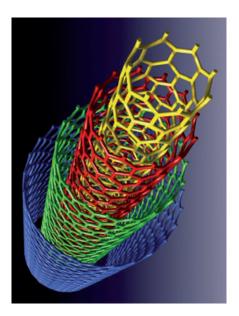
6.1.6 Signal Processing Rate

Higher clock rates, logic and memory density, as well as cost per function are the main drivers for ever increasing information processing and transport requirements. Here the combination of electronics and photonics at chip or packaging level offers the path to overcome current bottlenecks. As mentioned earlier, this includes most advanced CMOS on the one hand, but integrated devices with near-THZ Radio Frequency (RF) performance would also be highly desirable (e.g. SiGe нвтs, hetero-integration of III/V devices). Though much research is still needed, the expectations in realising "silicon photonics" are very high because such a technology would make possible functionalities such as terabit-onchip as well as integrated and fully functional coherent and non-coherent opto-electronic transceivers for shortto long-range data links. Once the limits of More Moore are reached, technologies such as the ones mentioned above are the solutions for future developments of micro- and nano-electronics and should therefore get the highest attention.

6.2 Carbon based Nanostructures

The International Technology Roadmap for Semiconductors (ITRS) has identified an end-of-life for scaled complementary metal-oxide-semiconductor (CMOS) technology around 2022 /ref ITR/. In a recent Workshop, sponsored by ITRS on "Beyond CMOS" technology, carbon has been identified as the most likely next platform for microelectronics, because of the huge development in the science and technology of carbon-based materials (fullerenes, nanotubes, graphene and graphene nanoribbons) for MOSFET applications. One of the most peculiar and interesting aspects of carbon is the fact that it exists in a large number of modifications which show different structural and electronic properties. For a series of recent review articles covering all modifications of carbon see /ref MRS3/.

Carbon in its three-dimensional single crystalline form of *diamond* is a wide gap semiconductor and in principle useful for high frequency, high temperature, and high power electronics as well as a material for exploratory work for room temperature quantum communication and computing. *Nanocrystalline diamond* films find applications in NEMS and MEMS devices.



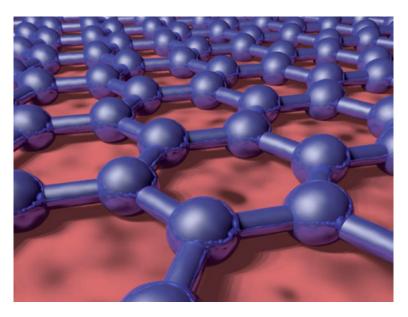


FIGURE 6.2.I. Carbon Nanotubes (left) and Graphene (right). Sources: Science Photo Library (left) and V. Palermo, ISOF, Bologna (right).

As a strictly two-dimensional material "graphene" is a zero-gap semiconductor which has already been used to fabricate transistors for radio-frequency applications with cut-off frequencies of up to 155 GHz, as realised by IBM researchers /ref NAT/. With rolled sheets of graphene quasi-one-dimensional structures (with respect to their electronic conductance) can be formed which are called carbon nanotubes. These exist both as metallic and as semiconducting nanotubes of different size and structure. High performance field effect transistors operating up to 80 GHz with on-off ratios of 10⁵ and even circuits (ring oscillators) were fabricated and furthermore the suitability of carbon nanotubes for photonic devices has been demonstrated as well /refs MRS4/, /MRS5/. A major obstacle for their wide-spread use is that, to date, it is difficult to produce large amounts of identical carbon nanotubes. Most synthesis methods yield nanotubes of different sizes and structures. Recently some progress has been reported, based either on separation techniques which discriminate between different sizes and structures, or following another route employing selective growth in order to maximise nanotube alignment and minimise their diameter distribution /ref MRS7/. Finally, in buckyballs or fullerenes the electrons are confined in all three dimensions of space and thus in this form carbon exists as a quasi-zerodimensional material. Derivatives of these fullerenes have found applications in organic electronics and optoelectronics.

A discovery, which recently has generated great attention, is *graphene*, a strictly two dimensional material, in which carbon atoms are arranged in hexagons in a single atom plane with electrons confined strictly to this two-dimensional plane /ref SCI5/. Theoretical mod-

els have predicted that graphene could make transistors more than a hundred times faster than today's silicon transistors. Arrays of hundreds of graphene transistors have already been made on a single chip /ref MRS6/.

Although today's transistors based on graphene still fall far short of the material's ultimate promise, there is evidence that graphene, because of its properties, could be practical for future generations of electronic applications.

From a fundamental standpoint, graphene's most exiting capability is the fact that its conducting electrons arrange themselves into quasi-particles moving at 1/300 of the speed of light, mimicking relativistic laws of physics /refs SCI5, MRS6/. Graphene is a gapless semiconductor and with an applied gate voltage both the conduction type (n-type or p-type) as well as the carrier concentration can be changed. Most notably devices fabricated from graphene show characteristic properties such as room temperature mobilities superior to those in well-developed CMOS transistors /ref MRS6/.

If the extrinsic disorder in graphene is eliminated, higher room-temperature mobilities than for any known other semiconductor are expected over a technologically relevant range of carrier concentrations,

Furthermore, graphene has an extremely *high* thermal conductivity up to 5 000 W/mK at room temperature, which is about 20 times higher than that of copper and can sustain current densities up to $5 \times 10^8 \text{A/cm}^2$. The combination of these properties could ensure almost no heat generation in the devices.

Because of its gapless nature, graphene based field effect transistor (FET) devices exhibit on/off ratios of approximately only 100:1 and this fact renders them not directly suitable for digital electronics, however, it

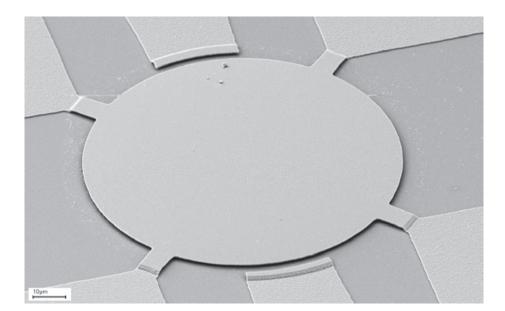


FIGURE 6.3.I.

Low-temperature thin-film
hydrogenated amorphous
silicon bulk MEMS resonator
on a glass substrate.

Courtesy of INESC-MN,
Portugal.

is sufficient for *analog* device applications /ref MRS6/. High frequency FETs with cut-off frequencies of about 100 GHz were reported in 2010 by the Avouris group at IBM /ref SCI6/. Quite recently this group has reported even higher cut-off frequencies of 155 GHz for 40 nm gate length devices using chemical vapour deposition techniques to grow single layer graphene on copper foils which was subsequently transferred to diamond-like carbon films grown on SiO₂ /ref NAT/.

Graphene holds promise for use in *high-frequency transistors* even in the THz regime.

To widen the possible electronic applications of graphene efforts to introduce an *open energy gap* have been made. Three routes have been followed so far / ref MRS6/:

- a) Graphene nanoribbons
- b) Chemically modified graphene as *graphane*
- c) Bilayer graphene sheets to which a perpendicular electric field is applied

Graphene nanoribbons are produced using lithographic and etching techniques whereby a band gap is created by carrier quantum confinement. For the chemical modification of graphene a reaction with atomic hydrogen is used, whereby "graphane" is formed, a semiconductor with a gap of about 3.5 eV. The third possibility is to use bilayer graphene and applying an electric field perpendicular to its layers which opens a gap of about 200 meV.

Graphene-based open gap materials hold the promise for future CMOS logic devices. Graphene is now also being studied for applications beyond conventional CMOS, like *spintronics*.

Among its further extraordinary properties is its extremely *high mechanical strength* with a breaking

strength of about 130 GPa (about 2 orders of magnitude higher than that of steel).

Apart from the exfoliation technique, epitaxial growth of graphene on silicon carbide has been demonstrated successfully and lately large graphene sheets about 30 inch (75 cm) wide have been deposited by chemical synthesis from a methane and hydrogen mixture on polycrystalline Ni and Cu substrates, paving the way for large scale graphene based electronic and optoelectronic devices/refs NATNANO, NPH7/.

Graphene with its high optical transparency combined with its high electrical conductivity and its flexibility makes it extremely appealing for future optoelectronic applications. Currently, graphene is one of the most exciting materials and all efforts should be taken to study this material on a broad basis to assure a leading European role in the industrial exploitation of this material.

