POSITION PAPER

Chemistry – Driving Innovation in Materials Science

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Electrospray ionization (ESI) now makes it possible to deposit individual macromolecules on any surface. Coatings < 10 nm made using this technique have no voids. A few macromolecules are able to penetrate quite deeply into the carbon fiber bundle, completely encasing the fibers without leaving voids. That is important for application of polymer adhesion promoters. During the deposition process, the polymer molecules remain intact and no decomposition takes place.
(© BaM Federal Institute for Materials Research and Testing)

1. Introduction and Goals

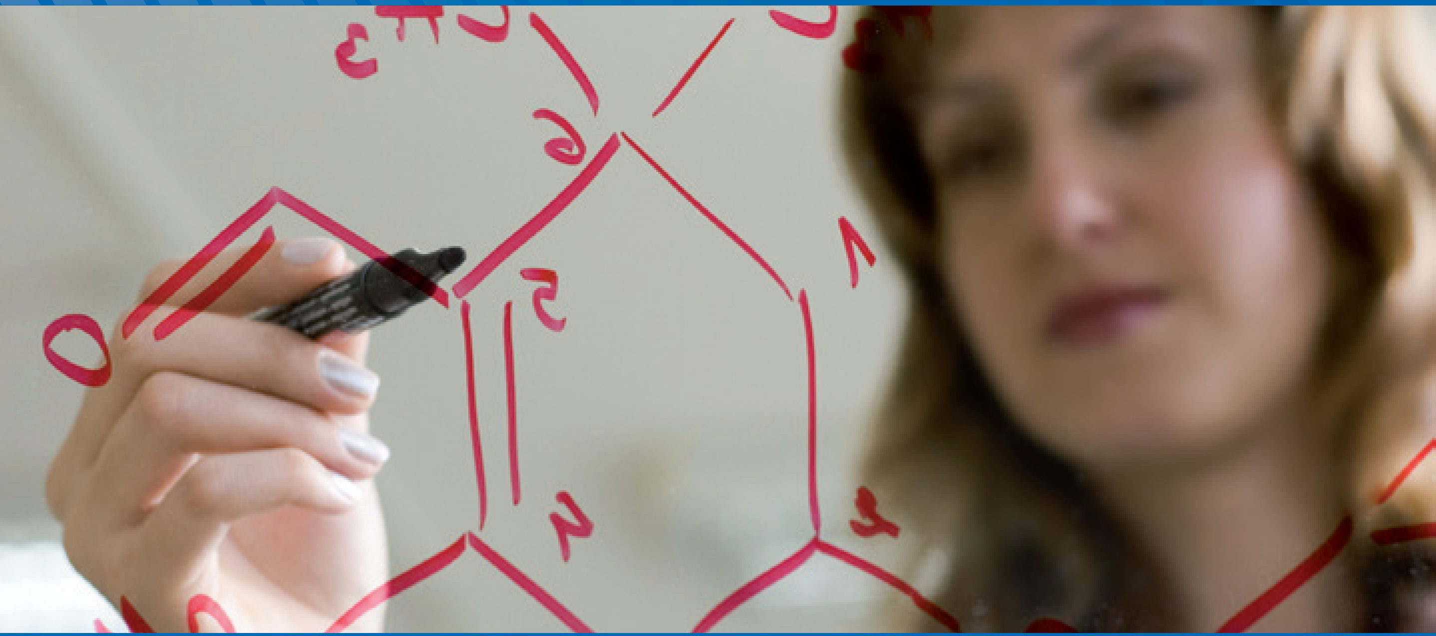
The development of new materials to address pressing future needs is one of the biggest challenges of the 21st Century. These new materials will play a key role in shaping the future. Among other things, they will have to provide pathways for sustainable resource management and energy supply, mobility, the future viability of the consumer society and new diagnostic and therapeutic procedures in the healthcare sector. A deeper understanding of materials and their chemical make-up, architecture, functionalization, processing and potential applications creates the foundation which the manufacturing and process industry in Germany and Europe needs to remain competitive. Strengthening of the industrial base is currently being discussed at the European level, and the success of this strategy depends on further intensification of Materials Science. Because Materials Science and engineering are so important for the future of our society, they have been given a prominent place in the German government‘s high-tech strategy. The 10-point program introduced by the Federal Ministry of Education and Research is one indication of the importance which is attached to this branch of science.

Materials Science is a dynamic undertaking, and interdisciplinary collaboration is needed to achieve successful outcomes. Depending on the particular research objective, chemists, physicists, material scientists along with biologists, health professionals and experts from other disciplines work together to develop solutions based on innovative materials for virtually all sectors of society. This position paper focuses on the role of chemistry in the development process. Chemistry makes a vital contribution to market establishment of innovative materials.

Chemistry is “the science of substances”, substance transformation and the relationship between material structure and material properties. It describes how individual substances interact and studies their stability and reactivity. To optimize material properties, researchers need an in-depth understanding of material structure and composition including how additives work, along with much more. That is why many new materials have their origins in chemistry labs. Experience in chemistry is also needed in order to understand how to optimize the functions and quality of materials production, processing and applications, and it makes an important contribution to materials science all along the value-added chain.

This position paper outlines the contribution made by chemistry to Materials Science in meeting a variety of needs. It summarizes the development potential and research needs over the next ten years.

Specific funding programs which energize chemical and Materials Science carried out in collaborative networks involving all of the related disciplines can lead to the rapid development of solutions for the challenges which will have to be addressed as a matter of urgency in the future to meet the various needs. The programs must encompass both basic and application-oriented research, and it is particularly important to build a bridge between these two research domains in Germany. This is essential to ensure that Germany is well positioned as a hub of high-technology expertise to meet future challenges in the field of Materials Science and to safeguard the competitiveness of its industrial and manufacturing sector.



2. The Role of Chemistry in Materials Science

Chemistry is playing an increasingly important role as an innovation driver in Materials Science. As a branch of science which strives to encompass and understand the entire world of materials, chemistry is always a major port of call in the search for new materials.

The ability to understand and control elements, compounds and architectures at the atomic and molecular level produces a basic understanding of material properties. This expertise is absolutely essential in the search for materials which must meet specific requirements profiles.

Because chemists have expertise in material conversion, understand how various substances and materials interact during production and actual use and can identify the best recycling strategies for end-of-life, they play a vital role in the search for totally new pathways and solutions.

Also, chemists are often asked to help assess compliance with regulatory requirements on Materials Science projects. They make an important contribution along the entire length of the Materials Science value-added chain, and in collaboration with researchers from other disciplines they help achieve innovative breakthroughs in materials science.

Economic prosperity in Germany is increasingly dependent on advanced, sophisticated products with high value-added. Production of basic materials is coming under increasing cost pressure. The development of high-performance materials and materials with innovative properties is becoming an increasingly significant factor in Germany's ability to compete in world markets. To a greater extent than ever before, chemists are working on material solutions in technologies along the entire length of the value-added chain in many different fields of application. Modern technologies are also becoming increasingly complex. Many of the challenges can only be overcome through interdisciplinary teamwork. Chemists in particular have the expertise and networks which are needed to develop effective solutions in collaboration with neighboring disciplines. They fully understand the capabilities and limitations of chemistry.

Chemical engineering curriculums must provide a broad, in-depth insight into a large spectrum of materials, so that students acquire the skills they need to build bridges to a wide range of disciplines, for example to provide pathways between inorganic chemistry and medicine and between polymer chemistry and metallurgy. Chemistry is playing an increasingly significant role in Materials Science, and it is important that a basic introduction to materials science is included in the chemical engineering curriculum. By the same token, chemistry must be given greater emphasis in the Materials Science and other engineering curriculums. Communication between the disciplines involved in Materials Science needs to be intensified.

Funding for chemistry research and education must be available if Germany is to retain its scientific and industrial leadership in Materials Science.

The following action needs to be taken:

1. Chemistry drives the development of innovative materials. It is more than just a “supplier” of new materials. Through knowledge-based functionalization, chemistry creates new pathways to tomorrow’s technologies. Increased R&D in collaboration with neighboring disciplines is needed to fulfill that role.

2. A broad-based basic education in chemistry with emphasis on Materials Science must be retained in the future to strengthen the position of chemists as materials experts.

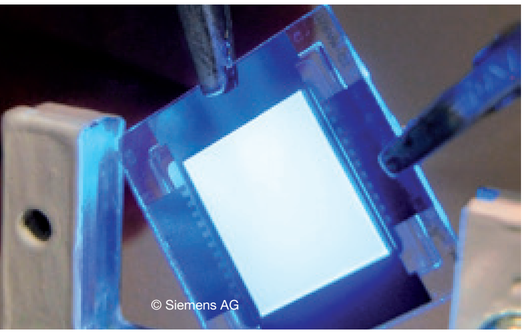
3. Collaboration with all of the organizations which are actively involved along the entire length of the value-added chain from basic research to process engineering and production must be intensified.

3. Innovation Potential of Chemical Materials Science – Examples

There is a definite relationship between new materials and the development of products which are based on new technologies. Developments in metal alloys and nanostructuring, for example, played a role in the discovery of materials with special magnetic properties that make it possible to produce hard disks with terabyte storage capacities.

However the importance of enhanced functional materials goes beyond the world of ICT. In order to provide tomorrow's solutions, new materials will be needed in other areas which have been identified in the German government's high-tech strategy.

In the chemical industry, catalysts increase the efficiency and sustainability of plastics and fertilizer production. The list of typical chemical products also includes paints, dyes, lacquers, pharmaceuticals and cleaning agents. However beyond that, chemistry plays an enormously important role in materials science, even if that fact is not always readily apparent. The following sections contain some examples of technologies where chemistry makes a particularly valuable contribution.



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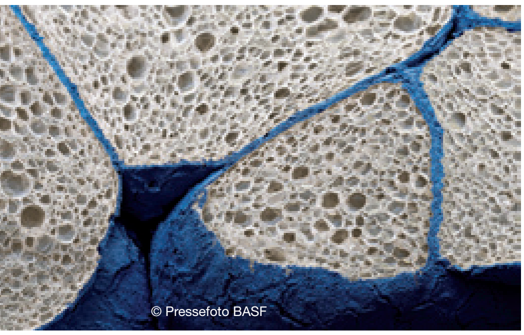
Functional materials for the electronics and energy industries

High-performance materials are needed in electronics (e.g. organic LEDs) and the power industry (fuel cells, photovoltaics, batteries, electricity storage). The purity standards for these materials are extremely demanding. Chemists are heavily involved in the development of polymers for OLEDs used in new display applications, electrolyte materials for mobile and stationary electricity storage and membrane systems for fuel cells.



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Lightweight materials

The development of lightweight materials is one of the top priorities in chemical materials research. A sustainable society which acts responsibly to ensure energy and resource efficiency has a vital need for lighter materials which are both rigid and strong. Expertise from the aerospace industry is already being applied in the automotive sector. The urgent need for low-cost, high-performance lightweight materials which can be produced in large volumes goes beyond the mobility sector. New solutions are also vitally important for other branches of industry such as power generation (wind turbines, etc.), civil engineering and housing construction. The chemical industry is continually developing high-tech materials such as carbon fiber, special foam products and coatings which protect lightweight materials against the effects of weathering for many years. The chemical industry also helps create adhesives. The new generation of composites could not be produced without adhesives and special resin hardener systems. These adhesives must be tailored to the specific application and they have to remain stable at a range of different temperatures under exposure to UV radiation. Intensive research will also be needed to develop new types of plastics and polymer-based composites. To make the use of the adhesives more cost-effectivly, they also need to dry faster under milder conditions. This will result in lower energy consumption and higher productivity.

Corrosion protection

Chemical solutions are also needed which provide corrosion protection to prevent material degradation and the associated costs. Total damage caused by corrosion is equivalent to 3% - 4% of Gross Domestic Product (GDP).

The problem is not limited to the conventional power industry, e.g. corrosion on high-temperature boilers and turbines. Equipment in the renewable power sector is also susceptible to corrosion. Offshore wind turbines are exposed to very high stress. Rotor damage caused by wind and weather can reduce the energy yield by more than 20%. Innovative corrosion protection solutions are also vitally needed for other applications such as geothermal and solar power, fuel cells, the maritime industry, internal combustion engines and much more.

As the requirements for technical systems become more demanding and operating conditions continue to evolve, there is a need to drive the development of coating materials. Additional research effort will have to be invested in chemical nanotechnology and the development of eco-friendly corrosion inhibitors and self-healing materials which provide corrosion protection. Even more importantly, in-depth studies using high-resolution analysis techniques (especially in the field of electrochemistry) will be needed to attain a better understanding of the corrosion process.

Re-use and substitute materials

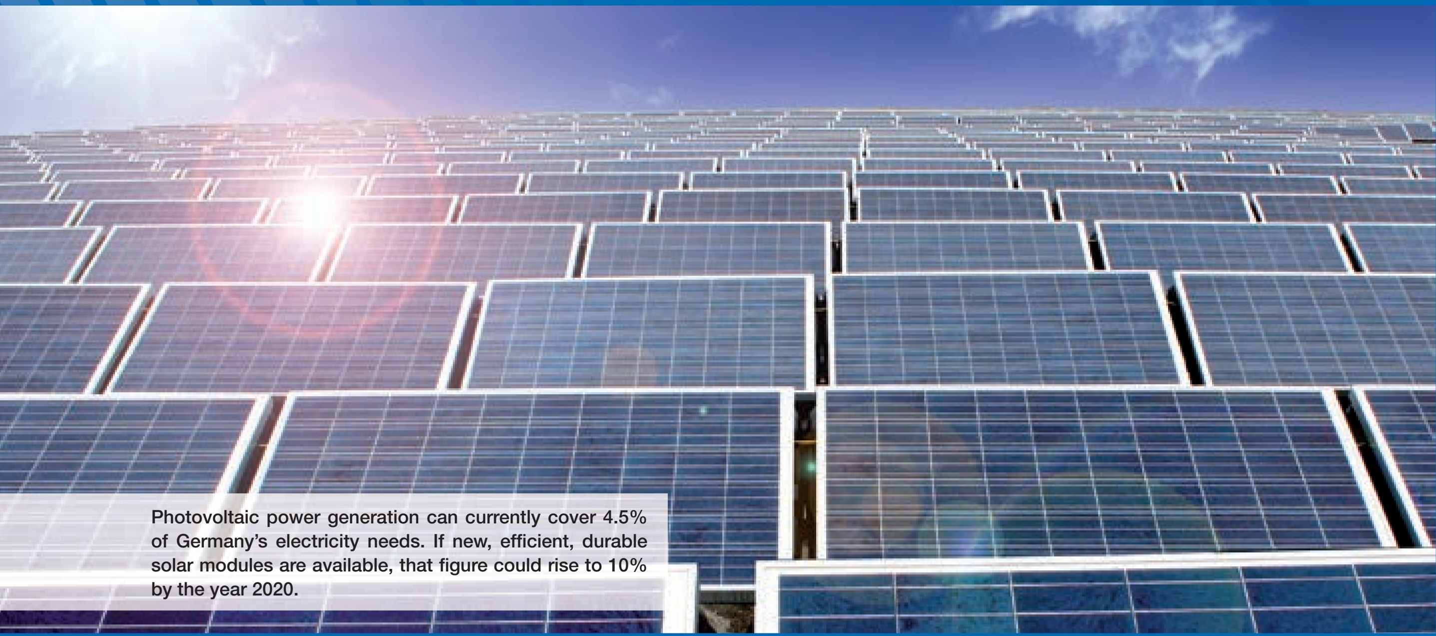
The role of chemistry goes beyond the synthesis of new materials, materials development and optimization for specific applications. It also makes a major contribution to material re-use (e.g. recycling) and the substitution of critical materials.

To produce materials and create infrastructure which are sustainable over the long term in a high-tech country like Germany, end-of-use and end-of-life are factors which must be taken into consideration right from the initial development phase. Chemists address these issues in the early stages of materials development and select the best materials for efficient recycling.

They also work hard to find substitutes for critical raw materials. If none can be found, chemical nanotechnology and other methods can be used to reduce materials consumption. All of this helps avoid materials shortages in Germany.

With an understanding of chemistry, it is possible to substitute capacitors containing rare earth elements with capacitors which are made without rare earth elements, making it possible to produce even smaller super capacitors for the ICT industry.

The challenge in the future will be to step-up development of substitute materials and develop more cost-efficient recycling methods using chemical treatment at end-of-life to recover high-value materials.



Photovoltaic power generation can currently cover 4.5% of Germany's electricity needs. If new, efficient, durable solar modules are available, that figure could rise to 10% by the year 2020.

4.1. Materials for Power Generation

4.1.1. Solar Energy Generation

4.1.1.1. Current state of technology

The installed photovoltaic base in Germany currently has a capacity in excess of 31 gigawatts. Due to inherent losses and the changeable weather in Germany, actual electricity generation nationwide seldom exceeds 70% of nominal capacity. The growth rate has been relatively high in recent years, and this is due in large part to subsidies granted under the terms of the Renewable Energy Act (eeG). More than 90% of solar modules currently installed are made of crystalline silicon wafers. The rest are thin-film solar cells which are expected to capture a 20% market share by 2020.

Organic solar cells (OSC) are relatively new to the market. Increased use of organic solar modules is necessary in some applications. Because these modules are cheaper, the expectation is that the costs and embodied energy will be recovered more quickly. Also architects have greater freedom of design, making it possible to place modules on parts of the building exterior which have not been used up to this point. Small, flexible modules have been on the market since 2009, e.g. in solar cell bags which can be used to recharge cellphones.

Solar energy is already making a substantial contribution in the effort to combat climate change, conserve natural resources and navigate the energy transition. Electricity generation in Germany from solar power was estimated to be in the region of 28,000 GWh in 2012, which is equivalent to roughly 4.5% of national electricity consumption . Based on the availability of new, efficient, durable solar modules, that figure could easily rise to 10% by 2020 and 25% - 30% by 2050.

4.1.1.2. Relevance

From what we know today, energy demand worldwide is expected to double by 2050 and a considerable proportion of that energy will have to be generated from renewable resources. Following the decision by the German government last year to phase out nuclear power by 2020, that scenario will have to become a reality even earlier in Germany. The potential wind, hydroelectric, biomass and geothermal generation capacity will not be sufficient to meet the challenge. In contrast, the amount of solar radiation reaching the earth's surface exceeds global energy needs by several orders of magnitude. The goal of solar cell development must be to provide affordable, efficient, durable technologies which utilize the sun as an energy source.

In the future, organic solar cells in particular are expected to increase in both size and performance. As efficiencies and service life continue to increase, the goal is to expand into new markets in the near future. Photovoltaic systems which are integrated into buildings are one example. Off-grid generation with organic solar cells is another target market for the medium-term. The market for printable or potentially printable photovoltaics is expected to rise from 260 million euros (2011) to roughly 5.7 billion euros by 2021.[1]

4.1.1.3. Technological/scientific challenges

Chemistry is a major factor in the market dominance of **silicon wafer based photovoltaic** technology. The footprint of chemistry is evident in the production of pure silicon as well as in the high-purity dopants, cutting lubricants and coolants and the chemical baths which repair sawing damage and produce the desired surface structure. Wafer thickness and hence the amount of expensive silicon needed per surface area is a major cost factor. Over the past ten years, the thickness has been reduced by roughly half to 180 µm, and the expectation is that the wafers will become even thinner over the next few years. Module efficiency has increased to 15 – 20%, and the goal now is to move significantly beyond the 20% threshold.

Thin film solar cells are produced by depositing suitable semiconductor materials on large substrates (glass or heat-resistant polymer film). The systems produced so far are made of amorphous silicon (Si:H, current module efficiency: 5% – 8%), CdTe (9% – 10% efficiency) or $Cu(In, Ga)Se_2$ (10% –12% efficiency). All three systems have a crucial advantage. Only a very thin coating (around 1 – 2 µm) is applied to the substrate, resulting in a cost advantage compared to silicon wafer based systems because substantially less active material is consumed. The cost advantage is only of consequence, however, if the associated efficiency loss is acceptable.