6.3 Micro- and Nano Electro-Mechanical Systems Technology (MEMS and NEMS)

During the last two decades MEMS technology has gained in maturity with a variety of materials and architectures never encountered before in CMOS technology. The new challenges concerning the control of mechanical properties of self-standing multilayered microstructures or the integration of multi-physics effects in a single device have been taken up by tuning materials properties such as stiffness, stress, refractive index, as well as chemical or biological affinity. However, the demand for even smaller and more power efficient devices pushes forward the limits of MEMS performance with a pace imposed by new

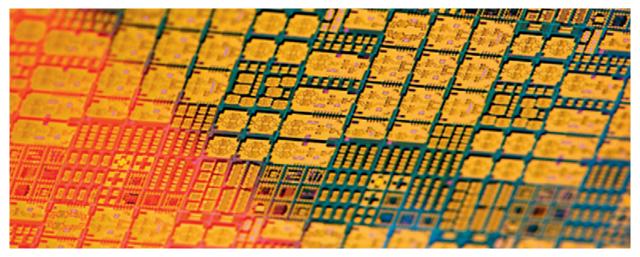


FIGURE 6.4.I. Processed GaN-based amplifier circuits. Source: © Fraunhofer IAF

societal needs in sectors such as transport, telecommunications, energy, videogames, health and security. This trend calls for new requirements in terms of size reduction and design of materials with very specific and well controlled properties such as ultra-thin or nanostructured chemical or biological films for biosensors or bio-MEMS, porous materials with very high specific surfaces for lab-on-a-chip functions and also micro-machined nano-cantilevers or rotating nanostructures for power MEMS devices that can withstand millions of deformation cycles without breaking. In addition, packaging at the wafer level is a critical issue to achieve reliable and low cost devices and thus requires careful design of protective materials mostly for in-vivo or harsh environments.

Progress in the microelectronics or MEMS industry will continue alongside a steady effort in materials science, with the main following scientific objectives:

- Materials multi-scale processing (combined top-down and bottom-up approaches)
- Nanoscale characterisation and modelling of materials (e.g. nanoprobes for surface and bulk measurements)
- Study of surface and interface physics and chemistry of materials
- Nanostructured active materials (nanoelectronics, spintronics, nano-optics, nano-sensors and nano-actuators)

6.4 Power Electronics

Power microelectronics currently represents 30% of the semiconductor industry. Europe's largest semiconductor industries (STMicroelectronics, Infineon), are considered world-wide market leaders in *power electronics* with a broad portfolio. In addition, there are many SME dedicated to equipment (LPE, etc.), materi-

als (many new companies are arising such as SICrystal, Azzurro, etc.) and device fabrication. This collection is of strategic importance for many areas such as automotive (future electrical and hybrid vehicles will reduce power consumption and CO₂ emission by the use of advanced electronics for engine control), energy production and use (wind, photovoltaics), communication (power servers, cellular bridges, base stations), power transport and transformation (from the grid to the system AC/DC and DC/DC conversion), consumer electronics and electrical household appliances. Many of these applications require high fidelity components (for safety, for example in automotive, security in industrial, and longevity in consumer products) and low cost.

Certainly, energy consumption is going to become a major issue. At present about 2% of electrical energy consumption is due to products related to the information technology industry like data centres, computers, wireless routers, etc. Within the next 10 years this share is expected to increase to 20%. While energy management of many products like cell phones is an important asset, many "side products" like chargers for mobile phones, MP3 players, etc. are only optimised for low production cost, with energy consumption not taken into account. The use of high efficient GaN/AlGaN High Electron Mobility Transistors (HEMTS), for example, can reduce power consumption in wireless base stations by up to 30%. In addition, these technologies are also extremely desirable for energy efficient RF power amplifiers (wireless base stations, mobile phones, tablets, etc.). For the development of a "zero power dissipation technology", systems are required that work with power off during stand-by, which allows for significant power savings: currently, for instance, many wireless routers are on 24/7 for convenience reasons, but actually used only for a small fraction of this time; standby power consumption accounts for a large fraction of the total power consumption of many such devices. As in many other areas, hetero-integration of III/V devices with silicon will solve most of these problems, which makes this technology one of the most important technologies for future microelectronics.

New and advanced power devices can successfully address at least two sectors: the transformation and the use of energy, but also transportation can take advantage by more efficient solid state switching power cabins. Power production by both photovoltaic and wind requires DC-DC and DC-AC converters. They exhibit up to 99% efficiency in the best working conditions, but this value can decrease to 80% in a poor environment and working conditions (high current, low dissipation).

It can be argued that the systematic and progressive introduction into the market of systems based on new high efficiency and intelligent power electronics will allow the EU to save about 3% of power consumption per year, allowing to meet the request of an increasing energy demand by power saving.

As a consequence, power saving will become a need, and the energetic class will be *the* characteristic defining the products on the market, which is so far only established for household appliances. Energetic restrictions and requirements that determine products' characteristics will become increasingly stringent.

For these reasons, it is tremendously timely to develop research activities in material science to engineer power saving and energy efficiency in power microelectronics.

The research trends in wide band gap semiconductors are based on high quality large dimension 4H-SiC wafers and high power switching devices, GaN HEMT on SiC for power applications and GaN on Si for low power applications. Advanced research is needed to improve the power device performances using nanotechnology but starting from the needs of specific power applications and systems.

6.5 Silicon Photonics

The enormous upsurge in communication industry has increased the demand for efficient and low-cost optoelectronic functions, while integrated photonic devices are also becoming of increasing importance for molecular sensing. In addition microelectronics is facing the interconnect bottleneck where due to increased integration signals transmission is the limiting factor in the device speed and a solution is forecast in the use of optical interconnects. All of these aspects require the development and fabrication of cheap, integrated, and CMOS-compatible photonic devices. Indeed, silicon-

based microphotonics has been under great scrutiny in recent years. The prospect of extending a massive, low cost electronics manufacturing platform into the photonics domain is the subject of much research and debate. It has become obvious that an important driver for the debate is the intrinsic distance × bandwidth limitation of electronic communications links. In other application domains, typically, photonic links are utilised once these electronic limitations have been encountered. Photonic link standards of many kinds have been developed to support such demands in the past. These standards represent a historical context for a silicon micro- and nanophotonics roadmap – and yet they may impede its development. A roadmap is starting to emerge focused not on how silicon micro- and nanophotonics can implement existing standards, but rather on how silicon micro- and nanophotonics can support the advance of network bandwidth in an important way.

Silicon photonics, *i.e.* the integration of *photon*ics and silicon technology /refs NPH, PHO, IEEEQE/ includes the generation, emission, transmission, modulation, signal processing, switching, amplification, detection and sensing of light. This is one of the key issues for the future development of micro-and nanoelectronics /ref ITR/. Since the material properties of silicon do not allow to fulfil all these requirements, it is obvious that incorporation of other materials into silicon technology is a necessity. To provide a truly compelling solution, silicon micro- and nanophotonics will likely need to achieve a high degree of monolithic integration with at most a small degree of hybrid integration, in order to offer both low cost and increased functionality. This will probably involve new photonic materials, (e.g. Ge, BaTiO₃, SiON, etc.) and nanomaterials (nanocrystals, nanowires). Although this adds manufacturing complexity, this trend is also occurring in advanced CMOS to allow Moore's Law scaling and new functionality, such as high-k gate dielectrics and MRAMs.

The main drivers for this technology are twofold:

- (i) High speed data transmission both for short, medium and longer range data links
- (ii) High performance interconnects

The final aim will be to integrate waveguides, modulators, multiplexers, photodetectors and active devices like light-emitting diodes and even lasers and high speed electronics on Si based platforms /refs PHO, NPH, IEEEQE/.

Photonic solutions will also help to decrease the so far rather large and still increasing power consumption of electronic circuits and interconnects with the presently used copper links. It is foreseen that the traffic capacity on a multi-core central processing unit (CPU) of a computer will reach tens of Terabit/s (Tb/s) within

the next decade making optical inter-connects the most practicable solution /ref PHO/.

The lack of efficient Si-based light sources currently represents a main bottleneck for the development of silicon photonics and for the full exploitation of potential benefits from merging electronic and optical functionalities on the same chip /refs PHO, NPH, IEEEQE/. Silicon is a poor light emitter because of its indirect fundamental energy band gap. During the last twenty years many efforts have been made to develop new strategies to increase the efficiency of light emission in Si. New advanced materials (strained Ge or Si-Ge-Sn structures, porous Si, Si nanocrystals in a SiO₂ matrix, si-Ge islands, Si-based films and nanostructures containing Er or other rare earth ions, nanocrystals of optically active compounds) and nano-fabrication tools (e-beam lithography, nano-imprinting) are currently playing an important role in this field.

Although limits and perspectives of *Si nanocrystals* and Er-doped Si nanostructures for applications in photonics are clearly visible, additional efforts for improving their optical performance are needed. It is of extreme importance, however, to also explore other routes, for example Si nanowires and different rare earth elements.

For the future application of silicon photonics the proper *coupling of optically active species* (Si nanostructures and/or rare earth ions, SiGe islands, strained Ge quantum wells) with photonic crystals and nanocavities has to be mastered /ref NPH/. In this respect the SOI (silicon-on-insulator) platform should be explored in great details for photonic applications and the use of defects and dopants in single crystal silicon for light emission, in view of the strong enhancement provided by photonic nanocavities, should be revisited.

Efforts have to be mainly focused on novel strategies such as silicon nanowires, different rare earth elements, nanocrystals in novel CMOS-compatible hosts, defects and emitting centres in SOI. The strong coupling of active emitting centres and photonic crystal nanocavities needs to be investigated thoroughly.

For the successful implementation of silicon photonics it will be of utmost importance to fabricate such systems in CMOS compatible silicon-on-insulator platforms /refs NPH, PHO/. Any larger scale industrial application of innovative Si-based light sources will necessarily require *electrical excitation* of the active materials.