Organic photovoltaic technology is a very promising alternative to silicon-based solar modules. There are three basic types of systems: a) organic or polymer heterojunctions; b) dye-sensitized cells (Grätzel cells); c) hybrid organic-inorganic systems. 10% efficiency has been reached in the lab with systems in the first category. In order to be cost competitive with existing systems, module efficiency must be greater than 10% which is equivalent to a cell efficiency of roughly 13% – 15% in the lab. Cell efficiency is expected to increase to 12%[2] by 2015. Service life is a problem. A lifespan of several years is currently the maximum depending on cell type, but 10 years is the goal for real-world applications. The systems can be made using low-cost production techniques, e.g. printing or vacuum coating, which is a big advantage. Costs are expected to fall by a factor of two to three from current levels. The technology could be used to make completely different types of solar modules which are very light-weight. They are colorful and flexible and create a whole new range of possibilities in architecture and design. Three factors determine the long-term stability of organic photovoltaic systems, namely the intrinsic stability of the molecules in the active layer, the stability of cell nanomorphology and the stability of the contact between the organic elements and the conductive layer (indium tin oxide, ITO or metal). Also, the encapsulation must remain intact over the long term. If no adequate solution for this problem is found (e.g. if glass is used), the advantage of overall system flexibility would be lost. 11% efficiency has been achieved in the lab with dye-sensitized solar cells. The aggressive electrolyte system and the associated need for corrosion resistance is a major problem with this system.

1 Organic and Printed Electronics, 4th Edition, 2011, OE-A Organic Electronics Association, VDMA, Frankfurt

2 Die organische Photovoltaik holt auf, vdi-nachrichten, 2.12.2011

4.1.1.4. Possible approaches and improvement potential

In silicon wafer based photovoltaics, opportunities exist to further improve not only semiconductor materials production but also integration into the modules. Encapsulation using polymer materials in an aluminum frame with a layer of glass to provide protection currently accounts for roughly 30% of the cost of a module, and the amount of energy used is not insignificant.

In the thin-film solar cell sector, knowledge transfer from other industries (e.g. flat screens) is expected to lead to substantial advances in high-volume production technology. The price per module will come down because the relative unit costs of the production technologies will be lower. Simplification of module assembly and the possibility of using polymer substrates to produce flexible, low-weight modules are additional advantages that come into play.

In organic photovoltaics (organic/inorganic hybrid structures), efforts are being made to combine the favorable and easily manipulated light absorption properties of the organic layers with low-loss charge transport in the inorganic materials. Researchers are working on new morphologies for the inorganic components, e.g. enlargement of the layer surface area, creation of light scattering effects and increased absorption capacity of the dye molecules.

4.1.1.5. Need for further research

Silicon wafer modules

- Lower-cost production techniques for ultra-pure crystalline silicon
- Enhanced, less expensive production techniques for thinner wafers with improved surface texture
- New contacting techniques (from the rear side) including the use of conductive adhesives
- Cheaper encapsulation technologies using more resilient materials with improved optical properties
- New lead-free solder
- Reduction in/replacement of conductive silver paint

Thin-film solar cells

- New semiconductor materials with higher energy efficiency made using available raw materials (avoiding the use of indium)
- Better/less expensive production technologies, particularly those which do not require the use of vacuum: roll-to-roll, nanoparticle printing, electrodeposition and monograin layers (MGL)
- Cheaper transparent electrode materials with better electrical and optical properties
- Polymers and composites for permanent encapsulation of the active layer for the entire lifespan of the module
- Materials with different band gaps so that a large portion of the solar spectrum can be utilized (tandem and triple cells); designs which combine materials in the modules to meet the application needs
- Research on new ways of using the red and infra-red portion of the spectrum (two-photon up-conversion) or the short-wave portion of the spectrum (down-conversion to generate two low-energy photons). The use of nanomaterials and fluorescent dyes is being considered for both concepts.

Organic Photovoltaics

- Research into organic and organometallic materials with specially modified properties such as solution-processable low-bandgap and n-type semiconductors
- Development of materials with higher charge carrier mobility
- Refined morphologies produced by nanostructuring
- Increased service life based on thin-film encapsulation technologies with improved barrier protection to keep out oxygen and water, and process development for industrial-scale production
- Energy efficiency > 20% - 25% without appreciable heat loss based on multi-stage utilization of sunlight; development of multi-layer cells connected in series or conversion of excitation energies using 2-photon processes
- Research on alternative electrolytes for dye-sensitized cells
- Use of mechanically flexible substrate materials such as foils or semi-finished textiles

4.1.2. Fuel cell technology

4.1.2.1. Current state of technology

Many different types of fuel cells already exist. The lines of development are based on various materials combinations which work at different operating temperatures. Fuel cells can supply power to electric motors or provide a mobile source of electricity or a stationary source of electricity and heat. If they were available at competitive costs, fuel cells in combination with CHP technology could already be making a major contribution to enhanced energy efficiency without the need for new infrastructure. The list of fuels includes hydrogen for automotive propulsion systems, methanol and other liquids for low-power applications as well as natural gas and biogas for stationary applications. Hydrogen can be produced on an industrial scale from fossil-based resources. In many cases, low-power fuel cell systems can provide a distributed source of power at least as a transition solution until electricity from renewable energy sources is available for electrolytic production of hydrogen.

4.1.2.2. Relevance

Efficient energy conversion can help conserve fossil energy resources and protect the climate. Fuel cell systems are efficient right down into the low-power range. Because fuel cells have a lot of advantages (high electrical efficiency, low emissions, modular design, broad power and applications range and very well suited for CHP generation), a lot of effort is being invested in development of the technology around the world.

4.1.2.3. Technological/scientific challenges

The goal has to be to develop affordable fuel cell systems with a long lifespan as building blocks in a future energy supply architecture. That will require high current densities (up to several amperes per cm^2), safe segregation of the fuel gas and the load and (analogous to existing technologies) a long lifespan coupled with a substantial reduction in materials costs. These ambitious goals are only achievable in conjunction with the development of new materials. The membranes and optimized production of the membrane-electrode units are the biggest challenges.

Perfluorinated membranes for **membrane fuel cells** have high chemical stability, but they are still too expensive. They are conductive up to 80 - 100 °C and require careful water management. **Molten carbonate fuel cells** operate at 650 °C and use a molten salt electrolyte. Corrosion and solubility of the cathode material in the electrolytes are material issues that need to be addressed. Yttrium-doped zirconium oxide is a good conductor of oxygen ions for **solid oxide fuel cells**, but it can only be used at 900 - 1000 °C and that poses a difficult challenge for other materials mainly because in electrolyte-supported cells a relatively thick electrolyte layer is needed to ensure adequate mechanical stability. One way of reducing electrolyte thickness and thus the operating temperature (down to 650 - 700 °C) is to use anode or interconnect supported cells. Lower long-term system stability compared to electrolyte-supported cells is a disadvantage of this approach.

4.1.2.4. Possible approaches and improvement potential

Enhancement of existing materials and the development of new materials will be required for membrane, molten carbonate and solid oxide fuel cells. New electrolytes, inorganic-organic hybrid membranes and intrinsically conductive polymers play an important role in **membrane fuel cell** technology, and further optimization will be needed to increase their stability and reduce cost. Modification of new materials can reduce the corrosion rate in **molten carbonate fuel cells**. The search is on for new **SOFC** electrolytes which have sufficient ion conductivity at low temperature and also have good processability.

4.1.2.5. Need for further research

Membrane fuel cells

- Development of electrolytes and membranes with better conductivity and longer lifespan and which have working temperatures > 100 °C
- Development of inorganic-organic hybrid membranes and efficient manufacturing technologies for these membranes
- Development of corrosion-resistant catalyst carriers to replace conventional carbon black
- Increase in the catalytic activity of the cathode catalyst for oxygen reduction of stable and/or platinum-free catalysts
- Development of CO-tolerant catalysts
- Development of membranes with reduced methanol permeability and high conductivity for direct methanol fuel cells
- Increase in the conductivity and long-term stability of anion exchange membranes for alkaline polymer membrane fuel cells
- Further development of functionalized silicon organic membranes
- Development of intrinsically conductive, stable polymers for high, water-free (proton) conductivity
- Development of fiber or textile reinforced membrane systems, in particular for mobile applications

Molten carbonate fuel cells

- Modification of existing materials to reduce the corrosion rate
- Optimization of materials properties in long-term trials

Solid oxide fuel cells

- Development of new electrolytes with sufficient ion conductivity at low temperatures (e.g. cerium, gadolinium or scandium)
- Good system processability with suitable thermal expansion coefficients, low electrical conductivity and sufficient availability
- Increased oxidation stability and coking resistance of the nickel cermet anode for operation with natural gas or biogas
- Joint and sealing compounds with customized thermal expansion

4.1.3. Thermoelectric materials

4.1.3.1. Current state of technology

Thermoelectric power generation is currently only used to a limited extent, but the technology has been used in the aerospace and ICT industries for decades. Field tests got underway some time ago in the US to generate electricity from the heat given off by diesel engines to power on-board electrical equipment in vehicles.

4.1.3.2. Relevance

Around two-thirds of the energy contained in the fossil fuels which are currently used is lost as waste heat during combustion. Motor vehicles are the best example. As attention remains focused on CO_2, there is increasing interest in using thermoelectric technology to utilize the waste heat. The thermoelectric materials will have to become much more efficient to make commercial applications viable.

4.1.3.3. Technological/scientific challenges

The efficiency of the materials currently in use is significantly less than 10%. The main challenge here is to develop new innovative materials which are more efficient.

The lack of standardized thermoelectric converters (aka modules) which work at higher temperatures is an obstacle to widespread use. The availability of medium temperature modules which typically operate at around 500 °C is essential to convert vehicle waste heat into electrical power for on-board electronics on a broad scale. Significant effort is being invested worldwide in the development of suitable materials which are significantly more efficient than the best materials which are available today. Success so far has primarily been achieved in the academic sector.

4.1.3.4. Possible approaches and improvement potential

The goal has to be either to reduce the heat conductivity of known materials without decreasing their electrical conductivity or to synthesize new materials and optimize their thermoelectric properties. The objective is to increase the thermoelectric grade of merit (ZT factor), which is calculated based on the specific material properties and the temperature, from the current value of one to values greater than two. This could lead to widespread thermoelectric generation of electricity from waste and solar heat. Progress is expected particularly through the use of new thermoelectric nanocomposites.

4.1.3.5. Need for further research

- Standardized materials (nanocomposites) for use at temperatures up to 500 °C
- Development of hybrid materials which can be used to produce thermoelectric materials on an industrial scale
- Material combinations which make maximum use of large temperature gradients
- Electrical contacts for high-temperature materials, e.g. oxides and silicides
- Structural and interconnect technologies with long-term stability at high temperatures
- Materials which are resistant to temperature changes between room temperature and high temperatures
- Development of materials which work effectively at very low temperature gradients

4.1.4. Further development of power station technology

4.1.4.1. Current state of technology

Coal-fired steam power stations and gas or oil fired combined cycle gas turbine power stations with an installed capacity of around 3000 GW generate about 70 % of the world's electricity. Coal-fired power stations are currently responsible for around 30% of total CO_2 emissions in Germany. In contrast to an average 30 % efficiency worldwide, the figures for state-of-the-art power stations are as follows: anthracite steam power stations – 46 %, lignite steam power stations – 44 % and combined cycle gas turbine power stations > 60 %. Specific CO_2 emissions below 800 g CO_2/kWh for coal and below 350 g CO_2/kWh for gas are achievable.

4.1.4.2. Relevance

Coal-fired power stations will continue to make a major contribution to electricity generation for a long time to come. As a result, the ongoing development of power generation technology should be aimed at increasing efficiency to reduce CO_2 emissions. Underground CSS (Carbon Capture and Storage) provides one way of doing that. The technology has been under discussion for a long time, but it has generated considerable controversy in Germany. Passage of the Carbon Dioxide Storage Act (KSpG) in June 2012 created the legal basis in Germany for the first model CSS projects.

4.1.4.3. Technological/scientific challenges

To increase efficiency, power stations use the same basic process but operate at higher steam pressures and temperatures. New materials are needed to manage these higher states. Temperatures of 700 °C or more are currently envisaged.

To control CO_2 emissions, the big challenge is to develop high-availability processes which are cost-efficient on the scale typically found at power stations and which minimize energy losses in the overall process. Current research is focused on demonstration of suitable coal gasification techniques, development of oxygen combustion and development and trials of large hydrogen turbines. There is also a need to develop new scrubbing liquids for CO_2 removal and reduce energy consumption during regeneration of the scrubbing liquids. Major efforts are also underway to develop CO_2 capture technology which can be used to retrofit existing power stations (post-combustion).

4.1.4.4. Possible approaches and improvement potential

Development work and trials are currently in progress on new materials which are needed to increase power station efficiency. Efficiency improvements of up to 4 percentage points should be achievable.

Four different approaches to CO_2 removal are being investigated. Pre-combustion technology is based on the IGCC (Integrated Gasification Combined Cycle) process in which coal is initially converted to syngas in a gasification step. Steam is added during a subsequent conversion step, producing a fuel gas which consists mainly of CO_2 and hydrogen. The CO_2 is removed in a syngas scrubber prior to the main power station process. The energy contained in the hydrogen is used to generate electricity in a combined cycle gas turbine process.

The second route is the oxyfuel process. Nitrogen is removed in a preliminary air separation step, leaving only oxygen which is used for the combustion process. 70 % of the flue gas exiting from the steam generator is carbon dioxide. The rest consists mainly of steam which can be condensed out by cooling the flue gas. In the third process route, CO_2 is removed from the flue gas generated by a conventional power station process (post-combustion). Various flue gas scrubbing techniques are currently being considered. The fourth process is chemical looping. Metal oxides or limestone (carbonate looping) are used, producing a relatively pure stream of CO_2. Chemical looping is still at a relatively early stage compared to the other techniques discussed above, and it is of limited use for solid fuel.

All of the pathways to the CO_2-free power station have one thing in common. A power plant efficiency loss of between 5 and 14 percentage points has to be included in the equation. The loss is highest in the post-combustion process. As development work continues on the process technology and membrane materials, it can be expected that depending on the process, energy efficiency could be improved by between 1 % (pre-combustion process) and 2 % (post-combustion and oxyfuel process).

4.1.4.5. Need for further research

- Development and qualification of high-temperature (fiber-reinforced) materials (composites) and components made for example from nickel alloys, and coating systems to reduce oxidation and corrosion at steam power stations which operate at temperatures of 700 °C and above
- Further improvements in cooling for gas turbine components which come into contact with hot gas, and utilization of steam as a coolant in systems with high turbine inlet temperatures
- Increase the efficiency of stationary gas turbines using CMC materials (flame tubes, combustors, moving and stationary blades) which withstand higher operating temperatures than the metal-ceramic composites which are currently availably.
- Optimization of expansion and compression efficiency of the turbomachinery
- In general, a reduction in efficiency losses caused by CO_2 capture from today's level of 9 % - 13 % to 6 % - 11% in the future
  - Post-combustion process
    - R&D on chemically stable scrubbing solutions used to capture CO_2 from flue gas, minimize energy consumption for solvent regeneration
  - Oxyfuel process
    - Improvement of existing oxygen transport membranes
  - Post-combustion process
    - Reactor designs to optimize the water-gas shift reaction
  - Chemical looping
    - Enhancement of suitable oxygen carrier materials
    - Synthesis of stable calcium carbonate modifications
- Optimize system integration to improve efficiency, availability, cost-effectiveness and CO_2 capture capability
- Large demonstration plants for 700 °C steam power stations, lignite pre-drying and CO_2 capture process routes

4.1.5. Thermal barrier coatings

4.1.5.1. Current state of technology

According to the Carnot relationship, the efficiency of heat engines used for transportation and power generation, e.g. turbines, increases as the combustion temperature increases. Lower fuel consumption reduces CO_x and NO_x emissions. The maximum combustion temperature of a process is determined by the stability of the reactor and motor materials. For turbines, nickel-based super alloys protected by thermal barrier coatings (TBCs) made of stabilized zirconium oxide are currently state-of-the-art. Environmental barrier coatings (EBCs) are similar to TBCs except that their primary purpose is to protect against a potentially aggressive gas atmosphere rather than provide thermal stability.

4.1.5.2. Relevance

The exceptional mechanical stability of new thermal barrier coatings at high temperatures along with low density and high oxidation stability make it possible to increase combustion temperatures by around 150 - 200 °C, dramatically increasing energy efficiency and financial return, especially if the turbines no longer need to be cooled. If electricity output from a 240 megawatt gas turbine could be increased by 2 % at the same fuel consumption level, CO_2 emissions could be reduced by 24,000 tonnes a year.

4.1.5.3. Technological/scientific challenges

A new generation of Si-C based precursor-derived ceramics are better suited for use as protective coatings on combustion engines than conventional materials. Bond coats with modified thermal expansion coefficients applied between the substrate and the TBCs will, however, have to be developed. Mo-Si-B based refractory materials which have superior properties are being considered as new substrates. The oxidation stability of oxide-free high temperature materials needs to be improved.

4.1.5.4. Possible approaches and improvement potential

Besides the amorphous Si-B-N-C ceramics and Mo-Si-B alloys which have already been investigated, other refractory materials in boride, silicide and carbide systems have extremely attractive property profiles for these applications

4.1.5.5. Need for further research

- There is a particular need for further investigation into the corrosion stability of high-temperature materials in the presence of steam at high temperatures and analysis of the phase equilibria in multi-phase composites.

4.1.6. Materials for collectors

4.1.6.1. Current state of technology

Collectors which absorb and store solar or geothermal energy are needed for solar and geothermal systems. The efficiency of solar collectors is currently as high as 75 %. Different types of collectors are used including flat-plate collectors, evacuated tube collectors and concentrating parabolic trough collectors. Absorber materials, thermal barrier layers (polyurethane foam and/or mineral wool), reflectors and heat transport fluids are the main components in the collectors. Mixtures containing water and propylene or ethylene glycol are normally used as the heat transport fluid. The absorbers must be black and thin and they also have to be good heat conductors. Sheet metal (copper or aluminum) with highly-selective coatings or glass tubes are the materials of choice, and they are optimized for maximum absorption and minimum emission. The coatings consist of electroplated “black” chromium or “black” nickel electroplate with an absorption coefficient of up to 96% and an emission coefficient as low as 12 %. Aluminum, metal carbide or blue titanium oxynitride coatings applied through vapor deposition or sputtering under high vacuum are other alternatives. Very good emission coefficients of around 5 % can be achieved with the latter, resulting in a substantial performance increase particularly at high operating temperatures. Absorptance of 94 % and emittance of less than 6 % are achievable. The highly transmissive glass covering on the collectors is made of special low-iron, hardened borosilicate or anti-reflex glass.

On concentrating solar thermal systems, compound parabolic concentrator reflectors are being used to an increasing extent. CPCs collect the radiation within a specific range of incidence angles and focus it on the collector. White, diffuse reflectors made of high-purity aluminum also exist.

4.1.6.2. Relevance

The area covered by solar thermal collectors in Germany has increased in recent years, reaching 15.3 km^2 in 2011. Flat-plate collectors are installed on around 90 % of the surface area with evacuated tube collectors making up the rest. Heat generated with solar thermal systems has increased in recent years and now stands at 10.7 GW, but that is only equivalent to less than 1 % of heat consumption nationwide. Future innovation, installation of large solar thermal systems on multi-family dwellings, commercial applications and construction of large solar thermal plants should make it possible to increase the contribution from solar thermal heating. A figure of around 10 % appears realistic.

Small systems cover significantly more than 100 % of demand in the summer, but that figure is much lower in the winter. Seasonal storage systems will be required to utilize the excess summer energy in the winter.