Particular attention should be also given to the *electrical contacts* needed for the electrical excitation of the system, which should be made of transparent and conductive materials. To achieve this goal graphene-based contacts might turn out as a possible solution.

In the following the present status of the key elements for Si photonics is summarised, for further details see a series of review articles /refs NPH, IEEEQE/.

6.5.1 Present Status

Modulators: For the wavelength region used for telecommunication (1.3 and 1.55 μm) so far most Si-based modulators use a change of the charge carrier density by applied electric fields to modulate the refractive index. Carrier depletion based modulators with transmission rates > 40 Gbit/s were reported /ref NPHO $_3$ /. Recently the quantum confined Stark effect in multilayers consisting of Ge-rich quantum wells and SiGe barriers on substrates compatible with Si technology has been exploited for electric field induced changes in optical absorption /ref IEEEQEL/.

Detectors: Considerable advances have been made in high performance detectors which involve epitaxially grown Ge or GeSi layers on Si substrates /ref NPH4/ with high responsivity from near infrared to visible wavelength region together with comparable fast response time. Waveguide integrated detectors enable monolithical integration on a Si wafer. Integration with Si based read-out circuits makes such detectors suitable for both high performance data links as well as for infrared imaging. So far the highest reported efficiency bandwidth product for a waveguide coupled Ge detector is 30 GHz at a bias of 1 V /ref NPH4/.

For high bit-rate optical communication systems avalanche photodetectors (APDs) are used and recent progress has demonstrated that Ge/Si APDs can achieve at least comparable or even better gain-bandwidths products (approximately 340 GHz) and comparable sensitivity as the so far used III-V compound APDs, notably InP based ones / refs IEEEOFI, NPH6/.

Light sources: Since both Si and Ge have indirect fundamental energy band gaps there is no efficient radiative recombination resulting in very low internal quantum efficiencies for light emission in bulk crystals. However, for nanostructures an enhanced light emission has been reported for systems like Si nanocrystals, Si nanopillars, porous Si, Si/SiO₂ superlattices, Si nanowires and in some of these even optical gain was observed /ref NPH5/. Another route which is being pursued is based on MOS-like structures consisting of erbium doped silicon dioxide (or silicon nitride) layers containing Si nanoprecipitates. The carriers are injected in the structure through tunnelling and the recombination of excitons in the Si nanostructures excites internal transitions in erbium. In addition, efforts in exploiting electrically excited light emission from defect transitions in Si have been made and quite efficient emission has been achieved from the recombination of carriers confined at dislocation loops. While light emitting devices have been obtained, with all these approaches *no* continuous wave (cw) electrically excited lasing at room temperature has been reported so far.

Optically pumped lasing has been reported by exploiting stimulated Raman scattering in silicon. In this case particular attention was taken to remove carriers within a reverse biased p-i-n waveguide in order to avoid free carrier absorption. Gain and even lasing was also claimed to take place in optically pumped Si/Ge/Si heterostructures for a wavelength of about 1.6 μ m by exploiting transitions at the direct band gap in tensile strained and highly doped Ge layers/ref OPL/. Whether such structures can lead also to an electrically pumped diode laser remains to be seen.

Today injection lasers which operate in continuous wave (CW) mode at room temperature on a Si wafer are, however, only hybrid lasers. These are fabricated by bonding a III-V compound semiconductor wafer, usually InP, onto silicon on insulator (SOI) substrates. A typical structure consists of a p-InP active layer and p-InGaAs and n-InP cladding layers and up to six inch wafer sizes with such hybrid structures have already been realised /refs NPH2//NPH5/.

Photonic integrated links: Companies and research institutions like Intel, IBM, Hewlett Packard, Luxtera, Kotura, ST Microelectronics, Alcatel Thales, LETI, IMEC, the Microphotonics Center at the MIT, and others are investigating the implementation of Si photonics since an optical communication system between chips and possibly also within chips and cores allows for much higher bandwidths than copper interconnects. For future high performance computing systems companies like IBM develop on-chip optical interconnects and consider Si micro-and nanophotonics as the enabling technology for "exascale computing" and essential for the realisation of future 3D-integrated chips. This company has recently presented integrated CMOs and nanophotonics modules where for the latter already 65 nm design rules were employed /ref івм/. Intel has reported that it can integrate all the optical building blocks (hybrid lasers, modulators, multiplexers, optical couplings, and detectors) on single receiver and transmitter chips /ref INTEL/. An integrated link operating at 50 Gbit/s over a single fibre has been achieved using multiple wavelengths and wavelength division multiplexing and suggestions for further upscaling the bandwidth have been made /refs NPH2, IEEEQE, IBM/.

In this context it is foreseeable that there will be an important market for optical fibre links to connect PC devices with their periphery for data transfer.

6.5.2 Future Trends

Si micro- and nanophotonics is attractive since it is a scalable technology which offers high modulation speeds and a combination of electronic and photonic functionalities. The driver to implement photonics solutions on a large scale is the necessity to reach the bandwidth range of Terabit/s /refs PHO, NPH2/.

Apart from enabling the aforementioned applications, silicon micro- and nanophotonics will also have an impact in fields like imaging and sensing, and can be expected to have important implications for advanced imaging techniques, in particular for biological and medical applications.

Substantial impact can be expected also in the field of high-efficiency Si-based solar cells where nanocrystals and rare earth doping can be utilised to widen the range of spectral sensitivity by converting one short wavelength photon into two or by combining long wavelength photons to form one photon with shorter wavelength. A substantial increase in efficiency is expected from such techniques.

Si micro- and nanophotonics will provide high density integration of optical components at comparatively low cost for data processing and photonic communications and thus will play a key role for the European economy, and not only for the computer and communications industries.

6.6 Conclusions and Recommendations

From the examples above – many more could have been given – it is clear that micro- and nanoelectronics is probably *the* key enabling technology. Beside the technological and economic importance of electronics itself, almost all other fields depend to some extent on the developments made in electronics. It is also clear that in the next one to two decades the development successfully followed in the past decades will reach fundamental limits. Several promising solutions to overcome these limits, like graphene or photonics, are on the horizon, and pushing research in those fields could ensure Europe holds or regains the leading role, with obvious impact on the European economy and society.

7. BIOTECHNOLOGY

According to the reference documents on KETs, biotechnology here was taken in the restrictive meaning of "Industrial Biotechnology" or "Biological Engineering" ("Biotechnology brings cleaner and sustainable process alternatives or industrial and agrifood operations") / refs ECI, EC2/. Considered excluded from consideration in this particular KET at this moment are then aspects such as biomedical and health applications, environmental monitoring and mitigation, and nanobiotechnology, which are in general considered to be part of the field of biotechnology/bioengineering.

Although health sciences and technologies, for example, have not been included so far in the KET documents as such, some aspects are partially covered in the "Advanced Materials" and "Nanotechnology" topics. Nevertheless, the importance of this field is such that it is proposed that the KET on Biotechnology be expanded to include health sciences and technologies.

In the field of biotechnology related to health, Materials Science and Engineering (MS&E) can have an important contribution in:

- molecular and cellular diagnostics, where the ultimate goal is to identify disease at the earliest possible stage, ideally at the level of a single/few cells and/or single/few molecules, namely through the development of novel biosensors, Biomems/lab-on-a-chip systems, and analytical tools;
- <u>drug delivery systems</u>, where the long-term objective is the ability to target selected cells and/or receptors within the body and deliver a molecular payload, namely through the development of nanoparticle engineered systems;
- <u>regenerative medicine</u>, where the focus is to treat disabling chronic diseases and to help victims of disabling injuries, through the application of tissue engineering and advanced biomaterials.

It is proposed that the remit KET Biotechnology be expanded to include biomedical and health science and technologies. This KET would benefit from the recent MS&E advances in bioelectronics, bionanotechnology and biomaterials for applications in diagnostics, drug delivery and regenerative medicine.

From the point of view of the contribution that MS&E can bring to this KET as it is currently formulated, the input is limited. Although biotechnology reactors are obviously fabricated from specific materials, and, namely in the cell or enzyme support systems, the chemical and physical properties of the support materials is an important materials design issue, MS&E considerations are not dominant.

It is a different matter if one considers the <u>contribution that KET Biotechnology can bring to MS&E</u>. It is challenging to consider a *new paradigm* in which renewable agricultural and animal farming products can be made into an *important source of new engineering and functional materials*. This perspective is mentioned in some of the documents and would represent a significant change in outlook for MS&E.

Materials resulting from processing of renewable biosources such as wood, rubber, textiles, and paper have long been used. To achieve a qualitative change of the current situation, in which most materials are processed from non-renewable sources, the success of a KET in Biotechnology from the point of view materials production would have to combine the following factors:

- Advances in biosciences, namely in genomics, proteomics and systems biology, as well as in molecular and cellular engineering, which allow the design of novel organisms with specific characteristics, e.g., production organism and process development from raw material to chemicals and materials by cell factory concepts;
- 2) Development of MS&E structure-propertiesprocessing-performance know-how relating

- to engineering and functional materials from biosources;
- 3) Synthetic biology integrating different scientific disciplines and engineering and thus allowing designing and constructing new functionalities and building blocks for cell or cell chassis production of novel functional and structural materials.

The ambitious objective proposed in this KET to develop biotechnological industrial processes in which organisms would produce, either semi-assembled or in the form of building blocks, different designed advanced materials with an ambitious set of properties competitive with those of metals, semiconductors, fossil fuel-derived polymers, and ceramics and glasses, is strongly endorsed.

It is important to stress that currently there is no integrated scientific or technical knowledge on how to achieve the above-mentioned objective, although efforts in developing bio-based materials focused mostly on fibre production are underway.

At the current stage, it seems that the following two approaches could be taken:

- Support for basic research and development in the field of biotechnological production and characterisation of engineering and functional materials, both from a biomimetic point of view and also via the *de novo* design of microorganisms.
- Investment in the integration of a strong MS&E component in Biotechnology courses and, likewise, ensure a strong Biotech background in MS&E and engineering courses in general. The mutual understanding of these communities' knowledge basis is indispensable for progress.

8. GENERAL CONCLUSIONS

Innovation is often supported by invention, the *creation* of a new idea, made manifest, which only needs to be a theoretical concept and thus may not always result in a product. Invention is a highly creative process. An open and curious mind enables one to see beyond what is known. Inventors think outside of the box. Business people used to say: "Invention is the conversion of cash into ideas". Innovation is the conversion of ideas into cash.

In spite of receiving a large part of European research funding, the efficiency of the European Research Area (ERA) concerning innovation is questionable, considering that only 15% of high tech products originate from Europe. In the proposal for the decision concerning the 7th Framework Programme (FP7), the EU Commission has pointed out that "it is paramount to overcome one of the key European weaknesses the "European Paradox" – in generating splendid scientific knowledge and insufficient ability to convert this knowledge into innovation and commercial products".

Furthermore, in one of the European Commission's communications (2004-353), the Commission worries about the fact that "Europe lacks sufficient capacity to transform knowledge into products and services". As one of the reasons for these shortages the Commission points out that "today's infrastructure in Europe does not always meet the requirements of industry". In this context we refer to a recent report on "Creation and Transfer of Knowledge –The Critical Need for Closer Ties Between the Academic World and the Private Sector" submitted by the Committee for Research Structure of the Physics Class of the Royal Swedish Academy of Sciences /ref FFSK/.

There is an increasing consensus in the European scientific community that the core of this "European Paradox" lies in the weakness of the European research structures and coordination. In most European countries inventions are supposed to arise in the academic world, while the innovation process is taken care of by the private sector, but the lack of an effective and

constructive collaboration between these two sectors impedes the required transfer of knowledge. This difficulty is based, among other things, on the fact that the objectives and goals of the private sector are completely different from those of universities, and that communication between the two sectors is often hampered by the increasing interdisciplinary nature of science, which has become a dominant factor in many research areas. This is particularly true for the five key enabling technologies due to their interdisciplinary and multifaceted nature. In this context, KETs development and deployment will certainly depend upon the success in addressing the "European Paradox".

We support the results of the analysis and the statement of the High Level Group highlighting the "need to further reflect on the lack of appropriate financial ecosystems, along with limited financial instruments to address KET issues, risk taking in funding large-scale capacity expansions in KET production technologies and public strategic procurement and the current absence of a European IP patent"/ref KET./

As a final remark, the authors would like to note that new ideas are often created by research and are more easily generated through front line research than through improvements of existing ideas. Basic research and in particular curiosity-driven research are therefore important prerequisites for generating new ideas and seeing beyond what is known. In promoting innovation all efforts are therefore needed to ensure that scientific institutions are able to perform basic and curiosity-driven research at the highest level, even in the future. Furthermore, there is a critical need for closer ties between the academic world and the private sector and a very good example of where this is being implemented successfully is the increasing number of spin-out companies generated by University research.

Evolving research results into innovation (products, technologies, services, etc.), proof of concept demonstrated by prototypes and on pilot lines that meet the technical standards of modern production lines, accel-

erate the transfer of knowledge to production, *i.e.*: to the market. This is because adaption processes that are expensive and always fraught with risk are not directly necessary. However, this indeed requires that there are European research centres in the field of key enabling technologies that meet the high standards.

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APPENDIX

Knowledge Transfer in the field of PV: Ideas to Industry

Analysis of the present mechanisms for photovoltaic technology transfer in the USA

Written by Christine White for The European Materials Research Society

April 2010

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1 Overview

The aim of this report is to outline and understand the mechanisms involved in the transfer of knowledge from researchers and research institutions to industry within the United States photovoltaic sector.

Approach

It is evident that understanding the intricate details for the transfer of every idea or the birth of every start-up company that emerges in the PV sector would be overwhelming. However, this report simplifies the prominent and successful mechanisms in the US, to understand the general methods of technology transfer and the current policies and community initiatives available for facilitating the launch of new companies. In addition, the report briefly covers some of the barriers that can prevent certain research initiatives from reaching the market. The general mechanisms are introduced and discussed in the first chapter. In the following chapters, the report attempts to answer three simple but fundamental questions regarding photovoltaic technology transfer in the US:

- Where are most of the ideas generated and what is the relationship between academia, national laboratories and industry?
- What is the role of the inventor/researcher and who is granted the intellectual property rights and the rights for licensing the technology?
- Where does the funding come from and what pathways are in place for pushing these technologies to the market?

The final chapter is an overview of technology transfer is the final section is devoted to showcasing two prominent companies involved in state-of-the-art PV research and understanding how they emerged as PV leaders in the US.

In the end, this document is provided as a way to understand where PV technology ideas originate and the pathways from concept to manufacture in the US.

1.1 Technology Transfer in the USA

Now that alternative energy is emerging as a mainstream idea, the US government has expanded funding and created policies to quickly advance "green-technology." Private investors are also investing in promising PV technologies. The increased availability of funding has expanded research opportunities for existing companies, facilitated the manifestation of new solar research and engineering companies, and provided financial support for fundamental research in university and other laboratory research groups.

When looking at the origins of the innovative PV ideas, it is obvious that many cutting-edge technologies are derived from research performed at universities and federal or state-run research institutions. The amount of intellectual property that comes from such institutions is overwhelming. The dissemination of this intellectual property is facilitated with scientific journal publications, conferences and seminars as well as private collaborations, and is rapidly spread for others to read, understand and build upon. When ideas are recognized as having enough market potential to warrant patenting the technology could very well reach the consumer markets one day.

Over the past decade more than 24 new companies have been formed with photovoltaic commercialization as their primary mission. (See Appendix for list of start-up companies). Start-up companies formed by private researchers or investors make up about 65% of the new PV companies, while about 35% are developed as universities spin-offs. This number includes only those companies with active research and development, and aim to manufacture novel PV cells or panels. This number does not reflect any new departments or projects created within existing companies. It must be mentioned that the creation and dissemination of innovative technology in the PV sector is not limited to start-up companies. Therefore, for the sake of this report, the mechanisms explored are based on the acquisition of intellectual property for start-up companies and existing companies.

The Role of Government

Government plays a large role in the spread of new technologies through the institution of policies and programs that stimulate the growth in a particular market. In 2006, the US Department of Energy (DOE) began a program called the Solar America Initiative (SAI) whose aim was to boost the US-based solar energy industry. The DOE provided tax incentives and funding to companies and researchers in order to develop solar energy as a costcompetitive electrical energy source by the year 2015 [1]. This program ended in 2009, however, the Solar Energy Technologies Program continues to fund photovoltaic preincubator and incubator projects for emerging technologies [1]. (See chapter 3.3 for more details)

While federal funding is important, there are also local-government initiatives and public companies that provide local support and financial backing to boost the PV technology research in the state and help with commercialization of technology. For example, the program *Go Solar California* has funding available for "Research, Development & Deployment" [2], while in

Virginia the *Renew Virginia Initiative* was instituted to provide legislative and executive actions to stimulate the green-technology economy in Virginia [3]. The legislative and executive actions in Virginia included providing incentives for companies who manufacture green technologies, especially photovoltaics. In Pennsylvania, the governor granted state-budget funds for PV technologies [4] and the Pennsylvania Energy Development Authority (PEDA) continues to provide financing for renewable energy development and integration [5]. These are just a few examples of local actions that provide a favorable environment for emerging PV technologies.

The Role of Research Institutions

Universities and national laboratories are the main incubators of ideas, and much of the funding granted to them is geared toward fundamental, basic research and exploring undeveloped areas in the field. With this type of funding there is often much freedom to try new and innovative processes. While in academia and government funded laboratories, project goals must be reached and deadlines are normal, there is less emphasis on developing a product, producing revenue, and pleasing investors as there is in a business environment. The fresh ideas are a combination of innovative thinkers who are uninhibited by traditional corporate deadlines, and the abundance of necessary tools and resources available.

• Technology Transfer Offices

It is common for a strong research institution to have a technology transfer office (TTO). TTOs have been developed for facilitating the licensing agreements between innovators with their intellectual property and the entrepreneurs who can bring a product to the fruition [6], as well as providing substantial support to a researcher who is interested in starting a company – although under most circumstances the federal government does not permit employees to work for an outside company unless they leave their government position (this point is covered further in section 4).