4.1.6.3. Technological/scientific challenges

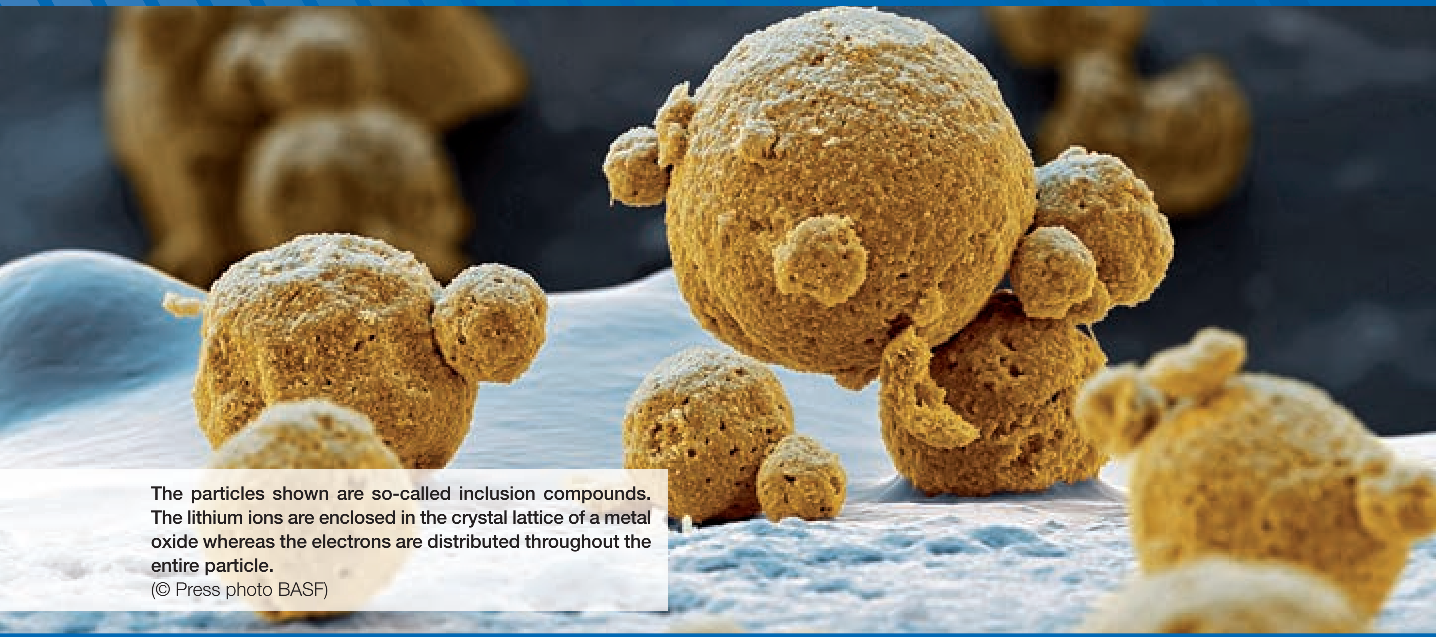
Actual system efficiency is less than indicated above, because optimal collector installation depends on architectural factors. Designs which reduce dependence on the incidence angle would make the process much more cost-effective. Evacuated tube collectors are an improvement, but they are prone to leakage over the long term.

4.1.6.4. Possible approaches and improvement potential

An interdisciplinary approach to materials synthesis and deposition of thin layers will lead to the development of new absorber systems. Conditioning and application must be modified to achieve greater tolerance in the solar radiation incidence angle.

4.1.6.5. Need for further research

- New polymer materials for solar thermal components and systems with specific mechanical, electrical and optical properties which are suitable for temperatures up to 250 °C
- Nanostructured dirt-repellent surfaces
- Storage materials with higher heat density
- Insulation materials with significantly improved thermal barrier performance (nano-porous foam)
- Reduction in insulation costs for seasonal storage systems
- Improved efficiency of high-temperature selective coatings / cost reduction



The particles shown are so-called inclusion compounds. The lithium ions are enclosed in the crystal lattice of a metal oxide whereas the electrons are distributed throughout the entire particle.
(© Press photo BASF)

4.2. Materials for Energy Storage

The upcoming modernization of the electricity supply network in Germany and government policies on expansion of renewable energy highlights the importance of electricity storage and the development of new storage technologies.

For the foreseeable future, the increasing penetration of fluctuating energy from renewable resources such as wind and solar energy in the electricity grid will necessitate the integration of electrical storage to balance supply and demand for electricity. The anticipated future need for storage technology to stabilize the electricity supply will arise at around the same time as increased vehicle "electrification". Both are expected to create a growing supply-side need for electricity storage systems.

Electricity is the most valuable form of energy. It can be converted with the least effort into other types of energy. The energy losses during conversion should, however, be as low as possible.

Because the infrastructure which is currently available in Germany (e.g. compressed air storage or pumped water storage) will not be able to compensate for demand in the foreseeable future and electricity will have to be converted to a form of energy which can be stored for long periods of time, the search for alternatives will have to be a top priority for the scientific and research community.

4.2.1. Electricity storage

4.2.1.1. Supercaps

4.2.1.1.1. Current state of technology

Super capacitors (supercaps) are a purely physical form of electricity storage. The principle is based on charging/discharging of the electrolytic double layer (Helmholz layer) which forms at the phase boundary of an electrical conductor in contact with an electrolyte. The first patents for the use of double-layer capacitors were granted in 1957. Compared to conventional capacitors, supercaps have a much higher storage capacity which is typically 100 Farad/g when activated charcoal with a specific surface area of around 1000 m^2/g is used as the active electrode material. Energy densities can be as high as 5-10 Wh/kg. Compared to batteries, super capacitors can release the energy very quickly during discharge and supply high amounts of electrical power > 20 kW/kg for short periods. Their specific energy is, however, significantly less than that of batteries. Compared to other electrical storage systems where electrical energy is stored statically or dynamically as heat or mechanical energy, supercaps are more efficient and have higher power density. The operating conditions are also an advantage. Supercaps can be used in mobile or stationary applications at relatively low temperatures.

4.2.1.1.2. Relevance

In a high-tech society, electricity plays a particularly important role because it is a nearly universal form of energy which can be used anywhere and can be transformed into other forms of energy such as light, heat or mechanical energy.

4.2.1.1.3. Technological/scientific challenges

Applications which use double-layer capacitors in combination with batteries or fuel cells are designed to increase the power rating and lifespan of the electrical components. Supercaps could also replace batteries in some applications, and they attracted a lot of attention when hybrid vehicles were being developed in the 1990's. Their function is to provide short-term storage which can boost the output of the fuel cell or battery to deliver peak power and they can also store brake energy. To capture a significant share of the market, a substantial improvement will have to be made to the specific energy and performance ratings of supercaps.

4.2.1.1.4. Possible approaches and improvement potential

One way to boost the energy and the performance density would be to increase the rated voltage from around 2.5 V to 3 V at a cycle life of around 500,000 charge/discharge cycles. Research into new electrode materials (high porosity carbon materials) and electrolytes including ionic liquids (currently too expensive) will be critically important to achieve that goal. Design optimization to reduce volumes and weight is another option. Tailored pore systems and functional properties in three-dimensional electron-conducting structures can also lead to improvement. Greater use should be made of synergies in the development of thin-film capacitors and batteries.

4.2.1.1.5. Need for further research

- Continued R&D on new electrode materials and electrolytes
- Design optimization to reduce volume and weight
- R&D on tailored pore systems with functional properties
- Exploitation of synergies in the development of thin-film capacitors, lithium-ion batteries and post lithium-ion batteries.

4.2.1.2. Stationary electricity storage

4.2.1.2.1. Current state of technology

Electrochemical storage is one of the major options which will be available for storing energy in the future. Only limited success was achieved in earlier attempts to store electricity in the megawatt hour range using lead batteries. Stationary sodium-sulfur batteries with ceramic electrolytes as separators are now making a breakthrough in Japan. Both of these modular systems are designed as conventional batteries. Each cell contains the entire redox-active compound, and that costs a lot of money. In redox-flow batteries, the electrolyte can be stored separately from the electrochemical cell, overcoming the constraints of modular design. The redox-flow battery is currently the only form of electrochemical storage where energy capacity can be scaled completely independently of the power rating. However redox-flow batteries have the disadvantage that they require large amounts of chemicals. So far, they have only been developed on a pilot scale, with Canadian, English and Japanese companies playing the leading role.

In recent years, the vanadium redox-flow battery has emerged as a very promising alternative. Vanadium-bromine compounds are used as the electrolyte.

Research continues on batteries which are based on lithium technology which is currently one of the best commercially available electrochemical storage technologies. The batteries have a charge/discharge efficiency of 95%, which no other technology can match, much less exceed. Lithium-ion battery technology delivers a high charge/discharge rate which can be used to good advantage in power and energy oriented grid applications. Compared to lead technology, the self-discharge rate is lower by a factor of ten and significantly less maintenance is required. Due to their high energy density, battery systems based on Li-ion technology are relatively compact. The growth of distributed power generation and storage increases the importance of modular scalability which provides the basis for assembling a network of many small storage units to create a large virtual storage system. This makes it possible to avoid many of the problems associated with grid expansion or at least to mitigate the problems through better grid utilization.

4.2.1.2.2. Relevance

The increasing importance of power generation from renewables, particularly in the wake of the German government's decision to phase out nuclear power, is pushing the existing power grids to their limits. The widening gap between electricity supply and demand can only be closed by putting more storage capacity in place. Because the wind parks and pumped storage power stations are in remote locations, it is necessary to invest in grid expansion. The cost of further grid expansion and the lack of additional hydroelectric storage capacity create the need to find other solutions such as stationary electricity storage systems.

4.2.1.2.3. Technological/scientific challenges

Multi-megawatt redox-flow batteries are very large and are on a scale with chloralkali electrolysis plants. Selection and evaluation of potential redox systems must be as meticulous as for any safe, cost-effective, large-scale chemical process.

Li technology is currently expensive, and there is uncertainty regarding the expected lifespan (10 – 20 years). Both of these factors are significant disadvantages. The basic thrust of future R&D efforts must be to find cheaper electrochemical battery storage technologies which offer high power density, high efficiency, high reliability and a high level of safety for stationary applications. Low-cost, efficient materials and larger electrodes are the key to better storage systems. The general scientific challenge is to develop efficient active and non-active materials and enhanced manufacturing technologies to ensure optimal functionality of these materials in the target system.

4.2.1.2.4. Possible approaches and improvement potential

Despite the fact that many of the technologies listed above were developed in Germany, the lines of development have been abandoned there. Much of the expertise no longer exists in the country. New innovative approaches will be needed to close the gap with what is happening elsewhere. The development of new solid electrolytes, innovative separators, electron conductors and electrode materials are high on the research priority list. Pooling of development lines for these materials will be absolutely essential.

It would be a welcome development if the intensity of future funding were to reach the same generous level as for the National Electromobility Platform (NPE). The market for stationary electricity storage systems will initially be the domestic market where there is significant potential for dynamic growth, especially for small and middle sized companies which develop and produce electrodes.

4.2.1.2.5. Need for further research

- Development of alternative, less expensive electrolyte materials
- R&D on new solid electrolytes, separators, electron conductors and electrode materials

4.2.2. Thermal Energy Storage

4.2.2.1. Current state of technology

Thermal storage media are used in many different applications. The requirements profiles for thermal storage materials differ depending on the application and temperature range. Water storage systems dominate in the low temperature range (20-120 °C). Phase change materials (PCM), which store thermal energy as a phase change (e.g. from solid to liquid), are another alternative. The energy is released when the phase changes back again. In contrast to sensible heat storage materials, PCM storage materials remain at the same temperature when storing or releasing energy. PCMs include such materials as paraffin wax blends which are used at 20-25 °C for passive air conditioning. PCMs are also used in high-temperature applications, e.g. as molten salts. The capacity and range of applications depend essentially on the enthalpy and the temperature of the phase change.

Sorption storage systems utilize reversible desorption/adsorption processes to store thermal energy in the 100 °C - 150 °C temperature range. At high temperatures (up to 1000 °C), heat is normally stored as sensible heat.

4.2.2.2. Relevance

The largest proportion of energy consumed in Germany[3] (58 % in 2008) is used for heating in industry, commerce, the service sector and domestic homes. Natural gas and oil are the leading heating fuels in low-temperature applications (up to around 120 °C) for space heating and warm water and in high-temperature generation of process heat (up to more than 1000 °C). There are a number of ways to significantly reduce fossil fuel consumption, for example by improving thermal process efficiency, making greater use of industrial waste heat particularly where intermittent operation results in high heat loss, using more renewable energy to generate heat (currently only 4 %) and substantially expanding CHP generation. To exploit this potential, it is essential that efficient, economical thermal energy storage is available. Thermal storage also plays a major role in making power from solar thermal power stations available during the full day and night cycle.

4.2.2.3. Technological/scientific challenges

Thermal storage systems are complete solutions which are tailored to the particular application. Because the storage materials are an integral part of the system, the complex requirements profile which is dictated by the application applies to them as well. The systems have to be economical, rugged, maintenance-free and user-friendly, and they also need to have high storage density, which is particularly challenging. The use of reversible thermo-chemical reactions is another option which is being considered to reach higher storage densities.

4.2.2.4. Possible approaches and improvement potential

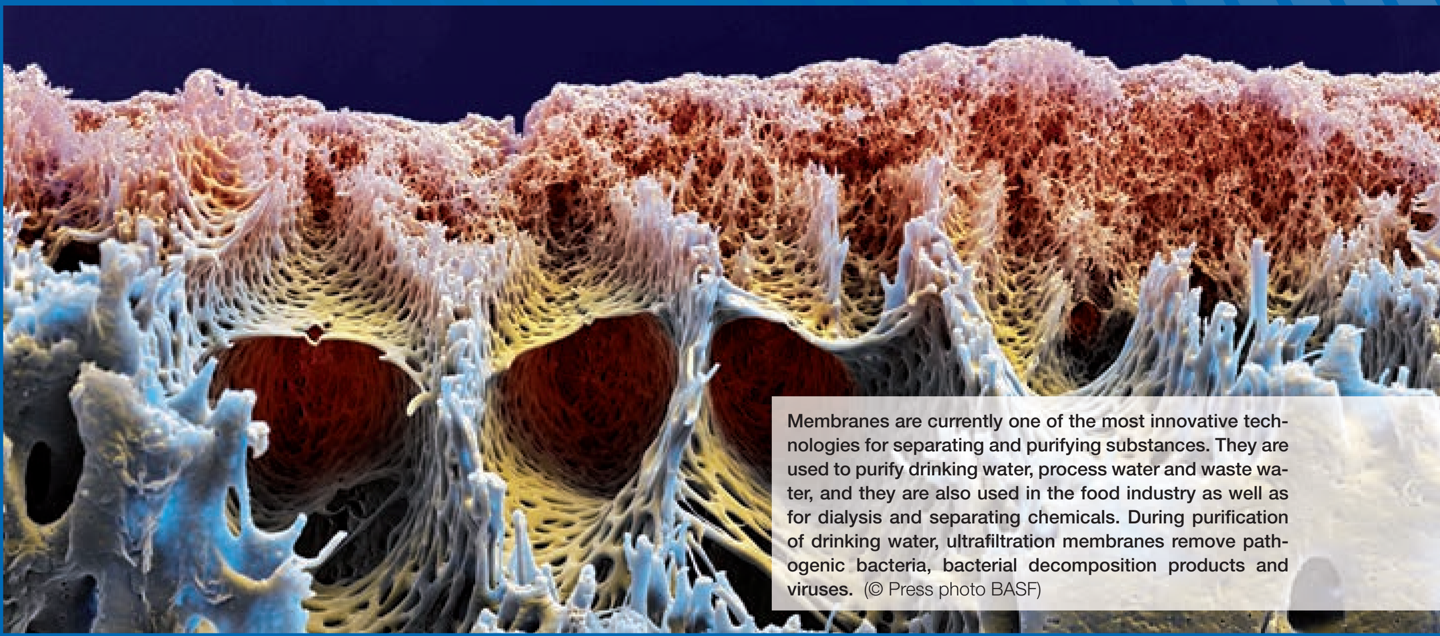
There is a continuing need to develop materials which cover a large temperature range. New ideas could lead to the development of completely new types of materials. Latent heat storage and thermo-chemical reactions have the greatest development potential. Systems which, for example, combine sorption with a thermo-chemical reaction could cover different temperature ranges, and they could be used for controlled generation of heat or cooling energy. A systematic approach is needed to the development of thermal storage. A narrow focus on the storage material alone will not produce a successful outcome for real-world applications.

3 Arbeitsgemeinschaft Energiebilanzen, erschienen in „Energiedaten“ des BmWi, Version 22 Jun 2011

Reversible chemical reactions are another option for thermal storage. The equilibrium of the reaction is shifted in one direction when heat is stored. The heat is released when the opposite reaction takes place until equilibrium is restored. Chemical reactions could potentially store large amounts of heat. The reaction enthalpies exceed phase change enthalpies and storage of sensible heat by a considerable margin. If the products are kept separate, chemical reactions could provide a safe, long-term, reliable method of storing heat in the form of chemical substances. In order to use chemical reactions to store heat, it is essential that the reactions are integrated safely and reliably into the storage system.

4.2.2.5. Need for further research

- Reduction of thermal storage investment costs
- Increased storage density
- Improvement of the relevant thermo-physical properties
- Increased energy efficiency (avoidance of heat and exergy losses)
- Better system integration
- Development of new materials with high sorption capacity
- Combination of active components and substrates
- Chemical reactions as thermal storage



Membranes are currently one of the most innovative technologies for separating and purifying substances. They are used to purify drinking water, process water and waste water, and they are also used in the food industry as well as for dialysis and separating chemicals. During purification of drinking water, ultrafiltration membranes remove pathogenic bacteria, bacterial decomposition products and viruses. (© Press photo BASF)

4.3. Materials for Environmental Protection

4.3.1. Material separation and purification

4.3.1.1. Current state of technology

Catalytic converters designed to control pollution have been effective in reducing different types of emissions for many years, particularly in the traffic and transportation (automotive catalytic converter) and power generation (flue gas desulfurization and denitrification) sectors and in many other industrial and commercial applications. Sophisticated catalytic treatment of industrial waste gas is well established in the industrialized world.

Many thermal separation operations are used in the chemical industry such as distillation, liquid-liquid extraction, crystallization and chromatography. Because these operations are energy and material intensive, between 40 % and 70 % of the investment and operating costs in the chemical process are attributable to them. As thresholds continue to decrease, materials separation and purification are migrating to techniques which are based on high-grade materials properties. Membrane technology is particularly relevant.

Adsorbents also play a key role in the material conversion and conditioning industry. Materials with tailored properties are used for physical and chemical sorption and as catalyst substrates in many materials separation operations. They make an essential contribution to the selectivity and yield of the production process, and they are a major tool for production-integrated environmental protection. They are also needed on a large scale in additive environmental protection. In addition, adsorption materials are being used to an increasing extent in energy systems (heat pumps, cooling).

4.3.1.2. Technological/scientific challenges

Sustained research on materials separation and purification is needed to meet or exceed new emissions standards, e.g. for emissions of organic solvents, nitrogen oxides, CO and CO_2. A continued focus on these types of materials is an absolute necessity. The shear breadth of the application spectrum in nearly all sectors of industry ranging from heavy industry, foundries and chemical and pharmaceutical production to electronics and the food and animal feed industry is a major factor which is driving innovation.

In catalytic post-treatment of (industrial) waste gas, combining multiple process steps is one of the strategies which could well lead to new breakthroughs in material separation and purification.

Membranes have only been used to a limited extent for organic media because the membrane materials which are suitable do not have sufficient durability. They are not resistant to solvents, and they lose their selectivity. The future challenge is to find alternatives to thermal separation which is currently the predominant technology for treating organic media. Membrane-based techniques would be much more energy efficient.

4.3.1.3. Need for further research

- Develop more durable membrane and filter materials with better resistance to solvents combined with higher selectivity and lower operating pressures
- Expand catalytic reduction of greenhouse gases (e.g. methane and N_2O) into new fields of application (sewage sludge combustion, fluidized beds, gas engines, cement and glass industry).
- Develop more efficient methods for adsorption of volatile hydrocarbons from painting and printing operations, etc.
- Develop adsorption and oxidation processes for trace gases in the semiconductor industry
- Develop new catalysts for low-temperature reduction of NO and N_2O and low-temperature oxidation of hydrocarbons which are difficult to oxidize, especially methane

4.3.2. Materials for water/wastewater treatment

4.3.2.1. Current state of technology

Water recycling and the recovery of valuable resources and residuals are becoming increasingly important aspects of industrial water engineering, particularly for German companies operating in a global market. Industrial water treatment and recycling make a vital contribution to environment protection.