TTOS provide a link between ideas and the "real world" industry and transfer their intellectual property through the licensing of intellectual property. The TTOS also provide a researcher with legal advice and market viability analysis for this new technology. In the case of a start-up company, the TTO provides (non-financial) assistance and often employs a knowledgeable "resident-entrepreneur" – someone experienced in starting companies. The researcher can find the support he needs through the TTO, which may also have connections to the financial realm, but which itself does not usually provide a large pot

of start-up funds. The role of the innovators in the continued improvement and advancement of the technologies they develop is also discussed in section 4.

The Role of the Private Sector

The private sector plays a very important role in refining ideas and processes that are developed by research institutions or envisioned by inventors. The private sector combines manufacturing engineering "know-how" with the business models of entrepreneurs, and often obtains substantial financial backing for marketable and promising ideas. All of this combined smoothes the process of commercialization and provides a pathway for technologies to eventually reach consumers.

Common Mechanisms

Technology transfer follows three basic mechanisms, which result in commercialization of state-of-the-art PV devices.

Outsourced Intellectual Property

One very common mechanism in the US for technology transfer in the PV industry is the outsourcing of patented ideas to existing companies. For universities and research institutions such as national laboratories, this provides a financial return on the intellectual property. An existing company benefits from the use of a profitable idea, while the research institution and researcher have little or no financial risk in such a venture. The existing company often has the manufacturing and business expertise to bring a technology to the market, and some of the revenue generated from the use of the patent is given as royalties to further other research in the research institution as well as compensate the inventor.

Researcher Start-ups or Spin-offs

Researchers are the brains behind advancing PV technology. Through a start-up or spin-off they have the greatest opportunity to push the research and development in a direction they see fit. Once they protect their ideas, either through a technology transfer office at their research institution or through a private means, the "researcher-turned-entrepreneur" chooses to create a company in order to bring their ideas to commercial reality. They then must find financial backing through venture capital firms or private investors. In this case the inventor approaches the investors with an idea. In addition, the inventor possesses the in-depth research knowledge to head a research and development project through the startup phase.

University spin-offs are less common these days for silicon PV research due to the saturation of companies in this field and the emergence of other technologies. However, recent market potential has increased for start-up companies who focus on state-of-the-art

second and third-generation solar cells, organics and flexible PV, and concentrating semiconductor materials (see Appendix). The federal, state and local incentives for green technologies provide a more favorable environment for start-up companies to get their feet on the ground and push past the start-up phase and eventually make it to a manufacturing and production stage. While starting a company is a great achievement for the inventors, it has been shown through significant research that if a researcher worked in academics prior to starting a company, it is common for him/her to return to academia once the company has a strong enough foundation [7,8]. Once he/she returns to academia, it is also common for him to continue do provide assistance to the companies, but he may often give up their role as chief technology officer.

• Investor Start-ups

In this case, investors or entrepreneurs (those outside of the research realm) see a potential market that is untapped and seek to create a company to address this commercial need. Once they identify the market demand and they develop a business plan and they either apply for the licensing of patented technologies that have not become commercialized in or they recruit researchers to develop the intellectual property they require to get their company off the ground. This is a fairly successful mechanisms of technology commercialization, however, the process from idea to commercialization can be lengthy and costly before their product reaches the market.

1.2 Common Technology Transfer Challenges

The challenges that are faced in the transfer and commercialization of new PV technologies are not limited to the PV sector. As with any new technology there is an entire step-by-step process that is involved from the invention and development side to the marketing and user side. In order to finally make the technology available to consumers the new idea or technology must make it through the entire process shown in Figure 1.1 can contain many roadblocks to success at each stage. These roadblocks vary depending on the type of technology or the nature of the project, but according to a report written by the International Environmental Technology Centre, some of the biggest challenges are "shortfalls in technology creation and innovation, underperformance in technology sourcing, sub-optimal enabling environments, and insufficient and unverified information" [9]. Small and medium enterprises are disproportionately impacted by these challenges, which can make it even more difficult for start-up companies.

One of the greatest challenges researchers and inventors face is deciding the best way to handle their intellectual property. While technology transfer offices at research institutions provide financial and legal assistance and attempt to smooth the pathway for technology transfer, impediments can occur at every link whether they are due to policy restrictions or the movement of information and materials, etc. [9]. It is well known that some academic researchers choose to bypass the technology transfer offices (TTOS) at their universities in order to increase the efficiency of the technology transfer and sometimes to increase their share of the profit [10]. Often the universities have specific policies in place that require a researcher to inform the university TTO of any invention or idea instead of selling the idea directly to industry. Bypassing the TTO is not an acceptable practice according to various university policies and could result in the loss of the researcher's job in some cases. But, there are some clearly stated reasons why this occurs. For instance, when universities merely encourage compliance with their policies without actually enforcing them, they signal tolerance of nondisclosure of inventions and discoveries [10]. Naturally, when compliance with employment guidelines does not enhance faculty's utility function – and when enforcement is rare – bypassing and private appropriation increase [11].

However, it is in the best interests of the universities to try to prevent this so-called "spillover" by negotiating for faculty departments and inventors to receive a larger share of the profits from the technology. A benefit of researchers using the TTO especially at a large research university is the access to legal advice and funds for patenting and licensing [8]. It is shown that for universities providing a large share of the return to the researchers and their departments, the researchers are less likely to bypass the TTO [10].

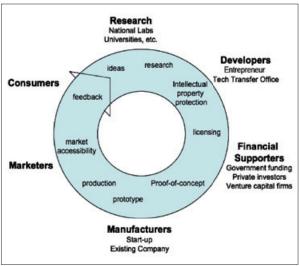


FIGURE I.I.

The cycle of commercializing technologies. [12]

Finding funding and financial backing for the advancement of an idea through the development and manufacturing stages is another large barrier to successful technology transfer. According to a report written by the Center for American Progress and the Global Climate Network, "Finance goes hand-in-hand with technology development and transfer" [13]. Because technologies such as photovoltaics often require a large initial investment it is important for the US government to institute funding and financing initiatives or subsidies in order to spur the creation of new technology ventures.

In the last two decades, favorable intellectual property policies have been instituted and more funding has become available to the green-technology sector. Private, public and federal incentives have been implemented; much as been done to reduce these barriers in order to maximize the economic and energy-related benefits provided by advanced cutting-edge technology.

2 Ideas and Innovation

Innovation is seen often in collaborative efforts. Cooperative agreements and collaborations happen throughout science and engineering, so certain laboratory policies and agreements have become standards for dealing with the legal aspect of technology transfer. As with any research and development effort there are many parties involved. When these parties are not part of the same institution, cooperatives, alliances and partnerships are formed in order to provide the legal backing for any intellectual property that is formed as a result. The focus of this section is primarily on the formation of research relationships. Intellectual property rights and ownership details will be described further in section 3.

In the early 1980s, the US political environment seemed to shift decisively in favor of permitting exclusive licenses of publicly funded research to encourage commercialization [14]. The Bayh-Dole Act was instituted to allow small businesses, non-profit organizations and universities, rather than the government, to pursue ownership of an invention or intellectual property even when federal funding grants are involved. This policy thereby allows the universities or small businesses to handle their intellectual property in a manner that they please. The federal government, however, still retains "march-in" rights to license the invention to a third party, without the consent of the patent holder or original licensee, where it determines the inventions is not being made available to the public on a reasonable basis [15].

In general there are three major sectors responsible for idea creation:

Universities

Due to the structure of academic research and the requirements for tenure-track professors, many researchers in academia are usually focused on publications and dissemination of knowledge. Often times, publications are required to improve the standing of the professor in his/her department and to fulfill productivity requirements in their contracts. However, the creation of patented technologies benefits both the research university and the economy. While these are not requirements of an academic job, researchers strive to created patentable ideas which in some cases can lead to the creation of a spin-off company, and adds recognition to the university, while providing a boost to the researchers professional standing in his/her field.

• Federal and State Research Institutions

The us government developed the national laboratory system as a research and development network for the advancement of technology. Additionally, the Stevenson-Wydler Technology Innovation Act of 1980 made technology transfer from federally funded national laboratories a mission and priority, and created a variety of institutional structures to facilitate this mission [14]. As a result these institutions are principally focused on developing projects that have large economic benefits, while still trying to investigate and explain the fundamental science. Research publications are often important in the national laboratory setting, as they can mark progress in research, however, when a technology is novel or a new discovery is made, it is commonplace to apply for patents and make the technology available for licensing to outside partners.

Industry

Private companies are largely "results motivated" and follow commercial benchmarks that must be met in order to pacify the investors and move from a R&D stage to a manufacturing stage and revenue-making stage.

It is common for academia, government run laboratories and the private sector to work together. With greater collaborative efforts more ideas are brought to the table and often the availability of resources is pooled. When an industry partner chooses to provide funding or to collaborate with a university or national laboratory, it is often necessary for the company to comply with the policies in place at the research institution and come up with an agreement that satisfies the policies of the institution and the company alike and likewise, it is expected that the researcher will comply with his institutions policy, otherwise he could lose his job.

2.1 Cooperative Agreements and Collaborations

Cooperative agreements for research collaborations are formed in many ways in the US. For researchers at universities it is mostly through joint journal publications that credit is given for working together. Researchers involved from both or all laboratories receive credit as authors based on the amount and nature of the work they perform to create the results. It is unclear exactly which university or TTO handles the intellectual property when a patent is filed. However, the people contributing most to the conception of the idea, providing funding through grant applications, and performing the research have a share in the intellectual property rights and the subsequent returns when the technology is then licensed. It is likely that the researcher who initiated the collaboration and provided the ideas also created a contract agreement to handle any patentable IP if it is produced while working together. Below is a brief explanation of the standard agreements that are made between collaborating parties.