As natural resources become increasingly scarce and expensive, these trends are likely to continue. In addition, water circulating through industrial facilities contains critical raw materials such as gallium which need to be recovered because of their strategic value. Recovery is legally mandated in Germany under the terms of the Recycling Act.

A whole range of treatment technologies including precipitation/flocculation, oxidation/reduction, ion exchange, membrane filtration, distillation and others used alone or in combination have an important role to play.

Around one billion people currently have no access to clean drinking water. Continued development of adsorbents for water decontamination in combination with catalysts, additives and innovative techniques is making a vital contribution to an improvement in quality of life and a reduction in the significant potential for social conflict. The possibility of extracting valuable (trace) elements from highly dilute media (e.g. strategic metals from seawater) can reduce supply dependencies for critical raw materials.

4.3.2.2. Ion exchangers/Adsorbents

4.3.2.2.1. Technological/scientific challenges

Much valuable research has been done in recent years on adsorption of inorganic substances. Water/wastewater engineering is now, however, confronted with a new set of challenges. Surface and ground water in many places has been contaminated with a variety of anthropogenic substances such as pesticides and their metabolites, halogenated or halogen-free hydrocarbons, nitrates and pharmacologically active and endocrine active substances. The situation will be exacerbated in the years to come, creating the need for research on technologies such as selective adsorption of organic compounds.

4.3.2.2.2. Need for further research

- A significant increase in the number of available adsorbers. New functional groups for selective ion exchangers, metal or metal oxide doped polymers and solids with specifically shaped adsorption centers (MIPs: Molecular Imprinted Polymers) are of particular interest
- Low-cost sorbents with high selectivity and capacity are needed for separation/recovery of alkali metals, rare earth elements, metalloids (e.g. selenium, tellurium, arsenic, bismuth, boron, gallium and germanium), anions (such as fluoride, nitrate, chloride, sulfate and iodide) and a large number of organic compounds with endocrine-active, carcinogenic, antibiotic, xenobiotic, persistent, antioxidant or therapeutic properties
- Further progress in the selective adsorption of organic compounds is needed

4.3.2.3. Membranes

4.3.2.3.1. Technological/scientific challenges

Besides the membrane itself, there is room for improvement of the membrane module as well in some applications. Flow optimization and selection of the right materials are issues that need to be addressed, particularly on large modules. Ceramic membranes will only become a viable option for a much larger group of users (e.g. pre-treatment of seawater for reverse osmosis (RO)) if the energy efficiency of the filtration process can be increased.

The challenge ahead will be to expand the range of possible applications for ceramic membranes, for example partial desalination of solutions, separation of different sugar fractions and the retention of small molecules in fluids to close the recycling loop. Polymer membranes can often be used in principle, but they lack chemical and/or mechanical resistance. Membrane cut-off, in other words the effective pore size, is the limiting factor for ceramic membranes.

(Industrial) wastewater treatment makes a huge contribution to our quality of life and can also recover critical raw materials from industrial water flows.

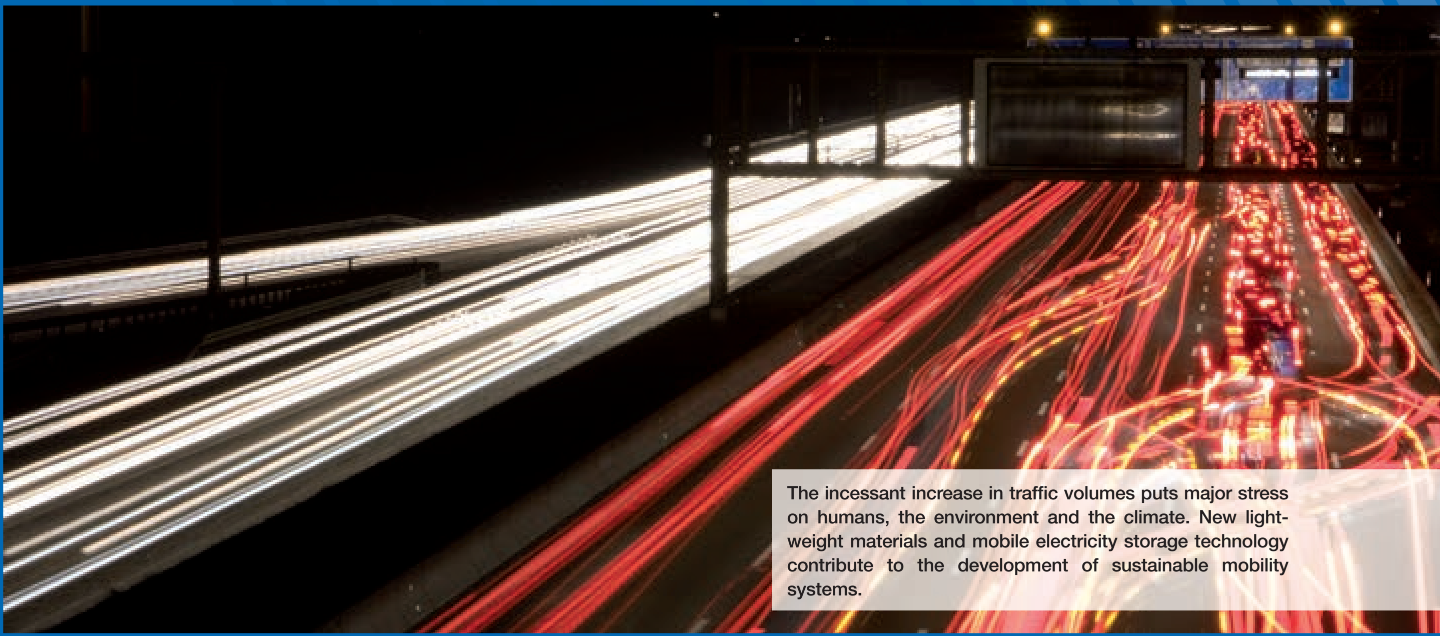
4.3.2.3.2. Need for further research

Further research on ceramic membranes is needed in the following areas:

- Development of membrane geometries with high volume-specific membrane surface area
- Process development to optimize filtration performance and energy consumption
- Development of ceramic NF membranes with 200 g/mol cut-off
- Ceramic ultra-filtration and nanofiltration membranes with high pH resistance
- Modification of ceramic membranes for use in organic fluids
- Process combinations

The following are seen as development priorities:

- High module throughput with low energy consumption
- Improved chemical, mechanical and thermal resistance
- Improved selectivity without constraints on productivity
- New module designs and membranes for applications which make better use of renewable energy (e.g. biofuel, biogas, syngas, natural gas scrubbing, osmotic distillation, direct osmosis, water recovery from combustion gas and much more)
- Improved anti-fouling properties and increased lifespan of polymer membranes



The incessant increase in traffic volumes puts major stress on humans, the environment and the climate. New lightweight materials and mobile electricity storage technology contribute to the development of sustainable mobility systems.

4.4. Materials for Mobility

4.4.1. Lightweight design

In the passenger and freight transportation sector, there is a pressing need for lightweight, safe, low-cost and eco-friendly designs which enhance competitiveness and maximize value-adding. Trade offs are inevitable, but we can expect to see continued development of hybrid designs which use a wide variety of materials to reduce weight. These designs will have advantages as well as disadvantages.

State-of-the-art lightweight materials are used in the mobility industry to cut fuel consumption by reducing the mass that needs to be moved.

Compared to other alternatives such as a reduction in rolling and air resistance and increased efficiency of the drive train, lightweight design appears to be the most promising approach.

On electric or hybrid drive vehicles, the prime reason for lightweight design is to compensate for the additional weight of the batteries and electric motors.

Functional integration is another key aspect of materials for the mobility sector. Structural health monitoring, safety features (sensors), interior lighting (luminescence elements) and intuitive controls (switches) can have major benefits in passenger transportation. Thermal insulation, anti-fouling and quality control play a major role in freight transportation.

Much can be learned from the wind power industry (large wind turbines).

4.4.1.1. Current state of technology

A variety of different metallic, polymer and ceramic materials are used in state-of-the-art lightweight designs. These materials must withstand the mechanical, thermal and media-induced stress defined in the requirements profile. Because the properties of plastics can be manipulated over a wide range, more and more plastics are being designed into today's products. Fibers and particles are often embedded into the parts to enhance thermo-mechanical performance and dimensional stability. Specially designed fiber composites with a polymer matrix and continuous filament reinforcement made of high-performance fiber materials such as fiberglass and carbon fibers as well as high-strength polymers are used when lightweight parts and assemblies must meet demanding mechanical requirements. High energy absorption is an important design aspect, particularly for crash elements, in order to protect passengers.

In addition to continuous fiber reinforcement, reinforcement of polymers with short fibers followed by injection molding is often used to produce lightweight parts with complex geometries, particularly in the automotive industry. Roughly 1 million tonnes of these materials are produced in Europe every year, and the growth rate is currently in the double-digit range.

High-performance polymers, polymer blends, copolymers and sandwich designs are other options for enhancing the properties of parts. The design of the inner and outer interface regions is particularly important in sandwich materials. In addition to the standard lightweight design materials (titanium, aluminum and magnesium), state-of-the-art steels are being used to an increasing extent in lightweight design. The new steels are the solution of choice in automotive body manufacturing. High strength combined with good workability is the primary design goal.[4]

As yet, functional integration at the material level is not very widespread. Structural health monitoring has been introduced to a limited extent in the aviation industry. For example, sensors integrated into the structure monitor load cycles for condition-based maintenance. Maintenance costs can be reduced by a substantial amount compared to time-based maintenance.

4.4.1.2. Shortcomings and development goals

A thorough understanding of the complex stress conditions and the development of an engineering concept which is suited to the specific materials and structure giving due consideration to all of the manufacturing constraints are vital aspects of lightweight component design. From the design and material perspective, there is a general tendency to view the load-bearing aspects separately from corrosion and wear protection. The reason for this lies in the fact that the materials which are currently available are only able to meet the thermo-mechanical, media-related and tribologic requirements to a limited extent. As a result, coatings which provide corrosion and wear protection are applied separately to load-bearing structures. The goal of material and design development is to create a new generation of lightweight structures featuring advanced functional integration based on new lightweight materials and composites which meet the thermo-mechanical and functional requirements profile.

The black metal approach is still commonly used for high-performance composites. Metalworking designs are transferred directly to composites. However these designs are not suitable for composite materials and fail to adequately exploit the potential of new material combinations. The same is true for the production process.

Additional functionality is often not included in the structural elements due to a lack of experience with the new technologies and also because of issues related to production engineering. Contacting of the conductive layers and integrated sensors represents a major technological and production engineering challenge.

Cycle times have to be kept short when fiber composite based lightweight designs are introduced into volume production in the automotive industry, creating another major hurdle. New formulations for duroplastic matrix materials and low-cost thermoplastic matrices which have greater thermal and mechanical resilience are required. On top of that, there is also a need for new process sequences and technologies for cost-efficient, cycle-oriented production of fiber composite components. The interface between the reinforcement fiber and the matrix has to be designed specifically to exploit the strength/rigidity of high-performance fiber materials. High modulus fibers will only be used on a widespread basis in the automotive industry if the price comes down. Mid-tech carbon fibers are a develop-

4 AVK Composites-Marktbericht 2011, S. 10

ment goal in their own right. Their performance characteristics should be significantly better compared to glass fibers, but for cost reasons they cannot be on a par with Polyacrylonitrile (PAN)-based carbon fiber.

4.4.1.3. Technological/scientific challenges

While factors such as the specific application temperature limits of plastics and fiber composites with polymer matrixces limit their suitability for widespread use in process engineering, economic considerations are what prevent their broad-based introduction in the mobility sector. The material properties, production process and component characteristics mutually influence each other. A holistic approach is needed to manage the effects of those interactions and produce fiber composite materials and related multi-phase material systems at an affordable cost. Process auxiliaries such as polymer binder materials offer enormous potential for the development of reliable, cost-effective manufacturing, but their effects on the fiber/matrix interface and component properties have not been sufficiently investigated.

Research on alternative precursor systems will be needed to develop low-cost carbon fibers. The bio-based wood derivative lignin is currently the subject of in-depth investigation. The precursor spinning process and especially the development of customized, effective stabilization and carbonization are the major scientific and engineering challenges. Researchers are also looking at the process which is used to make the precursor for the coated carbon fiber.

Production engineering issues place constraints on widespread use of functional integration. In some cases satisfactory solutions have not yet been found for problems at the interface between the reinforcement elements or sensors and the material. The development of (molten) liquid coatings for the reinforcement elements to reduce mechanical stress and promote adhesion among other things will be another major step forward.

4.4.1.4. Possible solutions

Enhancements in materials properties must be cost-efficient, and trade offs need to be managed along the way. Close, sustained collaboration bringing together materials developers, design engineers and technologists along the entire length of the value-adding chain will be needed to find viable solutions. Besides the development of new types of plastics and polymer-based (fiber) composites with application-oriented features as well as alternative reinforcement fibers such as mid-tech carbon fibers, continued development of textile technology can provide another pathway to low-cost component production.

Special copolymers can be used to make new lightweight materials for a wide variety of industrial applications. The thermo-mechanical characteristics and functional properties (acoustic, tribologic or electrical) of the copolymers lend themselves to manipulation.

New types of stress-resistant textile reinforcement in plastics offer considerable potential. The variable, directional structural properties of the components made of textile composites are defined during concurrent materials and component design. Compared to conventional materials, there is an even greater need to ensure that the different process stages are well coordinated. In order to achieve reproducible quality and short cycle times, the development team has to gain an in-depth understanding of all stages in the value-added chain including the filament, hybrid yarn, semi-finished product, textile preform and assembled components and products which have integrated functionality based on hybrid designs.

Current research on metallic materials covers a very broad spectrum. The emphasis is on further optimization and a reduction in production costs.

Continued development of lightweight materials creates many opportunities to save energy. In the automotive sector, a 5 % reduction in car body weight would reduce fuel consumption by about 3 %.

The development of intelligent sensor materials facilitates new integrated designs. Structural health monitoring and integration of smart elements (switches and sensors) are two prime examples from automotive design. Functionalizing surfaces by adding antifouling properties could be very beneficial in shipbuilding and shipping container applications.

Comfort, safety, variability and functionalization are becoming increasingly important aspects of car interior design. The functions include acoustic insulation, functional integration, touch & feel, dirt repellency, variability of the interior configuration and design for recycling. When fiber-based materials are used in combination with other material systems and the production and assembly process is properly designed, functional elements which form part of energy-efficient air-conditioning, sensor, actuator, ambient lighting and driver assistance systems can be integrated into the interior. This type of approach will become increasingly common as the transition to e-mobility and adaptive/configurable vehicles gains momentum.

Materials for extreme applications

Extreme operating conditions, for example in the space industry, create a huge challenge, particularly for lightweight components which are made of organic materials (plastics and plastic composites). Because of their very favorable weight profile, these materials are obviously attractive, but they are highly susceptible to the extreme conditions of space travel (temperature, temperate change, high-energy radiation, collision with high-speed particles i.e. „space junk)". In order to design future transportation systems, satellites and mission modules which are affordable and have a tolerable environmental impact, organic and hybrid materials will have to be used to a greater extent than is currently the case. There is a particular need to improve bonding under thermochemical and media-induced stress as well as low-temperature impact resistance, high-temperature dimensional stability and radiation tolerance. The initial work has already been done in the civil and military aircraft industry, and a systematic effort is now needed to make major advances. The results will have spin-off benefits for systems that operate closer to earth.

4.4.1.5. Need for further research

- » New types of plastics and polymer-based composites
- » In-depth understanding of the value-adding chain for textile-reinforced plastics, so that specific structural properties can be created in a concurrent material development and component design process.
- » New production techniques for high-alloy steel
- » New techniques and coatings for hot forming of steel
- » Improvement or replacement of the titanium production process to bring down the price of the material
- » Development of aluminum alloys which are suitable for welding
- » Development of low-cost malleable magnesium sheet metal materials for car manufacturing
- » Intelligent sensor materials
- » Improved anti-fouling coatings, and in particular investigation of coating aging and fatigue, in order to find ways of achieving long-lasting, eco-friendly stabilization (including fire prevention)
- » New compounds to improve forming and dimensional stability for exterior applications
- » Development of new types of hybrid materials so that functional elements can be built into vehicle interiors

4.4.2. Corrosion protection

Corrosion is a deterioration factor in many technical applications, particularly in the mobility sector. Corrosion damage can impair functionality or even lead to total system failure, and the consequential costs can be considerable. Studies carried out worldwide indicate that corrosion causes roughly $ 1.8 trillion worth of damage, which is equivalent to 3 % - 4 % of GNI. (Gross Domestic Product) in the industrialized nations.[5]

4.4.2.1. Current state of technology

Corrosion protection can be active or passive. There are many established techniques and materials for coatings which provide good passive corrosion protection on technical systems. Organic, inorganic or metallic materials are used in the coatings depending on the operating conditions. The techniques used to provide corrosion protection include painting, lacquering, powder coating, galvanic passivation and thermal and vacuum coating. Depending on the operating environment and part geometry, highly developed multi-functional materials solutions may be necessary to withstand other types of stress (e.g. tribologic or thermal). As the requirements become more demanding (e.g. increased power density), the existing materials and techniques are being pushed to their limits. Environmental and safety requirements are another factor which create the need to find alternative techniques to established systems such as chrome plating.

4.4.2.2. Technological/scientific challenges

As the requirements for technical systems become more demanding and operating conditions continue to evolve, there is a need to drive development of coating materials. The challenge is to develop multi-functional materials which provide adequate protection for the life of the product. To make things even more difficult, further process development work is needed for a prospective material to ensure that the coating can be applied to the functional surface even if the geometric architecture changes. Engine production is a good example of this. The power density of state-of-the-art diesel engines is now roughly 100 kW per liter of displacement, and the engines are subjected to greater stress and more aggressive corrosion. The combustion temperatures are higher, and the engine components are smaller.

4.4.2.3. Need for further research

- Use high-resolution electrochemical research methodologies to achieve a better understanding of corrosion effects, e.g. on lightweight materials and in new fuels
- Develop tailored architectures, which combine different materials classes, as well as new customized joining technologies which are able to withstand local corrosion effects
- Develop composites, multi-layer and gradient structural designs and material combinations which deliver better performance
- Increase resource efficiency, e.g. through the use of self-healing materials which provide corrosion protection with the aid of chemical nanotechnology
- Use sustainable substances, which are natural, biogenic or can be produced with biotechnology, as coating materials (e.g. biopolymers, coating resins without fossil-derived carbon, bio-based binders, coating materials based on vegetable oil and sugar)
- Develop new chemical and plasma-chemical treatment methods for multi-metal applications to replace critical elements (chromium, nickel, etc.) in coatings, coverings and chemical conversion coatings

5 G. Schmitt: Global Needs for Knowledge Dissemination, Research, and Development in Materials Deterioration and Corrosion Control, World Corrosion Organization, 2009

4.4.3. Mobile electricity storage

4.4.3.1. Current state of technology

A number of different rechargeable battery systems based on proven technology are currently available on the market. Lead batteries have the largest market share. Engineering development and optimization of lead batteries for a wide variety of applications is more advanced than for any other technology. They are used in a wide variety of applications ranging from starter batteries and emergency back-up to the supply of power for aviation and marine electronics and propulsion motors in rail vehicles and boots. Lead batteries have a relatively low power density, which is a disadvantage. The power to weight ratio is too low for many applications. Rechargeable batteries which are technically more manageable such as Ni-cadmium, Ni-metal hydride and above all Li-ion are better suited for small mobile devices. They are found in high-tech electronic devices such as cellphones, digital cameras and video cameras and laptops.

As e-mobility rapidly expands, Li-ion batteries are being designed into alternative propulsion systems which complement or replace combustion engines in motor vehicles. The use of Ni-metal hydride batteries is also on the increase, but for technical and economic reasons, high-power, high-energy Li-ion batteries appear to be a better choice than standard technology over the medium term. In the long term, technology is moving in the direction of lithium-sulfur or lithium-oxygen batteries. The market for high-energy lithium batteries for mobile devices is dominated by manufacturers in the Asian region. However working in conjunction with established research organizations, a number of German companies are already involved in the lithium technology value-adding chain (materials supply, component production, cell production, battery assembly, system integration). Their intention is to become the technology and market leaders in large lithium batteries.

Lithium batteries utilize what is currently the best commercially available electrochemical storage technology. The batteries have a charge/discharge efficiency of 95 %, which no other technology can match, much less exceed. Lithium-ion battery technology delivers a high charge/discharge rate which can be used to good advantage in power and energy oriented grid applications. Compared to lead technology, the self-discharge rate is lower by roughly a factor of ten, and significantly less maintenance is required. Due to their high energy density, battery systems based on Li-ion technology are relatively compact.

4.4.3.2. Development goals

In the future, batteries will be used in more and more mobile applications. In the consumer sector, more cordless power tools (screw drivers and drills) and products such as garden appliances (lawn mowers) will be powered with rechargeable batteries. Improved high-power batteries with greater energy density will have to be developed for these applications.

Lithium drive technology is expected to capture about a 20 %[6] share in the automotive sector by 2017.

In addition, electricity storage systems and systems which act as buffers at distributed solar and wind power stations that do not provide a continuous source of electricity will be needed to manage peak grid loads. High-capacity rechargeable batteries for these applications are not yet available. R&D on state-of-the-art rechargeable battery systems could be considerably expanded to address this need as well.

4.4.3.3. Technological/scientific challenges

The work which has been done in the field of electromobility in recent years indicates that electric motors and not internal combustion engines will power the cars of tomorrow. Compared to the rest of the world, Germany has a very strong automotive industry, and the country is also a leader in renewable energy. Because it does not have

6 Energieversorgung der Zukunft, eine quantitative Potentialanalyse, October 2009

a consumer electronics industry however, Germany has fallen far behind in lithium battery development in recent years. This applies to both industry and the academic sector where a significant level of activity only got underway a few years ago.

Lithium technology is currently expensive, and there is uncertainty regarding the expected lifespan (10 – 20 years). Both of these factors are significant disadvantages. The basic thrust of future R&D efforts must be to find cheaper electrochemical battery storage technologies which offer high power density, high efficiency, high reliability and a high level of safety for stationary applications. Better materials are the key to better storage systems. The general scientific challenge is to develop efficient active and non-active materials and technologies which optimize the functionality of these materials in the electrode and cell system. There are also safety issues to consider.

The latest advances in materials technology appear to offer significant potential for enhanced reliability and service life.

Li-ion technology is at the center of attention at the moment, but it is important to look at other options as well. The comparative advantages, suitability for practical application and level of innovation compared to the current status will be used as the yardstick.

4.4.3.4. Possible solutions

New electrode materials and electrolytes are needed to improve the performance of Li-ion batteries. The search is on for anodes and cathodes with higher charge/discharge capacities (lithium intercalation). Higher cell voltage could also increase the energy density. Particular attention needs to be paid to the reactivity of the electrode/electrolyte interface (SEI = Solid Electrolyte Interface). Nanostructuring can provide alternatives to conventional graphite. Replacement of organic liquid electrolytes with polymer electrodes, the use of more stable electrolyte salts and electrolyte additives and new overcharge protection mechanisms could improve the safety and stability of lithium systems.

4.4.3.5. Need for further research

- Anodes and cathodes with higher charge/discharge capacities
- Higher cell voltage, e.g. using cathodes made of $LiMPO_4$ mixed oxide (M = Co, Ni, Mn)
- Alternatives to conventional graphite, e.g. new mesoporous nanostructured carbon
- For lithium systems: replacement of organic liquid electrolytes with polymer electrolytes, electrolyte salts and additives that have greater stability

Ceramics by the yard: ceramic separators enhance the safety of lithium-ion batteries (© Evonik)

4.4.4. High-temperature processes

4.4.4.1. Current state of technology

There are a number of hard, inert substances that have high melting points including oxides such as tungsten oxide and silicon carbide which are frequently used as refractory materials in processes which run at high temperatures. A broadening of the materials base would make it possible to increase the operating temperatures and enhance process efficiency. Titanium aluminide alloys are currently the most commonly used intermetallic compounds in jet engines.

If the existing alloys and refractory materials could be replaced with materials that are stable at higher temperatures, substantial efficiency gains could be made in air transportation. Total emissions (and contamination) from aircraft have been reduced by more than 15 % over the past 30 years. The reduction was due mostly to new materials, especially after design changes to the engines. For example the emissions from an Airbus 320, which has a fuel consumption of 2700 liters of kerosene/hour, contain seven and a half tonnes of CO_2, about 3 tonnes of H_2O and, depending on flight conditions, 5 – 40 kg of NO_x and 1.5 – 5.5 kg of CO.

4.4.4.2. Technological/scientific challenges

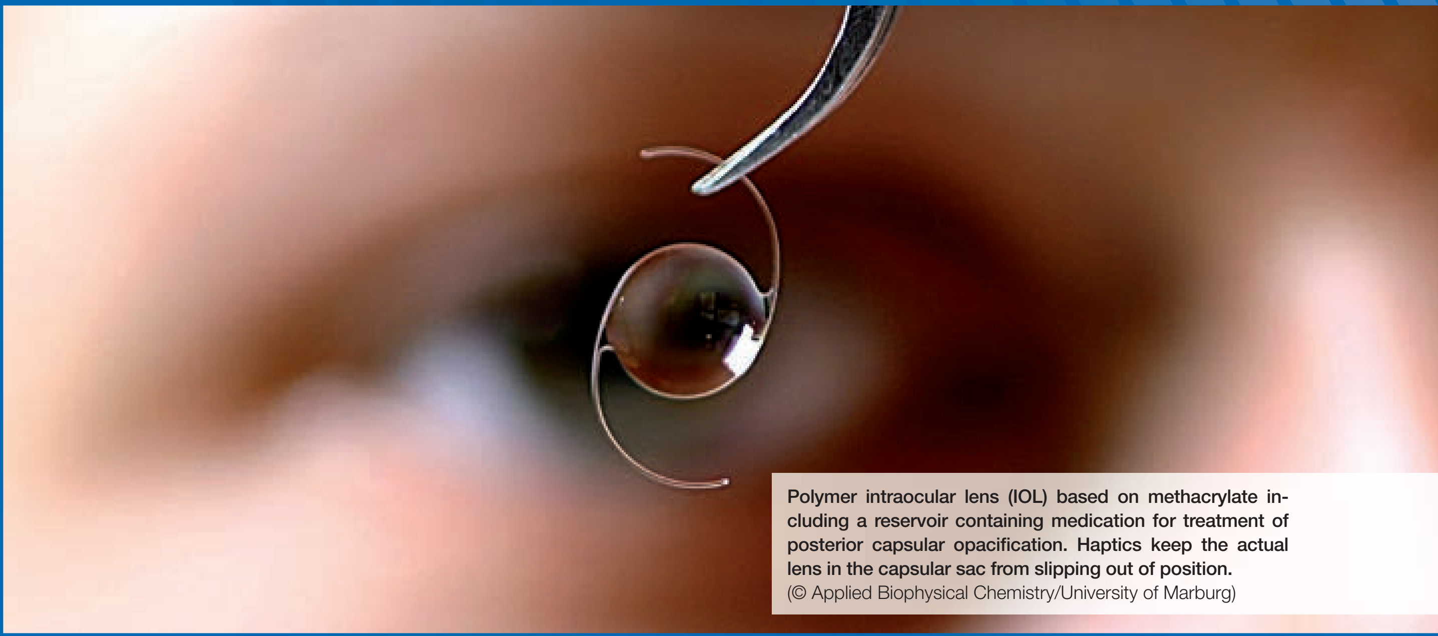
Apart from the established materials, the introduction of new materials will require extensive testing and modifications to existing techniques and methods. Processing of materials that have high melting points as well as reproducible production and reliable characterization of the materials are significant scientific and engineering challenges. Ultra-high temperature compounds like hafnium diboride, hafnium nitride, tantalum zirconium carbide and rhenium tungstide alloy are only reactive above 3000 °C and have low compressibility.

4.4.4.3. Possible approaches and improvement potential

The search for additional precursor-based synthesis pathways for high-temperature materials and continued development and establishment of state-of-the-art compaction and coating techniques could well result in the use of state-of-the-art high-temperature materials in real-world applications. Reactive sintering and plasma spraying are two of the technologies that need further development to get substances which appear to have great potential out of the lab and into actual products.

4.4.4.4. Need for further research

- There is a vital need for basic research on ternary borides, carbides and silicides. Scientists need to understand their mechanisms and electrical properties and determine their resistance to corrosion
- Research in materials science and during mechanical component development is also needed at the interface between synthesis and characterization of new substances to investigate the chemistry and compaction of these substances and their use in coating systems



Polymer intraocular lens (IOL) based on methacrylate including a reservoir containing medication for treatment of posterior capsular opacification. Haptics keep the actual lens in the capsular sac from slipping out of position.
(© Applied Biophysical Chemistry/University of Marburg)

4.5. Materials for Medical Equipment

4.5.1. Current state of technology

Materials made of ceramics, titanium and titanium alloys have been an indispensable feature of medical equipment design for many years. Titanium is often the solution of choice for implants because an oxide layer quickly forms on the implants inside the body, largely preventing an immune response. However, polymer materials are just as essential in modern medicine. Polymers are used in a wide range of products including disposable gloves, bandages, blood bags and syringes as well as contact lenses, dental materials, polymer-based heart valve replacements, ophthalmological implants and suture material. These are just a few examples chosen at random from a very long list of polymer applications in many branches of medicine. In medical applications with the largest market volume, polymers are used primarily as consumables and fabrication material. There is also a trend which has been gaining momentum recently to exploit the biomedical and pharmacological functionalities of polymers in increasingly complex medical diagnostic and therapeutic applications.

Sterile disposables can significantly reduce the risk of infection in nearly all fields of medicine. Blood bags, gloves, sterile packaging, catheters and tubing are just a few examples of products which can easily be disposed of following contact with materials which are infectious or potentially infectious. This has resulted in a major advance in medical hygiene.

Compared to glass or metal, materials made of polymer are much easier to work with because they are plastics. Using simple process techniques which readily lend themselves to mass production, medical items can be manufactured which have a wide variety of shapes and geometries and precisely defined properties. It is very easy to make disposable syringes with low dead volume, breathing (endotracheal) tubes which have the required mechanical properties and complex parts for use in medical equipment.

Besides their medical significance, polymer applications are also economically attractive. A simple, low-cost plastic can be made into a highly valuable and functional product suitable for use in medical applications. Companies with the right technical expertise can mass produce products which have extremely high value-added. There is probably no other area of medical research where innovative resourcefulness and excellent quality play such a vital role in market success.

Materials which come into constant contact with human (or animal) blood or tissue have to meet requirements which are on a totally different plane. In these applications, biocompatibility of the materials is a vital factor. Examples include dialysis membranes made of polymer fibers which enable patients with impaired kidney function to survive for a long time, often with a relatively good quality of life, and polymers in hip implants or artificial intraocular lenses (IOLs) where there is also intensive contact between the polymer materials and the patient's biological system. In the first example, haemocompatibility must be very good but only for a limited time, whereas in the other two examples the implants will ideally remain in contact with the biological system for many years. Careful consideration must be given to what is often a complex set of requirements. The edges of intraocular lenses must be populated with cells to ensure good integration into the eye. On the other hand, the central region of the lens must inhibit cell growth and migration to prevent lens opacification. This can be achieved through location-specific surface modification.

The range of applications is not limited to medical equipment and products. Polymers are also used in many biomedical and pharmaceutical applications. Contact with the human or animal organism is even more intense, because polymers become an integral part of the biological system. One of the first examples of this was the use of polymers like polyvinylpyrrolidone and perfluoropolyethers as plasma expanders during World War II. In the 1970's, polymer-based or polymer-conjugated APIs were introduced for the first time where the polymer was itself the medication or at least acted as the carrier for an API with low molecular weight. Following these pioneering developments, a very large number of materials have been developed for this type of application in recent years. They act as API carriers or masking agents, gene carriers, gene delivery agents and three-dimensional scaffolds in regenerative medicine and controlled drug delivery. Particularly in recent years, trans- and interdisciplinary efforts have created new potential uses for polymers in these branches of medicine, making an enormous contribution to the development of advanced life science applications.

4.5.2. Technological/scientific challenges

Medical applications for polymers have already reached very substantial economic proportions, and they significantly improve the quality of life for many people. What has been done so far, however, is only the beginning. Research over the next few years will considerably expand the range of medical applications for polymers and make a major contribution to personalized medicine, implants and biomedicine.

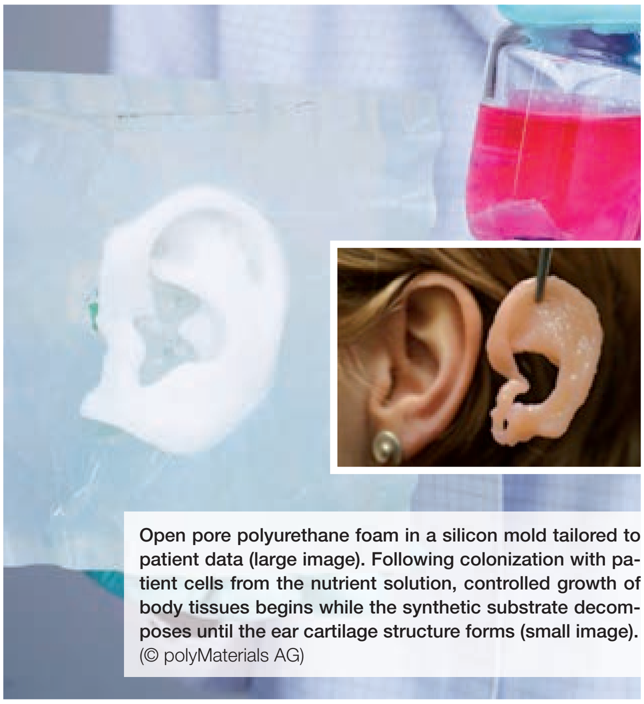
Improved biocompatibility is definitely still one of the big challenges in polymer medical application research. It is a vital factor for all materials which come into direct contact with the human body including polymers used in implants (e.g. artificial blood vessels, heart valves and prosthetic joints) and direct biomedical applications such as controlled drug delivery systems. The polymers must not have any harmful effects on the organism. They must be non-toxic, non-mutagenic and not cause persistent infection. They have to be well tolerated by the body or even better be accepted just like the body's own tissue. Biofilm (fouling) must not form on the surface, and that can be a very difficult challenge during long-term use. The assessment of long-term stability has so far been based on empirical data, and researchers have only very limited ability to predict the long-term behavior of biomaterials.

In many applications, it is quite possible that polymers will only perform a proxy function, taking over a bodily function until body regeneration has advanced to the stage where the body's own tissue is able to perform the function again. Polymer supporting tissue, bone screws and suture materials are a few simple examples of this. In this type of application, the polymer material completely decomposes once it has fulfilled its function and disappears virtually without a trace. In all of these cases, research on suitable biodegradable materials is vitally important.

Production of integrated systems is another major aspect of research on the use of polymers in medical applications. This includes bioanalytical systems such as biochips, cassette-based analysis systems and lab-on-CD platforms where a complete bioanalysis lab is installed on a CD. Another example is the production of implantable microsystems such as implantable insulin pumps, blood pressure meters and brain electrodes. The avoidance of unspecific adsorption is a major consideration in these systems. Miniaturization of implantable sensors and micro devices creates big opportunities for improved personalized medicine in the future. A miniaturized health monitor could be implanted into high-risk patients to keep a constant watch on their medical condition, and in certain critical situations such as an abrupt drop in blood pressure a warning could be automatically sent to a cellphone. From the microengineering perspective, it may not be too difficult to produce the systems, but the biocompatibility of the materials used is still a big problem which precludes routine use.

4.5.3. Need for further research

- Development of polymers with improved biocompatibility for medical applications
- Investigate the molecular and mesoscopic factors which cause the materials to change when they are used inside the organism
- Development of materials with outstanding properties for medical applications which are based on biodegradable substances; targeted control of material decomposition or possibly even inducement of decomposition by external stimulus
- Development of coatings for implanted microsystems based, for example, on biocompatible polymers



Open pore polyurethane foam in a silicon mold tailored to patient data (large image). Following colonization with patient cells from the nutrient solution, controlled growth of body tissues begins while the synthetic substrate decomposes until the ear cartilage structure forms (small image). (© polyMaterials AG)

Organic electronics will make it possible to create new types of totally flexible mobile products for a fully networked world.

4.6. Materials for Information and Communications Technology (ICT)

4.6.1. Organic transistors

4.6.1.1. Current state of technology

Research on organic field effect transistors (OFETs) has been ongoing for 25 years. OFETs are lightweight, compact, easy to manufacture and highly versatile, and they are expected to play a major role in future organic electronics applications, e.g. mounted on PCBs for displays or used as sensors (e.g. "electronic nose"). Printed OFETs are already being designed into portable electronics equipment such as RFID tags.

Because techniques such as printing make them inexpensive to manufacture, they can be used to make low-cost electronics products in all types of applications.

Transistors are functional building blocks found in nearly all electronic circuits, and they play an essential role in sensor systems. They are used to switch or modulate (amplify/attenuate) electrical or optical signals or react to changes in the surrounding environment (sensors). In field effect transistors (FETs), the current flowing through a semiconductor between two electrodes (source and drain) is controlled by an additional voltage at a third electrode (gate) which is physically and electrically isolated from the semiconductor. In OFETs, organic materials are used as the semiconductors.

4.6.1.2. Technological/scientific challenges

In addition to the possible development of low-cost manufacturing techniques for high-volume production, transistors with multiple channels (analogous to CMOS technology) are the next logical step which would enhance the competitiveness of OFETs and give them a solid foothold in the market. One of the biggest challenges is to maximize charge carrier mobility in the transistor when it is in the "ON" state and ensure fast decay of conductivity in the "OFF" state. New functional molecules, new processing technology and component pre- and post-treatment techniques are being developed for this purpose. As is the case with all other electronic components, researchers are constantly trying to make OFETs more rugged and durable.

The key parameters of OFETs are determined by the material properties, the end-to-end production process and the physical design of the device. All of the determining factors are closely related and have a mutual influence on each other. To produce transistors with properties which are tailored to a specific application, there are a number of parameters which need to be optimized. To make compact transistors which have optimal characteristics, the spacing between the source and the drain must be kept as small as possible. Also, the mobility of the charge carriers in the semiconductor should be as high as possible in the "ON" state and as low as possible in the "OFF" state (large On/Off ratio). Over the past 10 years, researchers have succeeded in increasing charge carrier mobility in organic materials by several orders of magnitude. OFETs now have nearly 10% of the carrier mobility of inorganic FETs.[7] However for widespread use in practical application, carrier mobility will have to be better than that, and the components made from these materials will have to be more durable. Researchers are currently working hard to find ways of achieving that. Increasing the detection sensitivity and selectivity of sensors, which are often transistorized, is another research priority.

4.6.1.3. Relevance

OFETs are unlikely to replace silicon-based FETs any time soon in applications with small chip sizes, high transistor densities and high operating frequencies, because inorganic FETs are a very economical option in these applications and development of the technology is significantly more advanced.

In the near future, OFETs will be targeted at other markets. They already have sufficient power and performance for small and medium-size flexible displays and simple RFID components. These are prime examples of markets which will be worth billions in the future. Estimates indicate that the RFID market in the animal, food and agricultural sector (with herd monitoring/animal identification and food traceability, sell-by date and continuity of refrigeration being the two principle applications) will reach roughly 3 billion euros by 2021.[8]

4.6.1.4. Need for further research

More research is needed to substantially improve the charge mobility, on/off ratio, processability from solution (printing), durability, etc. of functional organic materials for OFETs. Vapor deposition of small molecules has produced good results, but systems for processing from solution (printing inks, which are often polymer-based) still need a lot of work in terms of achievable performance. On the other hand, the simplicity and flexibility of processing from solution produces enormous cost savings and the components are cheaper. In addition to continual improvement of semiconductor materials, it is important not to lose sight of the need for extremely efficient insulators (e.g. gate dielectric). The availability of both types of materials is essential for a significant breakthrough. Process development must run in parallel with materials science. R&D is also needed on component architecture which does not necessarily have to be modelled on inorganic FET designs. A much deeper basic understanding of what is taking place inside the components is needed to create a much more rational basis for the ongoing development and improvement process (knowledge-based material and process development).