Material Transfer Agreements (MTAS)

A material transfer agreement is initiated when a transfer of physical resources (*i.e.* polymers, oxides etc.) is desired between two organizations. This is not strictly an academic agreement, but it is most commonly used in academic settings (non-disclosure agreement is more common for national laboratories). The agreement governs and defines the rights and privileges of the parties involved with respect to the usage of the materials and any derivatives. The MTAs are formed when the transfer of materials is required between two academic or research institutions, from academia to industry, and even when academia requests materials from industry.

Non-disclosure Agreements (NDAS)

Proprietary and confidential information is protected through non-disclosure agreements. An NDA is usually a policy of federal research institutions and industry to prevent any proprietary information about research goals, materials, or results from being discussed or presented in any form other than outlined in the agreement. These NDAs contain more protections than the MTA listed above but are often used in the case that proprietary materials are shared/transferred and incorporated into the research of the acquiring party.

Cooperative Research and Development Agreement (CRADAS)

In 1986, the Federal Technology Transfer Act allowed government-operated facilities to enter into cooperative R&D arrangements with industry as well as to grant outside collaborators the title to any invention that resulted [6]. In 1989, the National Competitiveness Technology Transfer Act of 1989 extended the 1986 legislation enabling the formation of cooperative research and development agreements (CRADAS) to government-owned contractor-operated facilities [14]. The intent of this legislation and the development of CRADAS was to provide legal structures to ensure the full use of the US Government's investment in research and development projects. Laboratories are encouraged to push for the transfer of federally owned and originated technology to state and local governments where appropriate, and to the private sector [6].

Under the CRADA, a collaborator with a national laboratory can choose the nature of their relationship to the project [16].

- Shared-Resources Agreement:

This is a joint research project between a national laboratory and a partner to develop, advance, or commercialize a national laboratory-developed technology without funds changing hands. It must fit within the scope of a project at the national lab, which is funded by the US Department of Energy.

- Funds-in Agreement:

This type of relationship allows for the partner to pay for all or some of national laboratories costs under the project. However, the national laboratory never provides funds to the partner. This is most commonly done for companies who seek assistance for a project they are currently working on which does not fall into the scope of a project at the national lab.

2.2 Alliances and Incubators

The formation of alliances and incubators is intended to develop networks of knowledgeable people in all aspect of the "energy business," to provide better access to business related resources, and to increase collaborative efforts in research so that the knowledge created can be disseminated for maximum economic benefit.

The Clean Energy Alliance

The National Renewable Energy Laboratory developed the Clean Energy Alliance with the mission of assisting clean energy entrepreneurs [17]. The alliance has developed into a network of investors, energy experts and industry leaders who are willing to provide assistance in the form of mentoring, financial support and introductions to the global energy community. By having a networking opportunity available for students, researchers, and entrepreneurs, the alliance enables easier navigation of the energy market, facilitates with the identification of opportunities, and provides important contacts for the necessary funding to develop and commercialize clean energy technologies. The Clean

Energy Alliance contains lists of research programs, equity firms, and development and commercialization centers, which are available to anyone with a CEA membership.

The Center for Revolutionary Solar Photoconversion (CRSP)

The Center for Revolutionary Solar Photoconversion is a part of the Colorado Renewable Energy Collaboratory, which provides unique partnership opportunities to businesses [18]. CRSP has six goals in its mission to bring energy technologies to the market. These goals include [19]:

- Affiliate Research Institutes

Establish a strong research collaboration between three Colorado universities and the National Renewable Energy Laboratory.

- Shared Research

Provide an interface for communication and participation between members of the collaboratory and the research institutes for any pre-competitive research.

- Sponsored Research

Provide a streamlined communication mechanism that facilitates the collaboration on member-specific proprietary projects.

- Basic Research

Develop an efficient network for performing basic research tasks under DOE funding.

- Training and Education

Provide educational opportunities and personal development to scientists and student to further develop knowledgeable researchers.

- Publish Results

Disseminate results of collaborative efforts created under the within the network of the CRSP.

CRSP has a scientific board that overseas the research projects that are performed as part of the collaboration. In addition, various scientific experts lead the research efforts to develop technologies with the greatest impact for global solar energy usage.

CEA and CRSP are just two examples of the types of networks in the US that provide assistance to those looking to network in the energy sector. Through these collaborations and alliances information is made available to a large number of institutions and businesses, further reducing the barriers to technology transfer.

2.3 Consulting and R&D support

When the research of a company does not align with the research of an academic group or federal laboratory, a consulting relationship can provide the necessary resources to the company. This type of relationship often results in a private company retaining the rights to the intellectual property, including any significant findings or breakthroughs.

Academia

Consulting and R&D support are common practice among academic researchers and their research groups. The consulting can be done on an individual or private basis with a single researcher providing help to a company, or an agreement can be formed with an entire research group to provide support for a commercial research project. In both cases it is normal university policy to require a contract commercial company for legal purposes, and if a researcher bypasses the contract and does not tell the university of his intentions, it is possible that he could lose his job if the university were to discover his outside work. However, most universities provide their employees with the freedom to consult for a specified amount of time as long as it the contract does not indicate a conflict of interest or prevent the researcher from performing the requirements of his/ her job.

Why do universities allow this? Researchers are the intellectual assets of the university. Retaining them is in the best interest of the university, and allowing academic researchers to consult and provide support to private companies not only lessens the possibility that a researcher will be recruited to work full-time for a company (although this does happen). Through consulting, a researcher can build a strong working relationship between academia and industry and facilitate the transfer of technology. MIT has formed an Industrial Liason Program (ILP), which acts to connect industry partners to research groups who can provide support to their research efforts [20]. By doing this they open communication pathways in industry, which may be helpful in the future when a researcher wants to commercialize a new technology.

National Laboratories

While national laboratories do not allow their employees to privately consult for any company whose mission is in line with that of the national laboratory (in the main case of this paper any type of renewable energy research), the national laboratories engage in Work-for-Others agreements (WFOS), which allow the national laboratory to take on a consulting or R&D support role. Various solar companies have used the support of NREL

and other laboratories for testing, troubleshooting, and certifying their innovations.

The Work-for-others agreement, like the CRADA, has variations in agreements based on the nature and extent of the work. Here is listed the types of agreements available from the National Renewable Energy Laboratory [16]:

- Interagency Agreement-Government (IAG)

A federal agency other than the US Department of Energy (DOE) provides funds to a DOE sponsored research laboratory to perform work directly. DOE and the other agency must enter into the agreement.

- Funds-in Agreement (FIA)

A nonfederal entity pays the national laboratory to conduct a research-oriented project. In this case, under certain circumstances, the agreement may allow for the non-federal project sponsor to obtain the title to inventions, which is different from the rights to the title when technologies are created through a CRADA.

- Technical Services Agreement (TSA)

A non-federal entity pays for the national laboratory to assist with an analytical problem. The national laboratory consults and provides basic technical assistance under this agreement.

- Analytical Services Agreement (ASA)

A non-federal sponsor pays for specialized, narrow analytical services performed by the lab in 13 different categories of testing or characterization services. This small-scale, "shrink-wrap" agreement has predetermined limitations on the duration and the cost.

3 Opportunities for Commercialization

The PV industry is full of motivated researchers intent of finding solutions. During this era of climate change awareness, "green" and "alternative" technologies have become more widely funded, researched, and accepted by consumers. The market is ready for energy solutions to avoid an energy crisis and curb global warming. As a result of this "green" technology acceptance, the market is seemingly booming with new companies and new missions for reducing our dependence on fossil fuels, jump-starting the economy, and of course making money. This chapter is focused on understanding when and how a researcher recognizes an opportunity for their discoveries, what resources they have to create a start-up or market their ideas, and what funding sources are in place to see that their ideas are given the opportunity to succeed.

3.1 Recognizing Opportunities

As mentioned in chapter one, researchers employed at universities and national laboratories have access to technology transfer offices that aim to provide them with the information they need to file for intellectual property protection. Since a researcher has many years of experience in his field it is easy for him to see the gaps in research or the lag in commercialized technology. It is these gaps and lags that motivate researchers to pursue the state-of-the-art research that eventually can lead to a technological breakthrough, or at least advancements in their field. Once the opportunity is recognized, the researcher then determines the best process for developing the technologies, what resources he must use, which professional contacts he must work with, and how to fulfill the gap or lag he has identified.

When he has done some initial research, it is possible that filling gap in research has provided nothing more than the knowledge that that particular pathway has been explored. But if a researcher has succeeded by finding a solution that is worthy of more than a scientific paper, he must then decide how to handle the intellectual property he has generated. If a patent has not been filed on a technology similar to his discovery, it is his responsibility to document his research and contact the TTO to lay claim to his discovery. Using the tools and resources provided by the TTO it is then up to the researcher and the TTO to jointly decide the next step; whether to allow the discovery to be licensed to an existing company or to form a startup around the new idea or ideas.