4.6.2. Organic memory

4.6.2.1. Current state of technology

Research on phenomena such as the ability to switch electrical resistance in polymers into relatively persistent ON and OFF states began back around 1970. The advantages of organic memory were recognized at a very early stage. Printed memory systems are highly versatile, and they are already being used in portable electronics and RFID systems. Cards with re-writeable memory which can be read with handheld consoles have been available since 2009, initially for advertising purposes but they are now used mainly for games applications.

Memory cells have at least two states, namely ON and OFF, which have to be "latched" for a certain period of time. It may be possible to erase and re-write them depending on the component type. An external electric field, which

7 Klauk H., Chem Soc. Rev. 39, 2643 (2010)

8 IDTechEx, $4.09 Billion Market for RFID for Animals and Food in 2021, 15.11.2011

can cause a physical variable (e.g. current flow) to take different states, is normally used to program the memory. In organic memory, this can be done for example by using a ferromagnetic polymer as the active component. The dipole moments of polymer segments can be aligned by the external field to increase or restrict current flow.

4.6.2.2. Technological/scientific challenges

Intensive research on ferroelectric organic memory has taken place over the past five years. There are various component configurations, but ferroelectric capacitors have now almost reached the commercialization stage in the low-end data storage segment. The biggest challenge at the moment is to design configurations which are substantially different and at least to some extent offer much better read, write and service life performance.[9]

4.6.2.3. Relevance

Printed memory is already being used in small, portable applications, especially in the toy and ID market segments. Anti-counterfeiting and intelligent packing, logistics and sensors are the main future target markets. The market for printed sensors or sensors that potentially could be printed is currently worth almost 100 million euros.[10]

4.6.2.4. Need for further research

- *Multi-level* storage to meet the need for higher storage densities
- Increase storage densities by storing multiple bits on one component (this could facilitate commercialization in additional markets)
- Material optimization to improve the ON/OFF ratio, rectification and stability (ON/OFF state retention time and cycling capability)

4.6.3. Organic LEDs

4.6.3.1. Current state of technology

The active optical and electronic elements in OLEDs (Organic Light Emitting Diodes) are partially (or in the best case scenario wholly) based on organic compounds. OLEDs have been around since the mid 1980's. They are extremely thin and produce brilliant colors with minimal energy consumption (at least in theory), making them ideal for today's displays. This innovative technology is already being deployed on a small scale. 30% of all MP3 players along with some cellphone models and digital cameras already have OLED displays. However, a lot of R&D work remains to be done before the perceived advantages can be fully exploited and the technology will be ready for broad-scale market introduction. Efficiency and durability are high on the research priority list.

In addition to flat displays, the applications spectrum for OLEDs also includes large, low-energy illumination. Essentially any color as well as white light can be produced by stacking luminous layers in an OLED.

There are two basic types of OLEDs: SMOLEDs where the active (luminous) layer is made up of small molecules and PLEDs which are polymer based. Production of SMOLEDs normally requires specialized vacuum manufacturing techniques for vapor deposition of the functional molecules. Highly pure active layers can be produced, enhancing efficiency and service life, but the production process is more expensive and less flexible compared to other, simpler manufacturing techniques, especially processing from solution. As a general rule, SMOLEDs are inflexible. Because polymer compounds cannot be vaporized and have excellent film formation properties, PLEDs can be produced from solutions or dispersions. Without the need for expensive vacuum equipment, semiconductors and light-emitting materials can be directly applied to, for example, flexible substrates, in the simplest case using commercially available inkjet printers. PLEDs can potentially be produced at low cost on flexible substrates, creating new opportunities for imaginative lighting and design.

9 Naber R.C. D. et al., Adv. Mater. 22, 933 (2010)

10 Organic and Printed Electronics, 4th Edition, 2011, OE-A Organic Electronics Association, VDMA, Frankfurt

4.6.3.2. Technological/scientific challenges

Relatively low material purity causes big problems at the component level during PLED production. Critical contamination is often inadvertently introduced along with the polymer and solvent. The contaminants cannot be subsequently removed and are hugely detrimental to component durability and efficiency. The additional cleaning step, which is not a problem with the small molecule vapor deposition process, cannot be performed in a solvent-based process. This is an area where there is plenty of room for improvement.

In general when talking about OLEDs, it is important to distinguish between displays and lighting applications, because there are significant differences in production, utilization and cost. OLEDs are a relatively new technology, and many aspects are still evolving. As a result, there are many significant challenges still awaiting resolution which are vital to future success.

Some of the current difficulties and limitations of OLED lighting are as follows:

- Low device efficiency (compared to conventional and LED lighting)
- Problems with the uniformity of the light-emitting layers on large surfaces
- Problems in maintaining high current flow on large surfaces
- Poor operating lifespan of various emitter materials
- Poor component shelf-life and poor component lifespan in long term operation
- Complex component design due to the limited selection of electrode materials available
- Low-cost production techniques not yet established for large OLED devices
- Device decomposition under exposure to UV radiation
- Utilization of the triplet states, which are electronically far more probable, to produce light instead of non-radiative deactivation which does nothing more than generate heat in the component

The Merck chemical research center in Darmstadt has one of the largest OLED displays with 9 sqm screen.
(© Merck KGaA, OLED Business Unit)

4.6.3.3. Relevance

A substantial portion of the energy consumed worldwide is used for lighting (> 2600 TWh). That figure equates to roughly 19% of electricity generation. Energy consumed for lighting translates to about 1,900 million tonnes of carbon dioxide emissions per year. It is estimated that energy-efficient lighting (mainly OLEDs and LEDs) would reduce energy consumption by about 40 % compared to current lighting technology. That would cut CO_2 emissions by more than 640 million tonnes per year.

Turnover in the European lighting industry is expected to exceed 3 billion euros by 2019, creating 115,000 new jobs between now and then. The expectation is that growth will be driven by the new OLED technologies and above all by the design, production and sales of OLED-based lighting. Current forecasts indicate that worldwide turnover in the OLED industry will increase to around $6 billion by 2015.[11] The ban on conventional incandescent light bulbs in Europe and the US and the increasing level of criticism directed at low-energy light bulbs are expected to promote growth.

Implementation of active matrix technology in OLEDs has stimulated substantial growth in the worldwide market (currently estimated at 1.6 billion euros) for printed or potentially printable OLED displays. Growth is expected to continue, with turnover rising to more than 13 billion euros by 2021.[12]

Successful OLED product and OLED display development depends largely on an iterative process involving the entire value-added chain “from the material to the product”, in other words material development, systems technology, device production, product integration and application development. Production and process engineering development will make an important contribution.

4.6.3.4. Need for further research

Further R&D is needed on various aspects of OLED technology including materials, devices, systems, standardization and production. The details of these activities are presented in the technology roadmaps of various interest groups and platforms.[13]

Development is currently focused on three key aspects of OLED lighting technology:

- Better OLED performance
  - Increased power and efficiency (20 – 40 lm / W in 2010)
  - Better light extraction and coupling (1000 – 3000 Cd / m2 in in 2010)
- Longer OLED lifespan
  - Improved reliability (5,000 – 20,000 hours at 1000 Cd / m2 in 2010)
  - Better encapsulation
- Price reduction (currently > € 1,500 pro m² in 2010)

11 OLED Lighting: An Eight-Year Market Forecast (2010), Nanomarkets
12 IDTechEx (2011)

A major effort will be required in Germany to gain scientific leadership in specific aspects of the technology. It is important to push R&D to the point where the technology can be turned into marketable products. The emphasis should be on the following:

» New materials such as high-efficiency emitters (particularly deep blue); new charge carrier and injection materials are needed for high light yield, and these materials must be particularly well suited or optimized for high-speed production (printing) or vapor deposition (good temperature stability) at high temperatures

» New materials and formulations to reduce production throughput times

» Materials with better electrical conductivity for production of thicker layers (more rugged devices)

» Develop techniques for applying coatings to large surfaces, use R2R (roll-to-roll) technology to significantly reduce investment and labor costs and increase process reliability in OLED production by, for example, a factor of 60 between 2011 and 2015.

» Develop new materials which are more resistant to degradation caused by water, oxygen and UV radiation, and develop new encapsulation materials for OLEDs

» Cost-effective alternatives to indium tin oxide (ITO), transparent electrode materials and low-cost substrates for OLED lighting, for example (a) transparent, conductive oxides (TCOs), (b) conductive polymers, (c) nanomaterials made with conductive nano wires (metallic nanowires and CNT) or graphene.

To make OLED R&D and implementation more effective, the organizations which have the necessary expertise in basic and applied research and materials, device and process development will have to work closely together and place significant emphasis on production and process engineering development, quality assurance and standards development. Any gaps in the knowledge base or the value-adding chain will delay the transfer process.

13 [A] Organic and Printed Electronics, 4th Edition, 2011, OE-A Organic Electronics Association, VDMA, Frankfurt

[B] Strategische Forschungsagenda für Organische und großflächige Elektronik, Für grüne Elektronik aus Deutschland, 2009, VDI-Technologiezentrum GmbH, Düsseldorf

Forschungsagenda OLED-Beleuchtung, Seite 19

Forschungsagenda OLED-Displays, Seite 33-34

[C] Towards Green Electronics in Europe, Strategic Research Agenda – Organic & Large Area Electronics, 2009

[D] Photonics Technologies and Markets for a Low Carbon Economy – Energy Efficient Lighting and Displays Technologies and Applications, 2011, European Commission

Protection of critical infrastructure is important to ensure public safety. Advances in materials science and analysis technology increase protection efficiency.

4.7. Materials for Security Systems

4.7.1. Detection systems

4.7.1.1. Current state of technology

The role played by chemical analysis in security systems should not be underestimated. It can be used to detect dangerous hidden substances before they can cause harm. Chemical analysis plays a vital role in preventing injury or damage and deciding what to do next in case of emergency. Protection systems must cover a broad range of possibilities and cannot be limited to selected substances.

Under the assumption that fabrication and placement of IEDs (improvised explosive devices) leave traces on the exterior, highly sensitive analysis techniques can be used to detect the devices unless they were made with extreme care and were then thoroughly cleaned. The high sensitivity of ion-mobility spectrometry (IMS) is the reason why it is probably the most widely used technique for detecting groups of substances in practical application.[14] Non-contact laser-based spectroscopic techniques used to detect trace substances on surfaces, laser-induced breakdown spectroscopy (LIBS), Raman spectroscopy[15] and IR laser backscatter work without the need to take samples.

Some analytic techniques work, generally speaking, by binding substance molecules to a surface inside a measurement instrument and then detecting the physical changes which take place. These techniques can be highly sensitive and selective even if only a few molecules are bound to surface receptors based on the lock and key principle. The contribution from chemistry in these systems is production of the coatings. Natural antibodies are also used for this purpose. That, however, has the disadvantage that the proteins involved have limited longevity. Molecular imprinted polymers (MIPs) appear to overcome that problem, but further development work will undoubtedly be needed.[16] MIPs can be used as receptors on physical sensors or for enrichment in an airstream. When heating is applied, the enriched substance can be de-absorbed again and directed towards an unspecific sensor. Zeolites and MOFs (MetalOrganic Frameworks) can also be used as specific adsorber materials in these applications.

14 G.A. Eiceman, J.A. Stone, Analyt. Chem. 2004, 391 A – 397 A, kommerziell angeboten u.a. von Bruker oder Smiths Detection
15 J. L. Gottfried et al., Anal Bioanal Chem (2009) 395:283-300
16 G. Bunte et al., Propellants Explos. Pyrotech. 2009, 34, 245-251 und J. Saloni et al., Polymer 52, 2011, 1206-1216

Even if a trace is detected, that does not necessarily mean the larger amounts of the substance are present. For example small amounts of an explosive are not dangerous, but the large amount which is normally hidden creates a huge risk. Because there is a real risk of triggering an explosion if the hiding place is opened, radiological techniques are the solution of choice for detecting and neutralizing the real source of danger. X-ray generators and image detectors are commonly used in these situations to inspect the items, and digital technology is making increasing inroads in these applications. A simple X-ray image, however, does not reveal much about the chemical composition of the items which have been inspected.

4.7.1.2. Technological/scientific challenges

There is a difference between trace detection, which indicates that large amounts of an explosive may be present, and confirmation that a lot of the explosive actually is present (which is of course the real risk). Trace analysis indicates that a certain type of explosive is present. Like explosive sniffer dogs, it warns of danger. Based on the results of trace analysis, closer inspection can be carried out on a piece of luggage or a container.

Protection of critical infrastructure such as the air traffic system is a very important aspect of public safety, but the security systems have to function as intended. There will be problems if the detection equipment generates too many false alarms. Air traffic operations must continue as normal without excessive interruptions. Development of remote detection technologies currently poses one of the biggest challenges in chemical analysis. Spectroscopic techniques such as laser-induced breakdown spectroscopy (LIBS) and Raman spectroscopy could well provide the answer.

The sensitivity and specificity of gas phase trace analysis can be improved right from the time when the sample is being taken. An enrichment step, in which the gas stream containing the target substance flows across an adsorbing surface, can enhance sensitivity. If only specific molecules are adsorbed by the surface, specificity improves as well. A desorption step is performed when the enriched substrate is introduced to the actual analysis stage. The simplest way of doing that is heating. This preliminary step can be used to good effect in combination with ion-mobility spectrometry (IMS). From the chemistry perspective, the engineering / scientific challenge is to design absorbent coatings for specific enrichment which are also able to withstand the desorption step. Fragile molecules such as antibodies are unsuitable for coatings which adsorb specific substances. Polymers such as MIPS (molecular imprinted polymers) which are better able to withstand heating for desorption are the better choice. This specific enrichment technique can also be applied when textiles are used to take swipe samples. The target material can be heated for analysis in a spectrometer. The analyte, the operating environment and all other materials which are present are key factors which need to be considered during development of adsorption coatings and wipes.

Efficiency, and at some point in time cost as well, will inevitably become major considerations when a routine analysis process is set up or new methods are introduced. The expectation is that nothing will be missed but no false alarms will be generated. The latter becomes increasingly probable as the sensitivity of the detection methods continues to increase. False alarms are particularly unwelcome during routine security checks at airports because they bring operations to a halt, create the need for additional measures to be taken and cost money. To make things even more difficult, the target substances are rarely present in a pure state. Other substances are present as well, and they can generate an analytical signal which is superimposed on the signal from the target substance, effectively masking it. In addition, some analysis techniques do not have sufficient specificity to distinguish between the target materials and similar or related materials. If a hazardous substance can be confused with something else which is harmless, it is highly likely that the harmless substance will be used to mask the dangerous material.

4.7.1.3. Need for further research

Suitable analysis standards and calibration reference materials will have to be made available. Because hazardous substances are involved, only very small amounts (as long as they are not toxic) or surrogates can be used in practical application to ensure safe handling of the samples. When surrogates are used, they must exhibit the same behavior as the real substance. Because different methods react to quite different properties of the substance, it is very likely that different surrogates will have to be available for the same original substance depending on which method is used. When only the elemental composition is involved as is the case in multi-energy radiography, it is relatively easy to provide a model substance. However, this will probably only be the case for relatively unspecific analysis techniques. The situation is different for highly-specific separation or adsorption techniques, and this undoubtedly is an area where a lot of research will be needed. In trace analysis, the problem of quantification can become quite serious during equipment setup. The long-term stability of volatile substances can be particularly troublesome. A substrate also has to be selected for gas phase detection. Researchers are attempting to simulate a dog's nose for ambient air analysis. Chemists will have to develop adsorption coatings which will be applied to the surface of sensors. These coatings will determine the specificity of the sensor system, similar to antibodies in physiology. If preparation of the test samples is necessary, the process should be miniaturized down to chip-size scale (lab on a chip). The "wet processing" aspects belong to the realm of chemistry.

The specificity of ion-mobility spectrometry (IMS) can be improved mainly by combining it with other techniques. That is the only way in which the unsurpassed sensitivity of this method can be fully utilized. This can be done using the specific gas phase enrichment technique as described above, and the same approach can undoubtedly be extended to a range of other substances which are being analyzed for the first time or which can be present with various other substances in different ways.

Research on other types of radiation such as neutron imaging is needed to improve substance detection in high-energy radiographic scanners used to inspect luggage at airports, etc.

So progress will be achieved both by improving and refining existing methods and by introducing entirely new techniques. Reliability in practical applications is a top priority, and issues such as measurement uncertainty need to be addressed.

4.7.2. Personal protective gear

4.7.2.1. Current state of technology

In textile-based ballistic protection, a distinction is made between stab protection, projectile protection and shrapnel protection. Hard body armor consisting of a polymer or ceramic matrix and high-strength fiber materials, soft body armor made up of many layers of fibers (e.g. aramids) or specially designed clothing can be worn depending on the application. The physiological aspects (heat and moisture transport/storage and UV protection) and easy care of the clothing are two of the big challenges. Some of the options include highly-stretched membrane systems, block copolymer systems and hybrid systems produced with electrospinning.

4.7.2.2. Technological/scientific challenges

Materials used to provide personal protection against various hazards are categorized by what they are used for, e.g. blast wave shielding, impact protection, body armor to protect against projectiles and stabbing, etc. They may have to be tear-proof or act as a heat shield. If they are worn, they have to be lightweight, not trap body heat and as far as possible not restrict body movement. Obviously, these are conflicting requirements. Adequate protection must also be provided if persons are exposed to chemical, biological, nuclear or radioactive hazards. In contrast to shrapnel protection or a protective vest, this means whole-suit, gas-tight protection.

One of the biggest challenges is to develop simple, automated manufacturing techniques for the production of low-cost systems which provide a maximum level of protection.

4.7.2.3. Need for further research

- The correlation between ballistic protection and the structure of the protective material (microstructure, the architecture of a composite system, hard-plate, backing) requires further investigation
- Improve the ability of ceramic protection systems to take multiple hits
- Bring down the cost of producing CMC materials (Ceramic Matrix Composites) by a substantial margin to enable use in protective clothing on a large scale

New detection systems help enhance the speed and efficiency of security checks.

State-of-the-art plastic packaging keeps food fresh longer. Selling grapes in trays or bags has reduced the amount of spoilage in the markets by 20%.

4.8. Materials for Consumer Goods

Consumer Goods include materials and objects which are intended to come into contact with food. Consumer protection regulations require that these materials and objects must not pose a health risk to consumers, and no substances may be assimilated into food items which could impair the quality of the food.

Other products that come into close contact with the human body such as toys, textiles, jewelry, wigs, cleaning agents, impregnation and finishing agents and air fresheners are also consumer goods.

Materials used to produce consumer goods must meet strict health and technical criteria.

The technical criteria refer to the mechanical and thermal stability of the material including the requirement that the materials be hygienic and chemically inert.

Chemical and technical suitability are closed related.[17]

The following four types of materials are used to produce consumer goods:

Silicate materials:	glass, ceramics (earthenware, porcelain)
Metallic materials:	aluminum, steel, copper
Paper, corrugated board and paperboard:	dried fibrous material, mostly of natural origin, with a wide variety of additives
Macromolecular materials:	thermoplastics (semi-crystalline and amorphous)
	thermosets
	elastomers and rubber
	coatings
	(film) composites

All of these materials are also used as fibers to produce semi-finished textiles.

17 Frede, W. (Hrsg.): Handbuch für Lebensmittelchemiker, Kap. 38, 3. Auflage, Springer-Verlag Berlin Heidelberg: 2010

A large range of macromolecular materials can be used to make consumer goods. No other type of material has gone through such extensive development in recent years. The advances were made possible by chemical research on precursor synthesis and material production.

4.8.1. Food contact materials and articles

4.8.1.1. Current state of technology

Ceramic and metallic materials are currently used for many different types of reusable drinking vessels and cutlery. It is also hard to imagine a world without plastics (e.g. macromolecular materials). These materials in particular have many, many properties which make them ideal for consumer goods:

- low density and heat conductivity
- good mechanical stability
- good electrical insulation
- good impermeability
- broad temperature range
- excellent processability
- can be used in many combinations with other materials

Plastic packaging is truly high-tech. Packing performance continues to improve despite a reduction in material s consumption. By making the walls thinner, producers are continually reducing the weight of plastic packaging items such as foil, yogurt cups, paint buckets, bottles and packaging for detergents and cleansers.

The entire range of polymer materials is used for some types of packaging ranging from polyolefins for foil and other types of packaging, PVC lamination film for cardboard, polyvinylidene chloride in composite foil and polyethylene terephthalate for beverage bottles.

Active packaging keeps food fresh until it is consumed. Oxygen scavengers, for example, absorb oxygen to extend the shelf-life of the food product. Intelligent packaging can provide information to the consumer about product shelf-life or freshness. Freshness indicators show whether the product is still fresh or whether the product has not been kept refrigerated at some point.

Most carbonated soft drinks in Germany are now packaged in PET bottles rather than glass bottles. PET bottles are also being used for many other beverages. PET bottles enhance consumer convenience because they are lightweight and not prone to breakage. Low weight also reduces fuel consumption in the distribution network. In addition, PET bottles can be recycled or upcycled (i.e. textiles can be produced with polyester fiber made from recycled PET).

4.8.1.2. Technological/scientific challenges

Possible heavy metal contamination from PET bottles has been the subject of public and government policy debate on many occasions in recent years. Although it is true that PET can release trace amounts of antimony, the low concentrations involved are currently believed to be harmless. Nonetheless, reduction or elimination of antimony and the development of alternative catalysts which do not contain heavy metals play an important role in efforts to enhance the sustainability of PET bottles.

Natural product chemistry offers a large number of reagents. Food packaging must remain inert in the presence of many different types of reagents. It must not release substances which alter the food by reacting with it, and it must not absorb volatile flavor compounds from the food or allow them to escape. The dream would be to combine the barrier properties of glass and porcelain with the technical advantages of plastics and metal in a recyclable material. The challenge is to find the best engineering/scientific compromise for the different types of food.

4.8.1.3. Need for further research

In order to preserve the quality and shelf life of food products, more effort will be needed to find very intelligent ways of tailoring the properties of materials which come into contact with them. The improvement of diffusion barriers and layers to enhance gas permeation performance will necessarily be one of the priorities.

Safety is another aspect where there is a lot of room for future research. Sensors can be used as food freshness indicators.

Given the great variety of foodstuffs, models are needed to investigate the interactions between a given material and the different types of food. Further development work is needed on the models which are used to verify the food compatibility of different materials. Simulation up to this point has been one-sided, focusing on migration of the material into the food. No models exist to simulate the loss of aroma compounds or other food constituents through contact with a material.

Recycling may be good for the environment, but there is a risk that material which is reused may contain contaminants which are impossible to define. Barrier layers in the packaging are intended to prevent direct contact between the food and recycled materials which may be unsafe. Further research is needed on the permeability of plastic foil to a wide range of contaminants.

More work is even needed on tin cans despite the fact that 2013 is the 200th anniversary year for this type of packaging. The inner linings effectively delay corrosion but they are not sufficiently protected from interaction with food.

4.8.2. Plastic packaging

4.8.2.1. Current state of technology

Polymer-based, functionally optimized packaging, ranging from simple carrier bags, plastic bags and PET bottles to multi-functional, multi-layer foil is an achievement of the modern industrial society. In Europe alone, around 18 million tonnes of plastic packaging were produced in 2009[18]. With the exception of paper, paperboard, etc., most polymer-based packaging is made almost exclusively from fossil resources. Polyethylene (PE), polypropylene (PP) and Polyethylene terephthalate (PET) are the principle plastic packaging materials.

4.8.2.2. Technological/scientific challenges

Despite the many advantages in terms of shelf life, hygiene, warehousing, logistics and of course convenience, there are sustainability issues which need to be addressed. Packaging polymers are extremely long-lasting under normal environmental conditions. They should not end up in landfill sites or the natural environment. Incineration is the best option for generating power at end-of-life, but CO_2 is released in the process and because the plastic is fossil-based there is a net increase in atmospheric CO_2. Re-use is the best solution followed by recycling which, however, results in material degradation and ultimately makes it necessary to revert to one of the other two options.

18 PlasticsEurope - Association of Plastics Manufacturers: Plastics – the facts 2010. An analysis of European plastics production, demand and recovery of 2009. www.plasticseurope.org

4.8.2.3. Possible solutions

Bioplastics are becoming an increasingly viable alternative to energy recovery and recycling. They are biodegradable (but are not necessarily made from renewable resources) or they are made from renewable resources or both. Governments (e.g. ban on plastic carrier bags in Italy, EU bio-based products lead market initiative) and industry are currently addressing both aspects, with increasing emphasis on bio-based materials. For years, BASF has been making Ecoflex, a fossil-based biodegradable polyester which is often used as a blending component in starch-based garbage and carrier bags. Operations recently started up at a new 60 kt plant. Coca-Cola introduced a "plant bottle" in 2009 made of PET with a bio-based ethylene glycol component (roughly 30% of the total polymer mass is bio-based). Danone recently began packaging its Activia yogurt product in a cup made of polylactic acid (PLA) which is a bio-based, biodegradable aliphatic polyester. Besides starch, PLA is the most widely-used bioplastic for industrial applications. Annual worldwide production is around 210 tonnes[19]. Growth in the global bioplastics market is currently in the double-digit range[20], making an important contribution to the sustainable society. Existing products have not by any means reached the market saturation point.

Polylactic acids (PLA) are polyhydroxy carbonic acids, and they are a major type of bioplastic. The properties of PLAs depend largely on molecular mass, crystallinity and, as the case may be, the proportion of comonomers. Polylactic acids have a number of properties which have advantages in many applications such as sportswear and functional wear, textiles, interior and exterior furniture and lightweight design.

4.8.2.4. Need for further research

In order to make further advances in bioplastic technology and gain a foothold in other market segments, more work will be needed to expand the property spectrum of bioplastics.

The ability to act as a barrier to gas and liquids is a key property in one segment of the packaging market. Packaging fresh fruit and vegetables in PLA film and trays is not a problem, but the same is not true for applications where higher gas and water barrier protection is needed[21]. Optimization of gas and water barrier protection for the specific application is an absolute research priority for PLA and other bioplastics.

Further work is also needed to optimize the production process for bioplastics to bring down the costs.

19 Estimate Fraunhofer IAP December 2010

20 http://en.european-bioplastics.org/market

21 E. Almenar, R. Auras: Permeation, Sorption, and Diffusion in Poly(lactic acid). Poly(lactic acid): Synthesis, Structures, Properties, Processing, and Applications. Edited by R. Auras, L.-T. Lim, S.E.M. Selke, and H. Tsuji, Wiley, 2010, 155-179

4.8.3. Textiles

4.8.3.1. Current state of technology

Textiles are fiber-based fabric materials made of natural fiber (e.g. wool or cotton) or synthetic fiber. The route to the end garment is as follows: yarn spinning, fabric weaving, dying / finishing and apparel manufacturing. The mechanical, physical and chemical properties of woven fabrics can be regulated over a wide range (elastic to stiff, water-proof and hydrophobic to porous and hydrophilic, etc.). The properties depend on the fiber materials and the production process. The main applications for consumer goods are clothing, home textiles and hygiene and medical articles. Organic synthetic fibers are based on natural polymers (cellulose or cellulose regenerate fiber, and in particular viscose fiber) or synthetic polymers. Polyesters, polyamides and polyolefins are the most prevalent varieties (especially PET, PA 6 or PA 6.6 and PP). A variety of other polymers such as HD-PE, high-temperature polymers including PEI, PEEK and others, fluoropolymers (e.g. PVDF) and bio-based polymers (PLA, PHB, Chitin, etc.) are used in technical and/or medical applications. Organic-based high-modulus fibers including aramid and carbon fibers play an important role in lightweight design and industrial applications. Glass, basalt, ceramics and metals are inorganic fiber materials which are used in technical applications. Spandex fibers are block copolymers made up of polyether segments or polyurethane sequences. By combining stiff and elastic blocks, extremely high elasticity (>700%) can be achieved.

The requirements profile for modern fibers includes mechanical strength, modulus of elasticity, elongation and elastic properties / return to original shape, physiological aspects of clothing (heat insulation/ transport, moisture transport), dyeing characteristics, abrasion resistance, UV resistance, resistance to alkalis or acids and biocompatibility. In the production of polymer-based chemical fiber, the following parameters are of vital importance to obtain the desired characteristics profile during use: transition temperature (glass transition, melt temperature), crystallinity and orientation of the molecule chains. The fibers are characterized by type of polymer, fineness (diameter), fiber cross-section, stretch, thermo-mechanical and thermal properties, water absorbency and dyeing characteristics.

4.8.3.2. Technological/scientific challenges

Some branches of science and technology have recently emerged or have experienced substantial development in parallel with the upsurge in the chemical fiber industry. This includes linear organic high polymer chemistry and fiber physics as a branch of high polymer physics. In process engineering, there was also a need to move into unfamiliar territory. Chemical fiber manufacturers design and produce some of the machinery and systems which are used to manufacture chemical fiber, with the rest coming from the machinery manufacturing industry.

Chemical fiber producers have an in-depth understanding of the process engineering aspects, the production equipment, the problems involved and ways of resolving those problems, and that is a vital aspect of their core expertise. Most of this expertise is described in patent documents, but after reading the documents it is often difficult to figure out exactly what the fiber producers are doing. The following list summarizes the essential requirements for polymer fiber materials:

- The polymer must be linear. There must be little or no branching in the molecules, otherwise spinning is difficult and drawing does not produce good orientation. For the same reason, the molecular weight should be at least 10,000. Also, the final product is not strong enough if the molecular weight is too low. There is insufficient cross-bonding between individual molecular chains and the adjacent chains which would prevent slippage under tensile load. In practice, the molecular weight is normally substantially higher than the minimum.
- The chemical structure and steric configuration of the molecular chains must allow cross-bonding between the chains. The molecule should not have any side groups which protrude so far that they inhibit tight packing (strength).

- The melting point or polymer degradation temperature (if lower) has to be high enough. Both depend on the chemical structure. The melting point also depends to some extent on the molecular mass and the crystalline structure of the fiber.
- The polymer must be suitable for spinning, i.e. the melt or solutions must be filament-forming. For this to be the case, the surface tension and melt/solution viscosity must be above and below certain values. Excessively low surface tension and viscosity inhibits filament formation. Excessively high surface tension and viscosity lead to melt fracture.
- The polymer should have maximum resistance to radiation and all types of chemical substances.
- It is very important that high polymer fibers for clothing and home textiles have good dyeing properties and are easy to care for.

Processing of standard polymers is particularly relevant. Individually modified and functionalized additives combined with appropriate process management strategies are used to create special property profiles. Examples include conductive polymers, piezoelectric polymers, photovoltaic polymers, integrated ingredient systems, etc. Another approach is based on the chemical modification of polymers which, for example, are processed using solvent spinning. The objective is to optimize material quality and processability. Precursors for carbon fibers, viscose-based fibers and polyurethanes are examples of this. With post-cross-linking polymers, cross-linking is activated after the spinning process, and improving the processability of these polymers is a challenge which still needs to be addressed. Aramids and the precursor materials are examples of this.

There is also a number of other challenges which need to be addressed starting with textile chemistry and the auxiliaries which are used in the textile production process to improve processability (tribologic and antistatic properties and resistance to mechanical stress). There is also work to be done on usability aspects: dirt-repellency, flame retardance, UV resistance, dyeing and coloring properties, anti-static and anti-bacterial properties, functional integration (physical, chemical, electrical/electronic) and smart textiles.

Economic considerations are another factor which determines whether a polymer is a suitable material for chemical fiber. This includes the availability of precursors and the cost of producing the starting material and converting it to fiber. Disposal and environmental problems are additional cost factors.

At present, polymer fiber is primarily based on petroleum chemistry. The limited availability of process routes and the high process costs currently impede migration to biological starter materials. The property profiles of biopolymers are not yet fully on par with those of established petroleum-based polymers. Cellulose and cellulose regenerate fiber (and in particular viscose fiber) are the exception among the polymers which are made from renewable resources.

4.8.3.3. Need for further research

Highly interdisciplinary, broad-based research will be needed to tackle the scientific challenges and provide solutions for state-of-the-art synthetic fabric applications. Continued advances in nanotechnology and a better understanding of molecular mechanisms in biology, medicine, physics and chemistry are blurring the traditional boundaries between the different scientific disciplines. New advances in material developments create pathways to active materials systems with functionality that was previously limited to living organisms.

Researchers will be working on the development of specialized fiber materials for lightweight design, medicine and the life sciences, smart materials, construction, energy harvesting/conversion, etc. The scope will include basic materials properties, process technology and interface/finish design. The primary research needs are as follows:

- Integration of nanoparticles as functional fillers, or bonding of nano-scale particles onto surfaces. Dispersion in the polymer and a reduction of the agglomeration tendency are the challenges which need to be addressed. The goal is to significantly improve the strength, modulus and resistance to dirt, UV radiation and abrasion
- Material models and modelling of processing behavior, e.g. for high-performance fibers with embedded nano-particles. Nanoparticles can be used to manipulate specific properties of the fibers only if the interrelationship between the process technology, the internal microstructure and the embedded nanoparticles is sufficiently understood
- Functional integration: sensors, fiber optics, actuators: e.g. modification of the polymer or management of the extrusion process, etc. to add piezoelectric, photochromic or electrochromic properties to fiber materials
- Production of nano-scale fibers, e.g. for medical and filtration applications
- Processability and product properties for bio-based polymers, chemical modification of biopolymers
- Development and production of integrated, functional layers and structures on textiles
- Development of functional materials adapted for textiles
- Wet chemical modification of fiber and textile surfaces
- UV treatment of surfaces, plasma treatment of textiles and fibers, electron beam treatment of textiles and fibers, boundary layer design
- Regenerated cellulose fiber: use of ionic liquids, reduction in the cost of the chemical pulp

To an increasing extent, interdisciplinary research teams will be brought together to work on the tasks listed above as well as other challenges which arise in the future The basic disciplines in chemistry, process engineering, textile technology and production technology will be heavily involved.

4.8.4. Detergents and cleaning agents

4.8.4.1. Current state of technology

The formulations for detergents and cleaning agents contain a number of different chemical products. The list includes surfactants, complexing agents, bleaching/optical brightening agents, alkalis or acids, dispersants, solvents, abrasives, enzymes, hydrotropes, corrosion inhibitors, colorants, thickening agents, preservatives and fragrance compounds.

Much of the development work in the industry is currently focused on sustainability and environmental protection. Because the products are disposed of as domestic waste which is emptied into municipal sewers, they can eventually be returned to the drinking water supply chain.

Surfactants are only fully effective in soft water, so a water softener has to be added to detergents. Phosphates were used for that purpose in the 1980’s but that led to eutrophication of rivers. Zeolites, citrates or phyllosilicates are now used in combination with polyacrylates to achieve the same purpose.

European market demand for polyacrylates which are used in detergents alone is in the region of 90,000 t/a. From the ecological standpoint, polyacrylates are relatively benign because they have low aquatic toxicity and adsorb to activated sludge.

Together with the zeolite, they can be extracted from the wastewater stream using activated sludge. Polyaspartic acid derivatives are a biodegradable alternative to polyacrylates. An eco-friendly complexing agent was developed during R&D work on the polyaspartic acid production process. The iminodisuccinate is also biodegradable, and as is the case with polyaspartic acid it has a good overall eco-toxicological profile.[22]

Detergent enzymes act as catalysts and break down natural stains. Despite the fact that only small amounts of enzymes are used in detergent formulations, enzymes play a vital role in today's detergents. The highly specialized biomolecules are very effective in removing specific types of spots and stains from the wash. Because they are activated at low temperatures, they reduce the washing temperature and thus energy consumption. Greenhouse gas emissions are lower, and consumers also save money on their electricity bills. Enzymes are also completely biodegradable. Proteases, lipases, amylases, cellulases, mannanases and pectate lyases among others are used in detergents.

These enzymes primarily break down proteins and are effective in removing stains left by eggs, milk, chocolate and mash potato residue or fat, and they also remove make-up and sun cream stains.

4.8.4.2. Technological/scientific challenges

It has been a legal requirement since 2005 that all surfactants used in detergents and cleaning agents have to be rapidly and fully biodegradable. Microorganisms are used in multiple stages for final biodegradation of surfactants. Only water, mineral salts and carbon dioxide remain at the end of the process. The bacteria also proliferate in the sewage treatment plants, and the activated sludge becomes "biomass". An increasing number of surfactants are being developed which are based on renewables such as palm kernel oil, coconut oil, sugar and starch. The search for alternative surfactants which deliver better performance continues.

New foods subjected to even more intensive processing are creating new challenges because they can cause new types of spots and stains in textiles. This creates the need for new detergent performance profiles.

4.8.4.3. Need for further research

The discovery of archaea bacteria presented the detergent industry with a new and potentially useful class of active agents which merit further intensive investigation. They have exceptional thermal stability because they have a large number of coordinate bonds which stabilize their molecular structure.

A significant need for research exists for the following processes and materials:

- Further compaction to reduce shipping & packaging requirements
- Improved performance at low temperatures
- Increased use of renewable resources
- Hygiene at low temperatures
- New sources of raw materials for renewable surfactants which do not compete with the food supply
- Polymers which have textile benefits (e.g. improved elasticity, color retention, easy iron)
- White biotechnology to develop more efficient enzymes and biosurfactants and also to improve production efficiency
- Ensure enzyme and bleach stabilization

22 http://www.baypure.com/imperia/md/content/fcc/baypure/friedrich_woehler_preis.pdf

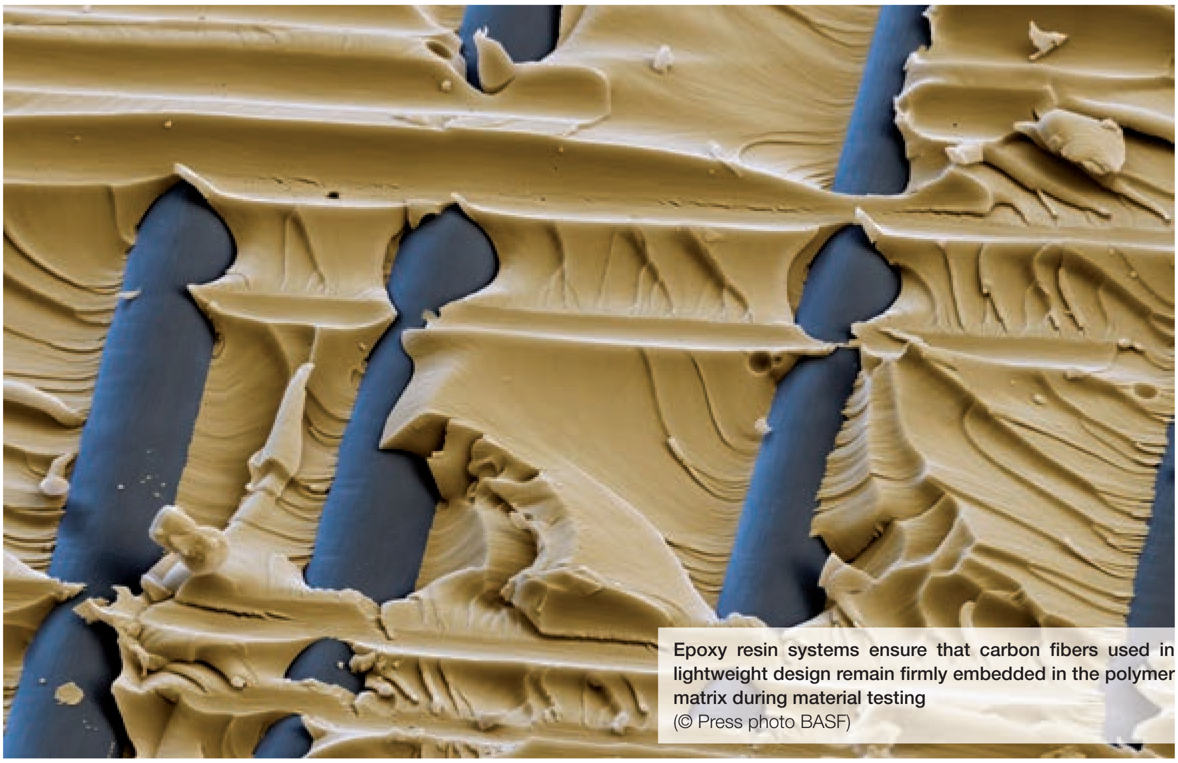
4.8.5. Adhesives

4.8.5.1. Current state of technology

Very few consumer goods are made of just one material, so in many cases there is a need to find ways of joining the different components. Adhesives are increasingly becoming the solution of choice due to their objective advantages. They can be used to join materials which are incompatible with other joining technologies. Engineers can design products which would be too expensive to produce with any other technology, and adhesives create an enormous amount of design freedom. The application spectrum covers a huge range extending from envelopes to the space station. It would not be possible to produce a new generation of composites (for lightweight design) without high-tech adhesives and resins. They create enormous value-adding in the economy. German adhesive producers and users are world leaders, and that is largely due to the country's outstanding institutional and academic infrastructure and the established courses of education. An estimated 20,000 adhesives are currently available in the German market for the various sectors of industrial production. Some are niche products and only a few kilograms are produced. A large portion of the value-added is created in the subsequent stages. There is a continual need for new adhesives, in many cases with additional properties, which are used in special products. The objective can, for example, be to create a more effective barrier and reduce the number of layers in food packaging foil or to improve durability and impermeability to fluids.