3.2 The Start-up

The staff of the TTOs often includes successful entrepreneurs, market analysts, technology transfer specialists, and intellectual property lawyers. This combination of expertise provides a pool of advice for determining the viability of a start-up or spin-off. Since not every patentable discovery has enough market strength to justify a start-up company, it is important to analyze the risk of failure involved with licensing a patent to a start-up. It must include a thorough analysis of the market need for the current technology and a projection of whether it will be accepted as a good solution to the problem it attempts to address, and whether there are any competitors.

While the patent is not devalued if the start-up company fails, the commercialization process is extended or slowed. However, if the company succeeds, the benefits to the university or research institute are often much greater than licensing to an existing company.

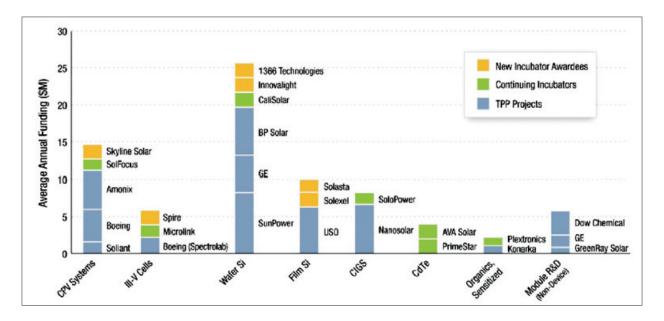


FIGURE 3.1. This is an illustration of the companies and amount of funding provided through the federal government during 2008 for the incubator projects and other on-going PV research projects [1].

In a start-up company it is common for the researcher becomes the chief technical officer to oversee the research efforts. Section 4.3 deals with the role of the researcher and compensation for his intellectual contributions.

3.3 Funding Sources

Funding for PV technology on the basic research and development level often comes from government grants for "green" technology or budgets also in place for furthering the research mission of a national laboratory. Sometimes, government laboratories and universities obtain funding form collaborations with industry partners and funding comes from the investors in the company rather than the government. Once a technology has become more advanced and shows market potential, private investors (such as angel investors, existing companies, or venture capital groups) become key to the success of the technology transfer from idea to commercialization.

• The Research Mission

Some universities and many national laboratories designate funds as "seed money" for innovative and promising research ideas. A seed fund provides a little financial backing to explore areas of research that otherwise would go untested and sometimes a clear research path is created. If a research group can show that further research could provide results influential to the field, it is possible that the research group

would obtain outside funding. Proof-of-concept is a strong promoter when applying for grants.

Industry funded partnerships are often the fastest mechanisms for transferring new technology discoveries. The company or industrial partner approaches a research institute with an idea but perhaps without the means to explore the idea. They provide the funding to explore and either the company can obtain exclusive licensing rights to any patented ideas or if negotiated the company may own the rights and is then free to use the information as they please.

• How is the Start-up Funded?

Start-ups in the US are funded during various phases by private, public or governmental funds. The government has the largest financial contribution during the early research and development stages of an idea. As mentioned previously, once the technology, whether it is a novel process, a new material or a combination, proves useful and unique this start-up seeks private funding sources such as venture capital investors. At this point they try to bridge the gap between a strictly R&D research company to a company with a plan for eventually manufacturing their products. However, all of this funding depends strictly on the company, it's founders and it's mission. Where the funding originates depends on how the company chooses to seek funds. It is possible that one company would not seek any public or governmental funds during any part of the start-up process, while another company could be funded almost exclusively by federal funds.

• Government Funding Strategies

Recently the US government has developed quite a few programs to push technology transfer especially in the PV fields. As an example the department of energy has created an incubator program, which provides funding for start-up photovoltaic companies. The program

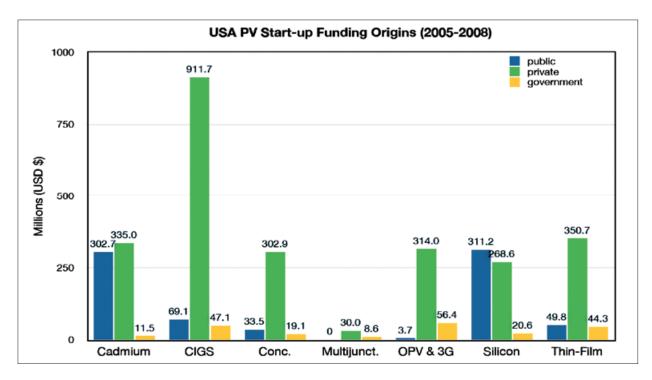


FIGURE 3.2. The public, private and governmental funds allotted to start-up companies in the US for various types of PV over the years 2005-2008.

also contains a *Pre-Incubator Project* focusing on moving ideas from concept verification to production of a commercially viable prototype. The PV Incubator project is aimed at accelerating prototype and precommercial technologies toward pilot and full-scale production [1]. Listed in Figure 3.1 is a graph of the companies funded and the amount of funding provided for the incubator projects as well as for on-going solar energy programs.

New incubator awardees are companies that demonstrate an idea that is aligned with the current industry trends, provide a strong business plan, and show strong initial performance. Companies that are listed as continuing incubators are those that have demonstrated the timely completion of scheduled deliverables, relevance to the current industry developments and likelihood of success [1]. The TPP projects are ongoing research projects that are demonstrated to be low-risk investments for the government while providing maximum market penetration of new technologies.

With the exception of Silicon technologies, which are funded largely by public funds, private investors have provided the greatest financial support for start-up PV companies in the US whereas the federal government has provided the least amount of funds, as shown in Figure 3.2. As is evident CIGS technology has the highest private investments of all types of technologies. New companies are emerging each year with the idea of

creating a cost competitive electricity generation using CIGS technology and efficient manufacturing processes [21]. While it is shown that the government does not provide the same capital as private or public entities, the US Government does create programs that attempt to provide start-up companies with extra funding to help them succeed.

4 Legal Aspects of Technology Transfer

Technology transfer involves a lot of legal aspects from intellectual property and licensing, to researcher compensation. This chapter discusses how the intellectual property is handled in academia, federal labs and industry (as well as during collaborative efforts), briefly explains the details of patent and licensing agreements, and outlines the roles of researchers.

4.1 Intellectual Property

The Owner(s) of University Funded IP

When a university researcher wants to protect his research results or ideas, the intellectual property protection is provided with help of the university technology transfer offices. They provide support and guidance for researchers, students and staff to apply for patents and other intellectual property protection methods (copyrights, trademarks, etc.). The university often assumes the rights to the intellectual property or invention created by any employee of the university, but compensation to the inventor is paid through a royalty agreement. As noted on many TTO websites,

research universities will pay for the patent application through university funds, but it is common for the fee to be reimbursed through royalty revenue if the technology is licensed.

Following the patent or IP protection step, two options are available for the use of the invention. At this point a license for use of the technology can be granted to an existing company, or the license may be granted to a start-up company if the invention is substantial enough to merit such an undertaking. As mentioned earlier, not more than 5-10% of inventions given to technology transfer offices are fit for creating a start-up company. Therefore, the majority of ideas are available to be licensed to existing companies. While this often provides a slightly lower return for the university investment the risk of failure is much lower and there is often less time to the commercialization of the technology.

• The Royalty Breakdown

Royalties are given as a percentage of the profit made by the company and these royalties are negotiated by the company and the university and signed into agreement when the licensing contract is formed. The royalties are then distributed to the university and the inventor according to the university policy and based on the profit of the company. Each university has its own policy for the percentage of the royalties given to the inventor, but large competitive research universities often offer the inventors a 25% share of the royalties. The benefits do not stop there, as some of the royalties are often paid to the research account of the inventor, the department for which the inventor works, and/or a university-wide research fund (as much as 50%). The TTO, which facilitated the patenting and licensing receives a portion (usually up to 25%). In final calculation, approximately 75% of the royalties received to the university are distributed again for research purposes, while the remaining 25% is used to cover the operating costs of the TTO.

National Laboratories and Intellectual Property Policies

Intellectual property at national laboratories is handled in a similar manner to that in academia. If a discovery is made that is worthy of patent protection, a patent application is filed. Since technology transfer is a large part of the mission of the national laboratories, they have set aside quite a bit of funding to cover the costs associated with patent applications. The TTO at the national laboratory then handles any licensing inquiries from industry. Once a company is ready to commit to a license the royalty agreement is created.

If a company is interested in working together with a research group at the national laboratory more

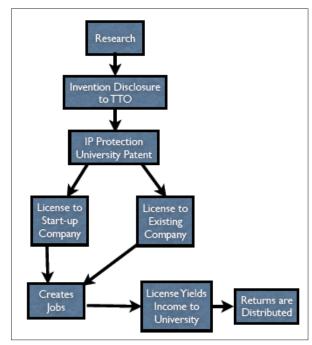


FIGURE 4.1. The flow of the intellectual property in universities.

care is taken in developing an agreement and protecting the intellectual property of both parties involved. Depending on the nature of the research, both parties start by listing any intellectual property that they own with regards to the project, prior to the start of any collaboration. Then a contract is developed stating the ownership of any subsequent intellectual property generated through the collaboration. In some cases, the intellectual property could belong solely to the national laboratory, solely to the company, or could be owned jointly. The details are often negotiated by the involved researchers and the company seeking to collaborate, and then are sent to the national laboratory TTO for approval.

Industry-based Intellectual Property

Inventors that create ideas on their own have much more responsibility with the legal and financial aspects than academic researchers or federal laboratory researchers who have an established TTO backing them. However, the rights to the intellectual property belong solely to the individual if he produces the idea with out funding. A researcher from a company may still receive a bonus for the good work he does at the company or research group, but when the financial support and resources are provided by that company, it is normal for the company to own the IP.

4.2 Patents and Licensing Agreements

In the US, successful technology transfer can often be attributed to the important role of technology transfer offices as commercialization liaisons. Technology transfer offices at universities and national laboratories provide the legal support and sometimes, the financial backing for patent applications and licensing agreements. When it comes to licensing an existing idea, the TTOs often provide lists of patents and technologies that have been developed within their institution. These are available for anyone to search and can be licensed under certain agreements between the institution and any interested company. The National Renewable Energy Laboratory, for example, maintains a database of intellectual property developed by all Department of Energy funded national laboratories. A database such as this makes it easier for the government to keep track of all the intellectual assets and maximize the benefits of these licenses and patents to advance technology and boost economic benefits.

4.3 Researchers Roles and Compensation

The researcher can take many roles in technology transfer and often it depends on which entity they are working for and where their funding comes from. A university professor or researcher often has the most freedom to decide what role he will hold within a start-up company or how their intellectual property is handled when a patent is involved. Whereas government employees who develop innovative ideas or demonstrate a unique process are often legally restricted to a particular role when it comes to technology transfer. Of course a private inventor has the most freedom available to do what he will with his ideas. However, without a TTO, raising capital and performing the market analysis is often more difficult to handle alone and may restrict the possibilities for the invention to make it to the market unless the individual has the means to do this on his own.

Technology Roles for Academic Researchers

At large research universities in the US, researchers are allowed to hold many roles when it comes to technology transfer. Most commonly a researcher creates the IP for a new technology and receives the royalties once the technology is licensed. When a market analysis is favorable toward forming a start-up around a technology or portfolio of technologies, TTOs provide resources and connections to those in the business world. At this point it is common for a researcher to seek out investors or form a company that is able to further the research and commercialize the technology.

During venture development in the PV sector it has been quite common for researchers to obtain approval for a leave of absence from their university or department, or to reduce their responsibilities at the university during the time when the company is getting started. They will have a title as a founder and may take on the role as a management partner in the venture or even as chief technical officer to advise the research and technical side of the operation.

• Compensation as a Founder

Many times the founders will create an agreement that dictates the roles of each founding member. But in the case of university-based intellectual property, any conflicts of interest (usually involving the issuance of equity) must be avoided by both parties, the inventor and the start-up (licensee) company. Often, the start-up issues founders' equity to the inventor in exchange for him serving on the management board, and this is issued as common stock. At the University of Alabama, as with many other universities, it is also possible that a founder could be issued equity in the form of stock, options, or warrants in exchange for exclusive rights to license the university-owned assets. [22] However, this is much less common. Although many founders' agreements are tailored to a specific company and situation, one details remains fairly consistent. The inventor is often not required to provide monetary compensation for any equity he obtains within the company. His intellectual property and management contributions are considered to have enough value to grant him rights to the equity without the requirement of purchasing them, however the percentage of equity he obtains varies from company to company and inventor to inventor.

After a leave of absence from his university job it is common for the researcher to return to his responsibilities at the university while continuing to consult for the spin-off company. He often continues to participate in an advisory capacity by serving on a management board or provide technical guidance to the researchers recruited to further the R&D stage. At the University of Colorado, the role the researcher has and the length of time spent working at the start-up usually depends on departmental policies and the needs of the company, but this can vary from university to university. And, according to the TTO policies of many universities, when the researcher returns to his position he is allowed to spend up to 1/6th of the year on work outside of his university obligation, as long as there is no conflict of interest

The number of technologies that are suitable for the creation of a start-up company is minimal. According

to various TTOs, estimates show that 5-10% of the ideas that are generated and patented at a university technology transfer office are suitable for the development of a start-up company, while even fewer succeed past the first few years. Therefore, the role of a university researcher is often just the generator of intellectual property and if possible then he can license the technology to an existing company.

Government Researchers Participation in Tech Transfer

National Laboratories in the Us offer some options for researchers to contribute to technology transfer. However, they do not provide the same freedoms as an academic setting. Federal policy often restricts employees from roles external to the laboratory where he is employed, but the policy does not prevent a researcher from contributing in other ways to the dissemination of research results and compensation as the inventor. The transfer of intellectual property is possible through any of the following agreements:

- Cooperative Research and Development Agreements (CRADA).
- Non-disclosure Agreements (NDA).
- Work-for-others (WFO).

These are further explained in section 2.1 and 2.3. When IP is created a researcher still has royalty rights to an invention licensed to an external company. It is also possible that the researcher would have a key role in advising a start-up company, if associates of the national laboratory create an investment venture. However, a researcher could not be an employee of the company while still working at the national facility.

5 Case studies: Mechanisms

5.1 Konarka: a University Spin-off

In 2001, a group of professors and scientists from the University of Massachusetts-Lowell teamed together to bring their on-going research in organic photovoltaics into a commercial setting. They began their research with support from the US military to develop a lightweight technology for soldiers and with this they produced an innovative manufacturing process for creating low-cost, and flexible, solar cells.

Through government funding and eventually the acquisition of financial support from venture capital firms, private companies and private investors, Konarka was able to successfully commercialize its ideas. Seven years after its conception, Konarka introduced Power Plastic to the commercial market [23]. In 2009, it opened

a pilot manufacturing plant and began producing panels suitable for use in microelectronics, and portable and remote power applications. Since the beginning, the company has increased from the core group of researchers to a company of over 80 employees. Konarka still works closely with US national laboratories and university research groups in the US and abroad to advance the technology further and continue to advance its commercial-scale manufacturing recipes.

5.2 First Solar: a Private Venture

In 1999, First Solar Inc. was formed when entrepreneur and inventor Harold McMaster decided to sell his solar research company, Solar Cells Inc., to an investment firm. As Solar Cells Inc. (SCI), the company worked largely on research and development efforts lead by McMaster's vision of affordable solar and efficient manufacturing [24]. Since becoming First Solar, the inventor-initiated company has set a great example for success in the solar industry. The company's main focus is to provide panels for commercial and utility scale projects, but it also provide panels for large residential projects as well. This is one of the most successful solar companies to emerge from the US in recent history and it continues developing cutting edge manufacturing processes and increasing the efficiencies of its cadmiumtelluride (CdTe) thin-film solar cells.

In 2004, First Solar began full commercial operation of its initial manufacturing line [25]. The First Solar's research and development department provides most of the research support for the company, but it has been known to work with national laboratories to further its research efforts. NREL's researchers provide years of experience solving critical issues for external companies and have worked closely on some accounts to help First Solar to solve problems, and to provide them with characterization and certified measurements of its devices.

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Appendix

Table of PV start-up companies and their origins (i.e. University or Private) and type of PV cell being developed

Company	Year Founded	Origination	Technology Researched	
1366 Technologies	2007	MIT	Multi-crystalline Si	
Abound Solar	2007	Colorado State University	CdTe Thin-films	
Alta Devices	2008	CalTech	Thin-films	
Bloo Solar	2008	University of California – Davis	Ultra-Thin-film (3 rd Generations Technologies)	
Covalent Solar	2008	MIT	Organic Solar concentrator	
Konarka	2001	University of Massachusetts – Lowell	OPV on roll-to-roll manufacturing	
PlexTronics	2002	Carnegie Mellon	OPV	
Solarmer	2006	UCLA	OPV	
Solasta	2006	Boston College	Mono-crystalline Si	
Soluxra*	2009?	University of Washington	OPV	
Suniva	2007	Georgia Institute of Technology	High Efficiency Silicon	
Ampulse	2007	Oak Ridge National Lab & NREL	Thin-film Si PV	
Blue Square Energy	2003	Private	High Performance Si	
CaliSolar	2006	Private	Crystalline Si	
Enfocus Engineering	2006	Private	Multijunction cells & concentrating solar	
First Solar	1999	Private	CdTe thin-films	
Heliovolt	2001	Private	Thin-film CIGS	
Innovalight	2002	Venture	Ink-jet printing Si-ink on Si wafer	
Inspired Solar*	?	Private	?	
Miasole	2003	Private	CIGS	
MicroLink Devices	2000	Venture	GaAs	
Nuvosun	2008	Private	CIGS	
PrimeStar Solar	2006	Venture with NREL technology	CdTe modules	
Semprius	2008	Private	III-V and Si	
Skyline Solar	2007	Venture	Concentrating solar on Si wafers	
Solar Junction	2007	Private	Multijunction concentrating	
Solaria	1999	Private	Crystalline Si Solar	
Solexel	2005	Private	Amorphous Si	
SolFocus	2005	Private	High-conc PV	
SoloPower	2006	Private	Flexible thin-film CIGS	
TetraSun*	?	Private	Crystalline Si Solar	
United Solar*	1999	Energy Conversion Devices spin-off	Flexible polymer-substrates, thin-film a-Si	

^{*} Information about these companies was limited or unclear

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