4.8.5.2. Technological/scientific challenges

In lightweight design, different materials are joined together. Adhesives are one of many possibilities. Adhesives are formulations made up of different types of adhesive raw stock, e.g. based on polyurethane materials. They distribute the forces over a large surface and hardly add any weight (in contrast to screws). Adhesive joints also have disadvantages. They make non-destructive opening and recycling more difficult.



Epoxy resin systems ensure that carbon fibers used in lightweight design remain firmly embedded in the polymer matrix during material testing
(© Press photo BASF)

4.8.5.3. Need for further research

- Better understanding of adhesive aging mechanisms to produce products with controlled durability
- In response to strong demand for lightweight design elements, develop new resins which are specifically designed to facilitate high-volume production of composite structures
- Develop adhesives which dry faster under milder conditions to reduce energy consumption and increase productivity; unlimited shelf life at ambient conditions and immediate hardening “in the blink of an eye” are research priorities
- Adhesives with built-in self-repair mechanisms or which allow the joint to be opened again “at the press of a button” for repair or recycling

More people now live in cities than in rural areas. State-of-the-art construction materials which reduce resource and energy consumption help improve the quality of life in urban living spaces.

4.9. Materials for Construction, Homes and Infrastructure

4.9.1. Current state of technology

A huge transition has taken place in the materials which are used in construction and civil engineering, but this has gone largely unnoticed by the general public. A lot of attention has been given to insulation of existing buildings and to low-energy or energy-plus houses, but the development of new construction materials and coordinated system solutions has been largely ignored by the media. There is no reason why this should be the case. Many advances have been made in state-of-the-art construction materials that are embedded into system solutions which enhance the functionality, energy efficiency, durability and recyclability of buildings. High-performance concrete and multi-functional wall plaster and road paving are a few examples of materials which have been developed in recent years. Interior plasters with built-in heat insulation are now available, and some exterior plasters keep harmful substances from penetrating into the house or even neutralize them. Coatings have been developed which withstand the aggressive conditions at sewage treatment plants or enhance the load-bearing capacity of fiber-based construction elements. Light-transmitting concrete is now available along with “whisper-quiet” paving concrete.

These success stories are primarily based on innovation in the construction chemicals industry and integration of these innovative products into construction systems. There are few other sectors where such a wide range of materials and production techniques are used alone or in combination as is the case in the construction chemicals industry. The general civil engineering disciplines provide the technical background, and a knowledge of physics is needed to understand how materials interact. Chemistry provides the basis for development and analysis of new materials.

German companies are world leaders in many product segments of the construction chemicals industry. Construction chemical producers make a wide range of products and additives for the construction, home and civil engineering markets, and they range in size from small companies to large corporations. The ability to consistently deliver excellent product quality and maintain a constant stream of innovation is crucial for the worldwide success of German producers. The industry’s innovative strengths are largely the result of close collaboration by everyone involved throughout the value-adding chain. Good availability of nearly all of the raw materials needed to make the products is a major advantage of Germany as a manufacturing location.

Looking at the larger picture, concrete chemicals and additives have historically been the dominant target market for the construction chemicals industry. When polymer chemistry, natural materials and environmental applications are added into the equation, opportunities for material development are created which can only be imagined at this point. We can expect to see a host of new products in the years to come. Hybrid materials, composites, multi-functional construction materials and complex construction systems are examples which can be foreseen at this point.

Many natural construction materials have outstanding properties, but they also have significant disadvantages. Clay is a good breathable construction material, but it is not very strong and is not water-resistant. Wool is a good insulation material but it is susceptible to insect infestation and is only available at certain times of the year. Direct use of natural materials is usually problematic. The composition and availability of these materials vary depending on the source and time of year, making quality assurance and continual supply to the construction site difficult.

Efforts began 80 years ago to develop chemical treatments for natural materials, e.g. casein, lignosulfonate and wood rosin extracts or completely synthetic imitations, e.g. citrates, tartrates, etc. A number of these products are still indispensable. Some construction chemicals are based on various other natural materials e.g. modified cellulose and amino acid salts.

One goal is to compensate for the deficiencies of natural materials by synthetically emulating and enhancing the useful properties of these biomaterials. Optimizing the chemical structure can increase the effectiveness of the materials. Nevertheless, biomaterials can increasingly act as models for new chemical agents or be conditioned for use as raw materials in the production of new additives. Biocomposites could be used in the construction industry at some point in the future.

4.9.2. Relevance

The German construction chemicals industry generates an annual turnover of around 5.1 billion euros which is more than 50% of the European total and is equal to roughly 1/3 of the world market. It is a major source of long-term employment. That in itself indicates the social and economic significance of the industry. Materials and energy make up a large proportion of the resources which are consumed to construct a building and maintain services in the building once it has been completed. The development of construction materials which conserve natural resources and energy will play an important role in the future. There is another very significant statistic. Construction materials are by far the largest category (> 80%) of construction waste in Germany. The phase-out of the nuclear power industry further increases the importance of energy efficiency in buildings and the use of advanced materials to save energy.

4.9.3. Health and ecological aspects

The hygienic and ecological aspects of construction materials have been the subject of public debate for some time. Production, preparation, installation, use, dismantling and disposal or re-use are the major phases in the lifecycle of construction materials. There are regulations and standards which apply to each one of these phases. The intention behind the regulations is to protect human health and the environment from the adverse effects of construction materials during the different phases of the product lifecycle and also to promote sustainability. The release of volatile organic compounds (VOCs), radon and nuclear radiation are the main concerns surrounding building materials which are used in the interior. The main issue with materials installed on the exterior is the release of substances due to the effects of weathering. The European Construction Products Directive and the European Construction Products Regulation, the remaining parts of which came into force in 2013, includes health and environmental protection among the essential requirements for construction products (ER 3 / BWR 3). The second-generation European product standards require declaration of the ecological and hygienic performance of construction products. These declarations will be based on harmonized European test and assessment standards which, however, do not yet exist. A large number of research activities are now directed at issues such as a) the health and environmental effects of construction products, b) optimization of the hygienic and/or ecological characteristics and c) replacement of questionable materials with others which have superior characteristics. Researchers are also looking for ways of reducing the amount of energy which is needed to manufacture construction products.

These developments are being driven to a considerable extent by advances in analytical chemistry and instrumentation. They provide the basis for methodologies which produce reliable and meaningful results in practical application and can detect and quantify potentially questionable constituents that often have no effect on the product characteristics. With the aid of analytical chemistry, new technological development pathways can be explored for reducing the proportion of undesirable secondary substances in construction products simply by making minor adjustments to the formulations. A profound understanding of the substances, formulations and processes is needed to make the intended improvements. Chemistry can make a vital contribution to the development and production of construction products which are not harmful to human health or the environment and for that very reason are sustainable.

4.9.4. Technological/scientific challenges

A large proportion of global energy and resources consumption is attributable to construction, ongoing operation, demolition and final disposal of buildings and infrastructure. As energy and natural resources become increasingly scarce, there is a need to change how we do things and explore new ways of reducing consumption.

Few efforts are currently being made worldwide to further functionalize the huge amount of covered land, roof space and building exteriors for other purposes such as power generation and creation of green space. More needs to be done in Germany to ensure compliance with future energy mix guidelines and keep CO_2 emissions below the maximum threshold. Brownfield sites in particular, but also rooftops and building exteriors will have to be used more effectively to generate energy.

There is also a need to reduce susceptibility to harmful or corrosive substances which attack, contaminate or decompose construction materials. The exteriors of man-made structures are very exposed to the effects of climate change and the more frequent extreme weather conditions. A lot of the building materials currently in use are unable to withstand the added stress. Many energy facilities are now located in remote areas with harsh climates, e.g. tidal power plants, offshore wind farms and energy extraction in oceans and deserts.

In the future, construction and insulation materials will have to be fully recyclable and easy to remove at end of life. The insulation and facing materials currently used in construction are bonded as firmly as possible to the substrate. When buildings are demolished, it is difficult to separate and recycle the various materials. Disposal is expensive and wasteful. Firm attachment of the insulation and facing materials to the substrate combined with the ability to easily separate and recycle the materials if the building is demolished is one of the biggest challenges facing the construction chemicals industry.

New life and work styles driven by factors such as the urbanization megatrend create new challenges for the industry, because they create the need for new, versatile building designs and development of the materials needed to construct them. More than 50% of the world population now lives in cities or 65 mega-cities with more than 5 million inhabitants. This gives a new dimension to sustainable construction.

4.9.5. Possible solutions, opportunities for improvement

The construction chemicals industry is one of the main sources of innovation in the construction materials sector. It will be a major contributor in the search for solutions or at least improvements across the full spectrum of materials.

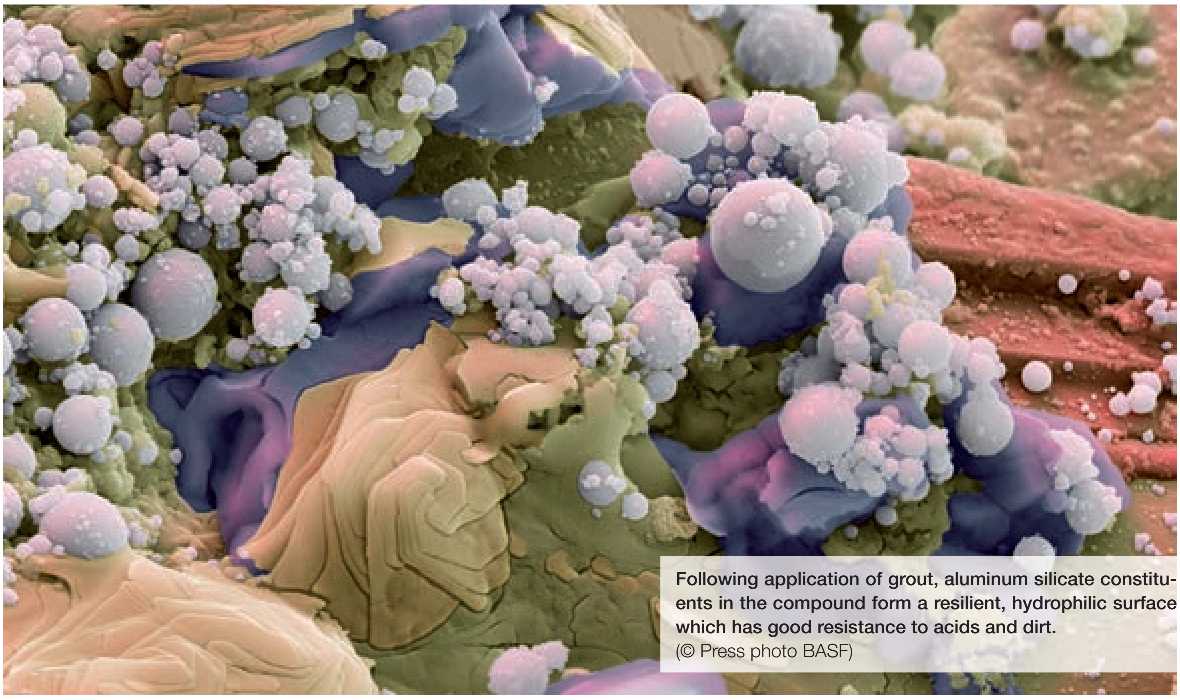
The general strategy is as follows:
Intelligent Materials will actively respond to changing ambient conditions such as temperature, moisture, contamination levels, etc. or indicate the presence of cracks, moisture or excessive stress. This includes materials which provide protection and enhance the durability of coverings and coatings, particularly in locations where access is

difficult such as renewable power generation (tidal energy plants, offshore wind farms and biogas plants), sewage treatment, building foundations, ocean cables, underwater pipelines, etc.

New work and life styles such as vertical farming, biomass power plants and the zero-emissions city create the need to make better use of construction materials or to provide **multifunctionality** which gives the materials added value. The large surface areas of functionalized construction materials can be utilized as an active environmental protection system (e.g. absorption of contaminants), or they can transfer energy or store heat and electricity. Development of low-emissions construction materials offers additional opportunities to minimize the release of pollution into the environment.

When **materials, buildings and infrastructure are viewed from a complete lifecycle perspective**, it becomes obvious that recyclability and reusability of insulation materials, coverings, etc. must be a development priority in order to avoid high disposal costs. This approach simplifies demolition work and does away with the need to separate materials which are mixed in together. **Materials which conserve energy and natural resources** also help reduce energy and water consumption. High-performance construction materials have the potential to reduce material consumption during the construction phase (i.e. equivalent stability using less raw material, lower primary energy consumption). Construction materials, especially high-mass materials, can be used to store heat and energy. High-performance insulation materials should provide good insulation in buildings which have thin walls and simple construction design (integrated systems) and offer a good quality of life. Research work should also continue on the development of improved glazing.

New manufacturing techniques and process designs based on bionics, biomimetics, nanotechnology and energy-efficient production as well as the development of technologies for separating and recycling demolition material, etc. can facilitate implementation of all the strategies described above and help exploit opportunities for improvement.



Following application of grout, aluminum silicate constituents in the compound form a resilient, hydrophilic surface which has good resistance to acids and dirt.
(© Press photo BASF)

4.9.6. Need for further research

The strategies described above for addressing current and future challenges create very significant future market potential for the construction chemicals industry. A substantial amount of research will be needed, however, to exploit this potential as described below.

To enhance **energy and resource conservation**, more research is needed to optimize heat insulation, climate control and the direct use of construction materials to generate heat. Research on grinding aids, activating/accelerating additives which facilitate the use of energy saving binders, crystal engineering to manage growth of hydrate phases and better utilization of clay and loam would allow producers to make better use of the energy which is contained in conventional binders. Because it is possible to continue using the existing infrastructure, there are no impediments to rapid industrial scale-up.

To improve **environmental protection** and reduce the effects of construction materials on human health, better methods are needed for detecting the potential release and spread of contaminants from construction materials in practical application. The technology can be used to ascertain the actual impact on water, air and soil, providing ecological and hygiene data for Declarations of Performance in compliance with future EU regulations. Photocatalytic breakdown of air pollutants and immobilization of contaminants by construction products also help protect the environment, but this is an area where more research is needed.

Intelligent materials have a very significant future market potential. More research is needed in the following areas: controlled release of active agents; materials and integrated systems which give an indication of inminent excessive stress or end of useful life (cracks, leaks, ingress of contaminants, excessive wear); self-healing building materials, coverings and coatings which maintain a good seal without human intervention; additives which bind corrosion-enhancing substances such as chlorides, sulfates and acids or release protective agents. Research on specific encapsulation of active agents is expected to be a crucial factor in the development and introduction of these materials. The processes and products will have to be suitable for the high-volume material flows in the construction products sector.

From the **materials lifecycle perspective**, development of demolition and recycling techniques must take place in parallel with product development. The identification of all construction materials without the need to refer to a separate document archive using techniques such as improved RFID chips (which contain no critical raw materials) makes it easier to sort the materials later on and achieve high recycling rates. Research is also needed on reversible joining and separation of materials “at the press of a button” to make recycling easier (or perhaps even possible).

New work and life styles such as vertical farming create opportunities to carry out research on **multi-functional surface utilization**. This includes such things as the development of construction materials for vertical farming, e.g. natural fiber based geotextiles with integrated nutrient supply. Investigation is also needed on the cultivation of plants and biofilms on building exteriors, for example to reduce air pollution by binding or breaking down contaminants or “probiotic biofilms” which protect against plants or biofilms that cause damage such as green or brown algae. Interdisciplinary research on new materials will be needed to take advantage of these opportunities.

The development of substitute materials and cost-effective, highly efficient recycling techniques has huge economic and ecological potential.

5. Securing Raw Materials through Recycling and Efficient Re-use

Economic prosperity in Germany depends primarily on high-technology production and exports, especially in the machinery manufacturing and chemical industries. This business model in turn depends on the secure supply of raw materials and commodities which are turned into consumer products and capital goods in a complex sequence of processing steps. Germany has few primary raw materials and extracting what little is there does not make sense from the economic and environmental standpoint, so the country is heavily dependent on raw material imports. As demand for raw materials continues to increase in the emerging and developing countries, the supply situation is expected to become even more tense. Shortages could occur which could hamper the introduction of new technologies and development of competitive products, for example in the electromobility industry.

It is also clear that extraction of natural resources will become more and more expensive and energy-intensive. This highlights the economic and ecological importance of recycling which must be firmly embedded in lifecycle planning for today's products in order to support an industrial society which is truly sustainable.

In addition, the export of new recycling technologies could become a significant economic factor for Germany.

5.1. Current state of technology

There are many different categories of waste:

- Compact material waste, e.g. pipe, sheet metal, castings, metal profile sections, panels, joining elements
- Easily deformed and fine particulate waste, e.g. rubber, foil, paper, fibers, chips and abrasive sludge
- Waste products and equipment, e.g. cars, machinery, electrical equipment and appliances that consist of various parts and assemblies which in turn contain various materials.

The items have to pass through different processing steps to selectively sort waste into lucrative materials fractions at a reasonable cost. The general sequence is shown in Figure 1.

The first step in a recycling process is waste collection. Initial visual identification of the material type takes place at this stage, and the waste is generally sorted into basic categories which are easy to distinguish (paper, plastic, metal, etc.).

If the waste products are more complex, they often have to be disassembled and sorted before the materials can be identified. Different techniques (screws, welding, riveting, adhesives, etc.) were used during production to connect the various parts and materials. The products also may have coatings and composites which require separation.

Disassembly, cutting, breaking and grinding are used to separate and break up materials which are joined together. Coatings are usually removed chemically or by melting. Separation of composites into their constituent parts is very complicated, making it difficult to completely separate and sort all of the materials.

The fact that materials have different physical properties is exploited during the sorting process. The main techniques are density sorting, magnetic sorting, electrical sorting and eddy current sorting. The physical shape and size of the materials have to meet certain criteria for these techniques to be viable. The techniques used to break down the materials must be designed to facilitate the sorting processes. Classification may also be necessary. Besides sorting the material into different fractions, contaminants (lead compounds, chlorinated organic compounds, oils, solvents, etc.) also have to be removed to keep them out of downstream processes for health and safety reasons.

To improve the quality of the target fraction, the fractions which have been sorted out are homogenized and impurities are then removed. Depending on the type of material, filtration, vaporization, precipitation or chemical / electro-chemical reactions have proven to be very effective for removing impurities. The cleaned fractions are then turned into marketable recycling products such as metal blocks, metal powder, plastic granulate, salts or liquids.

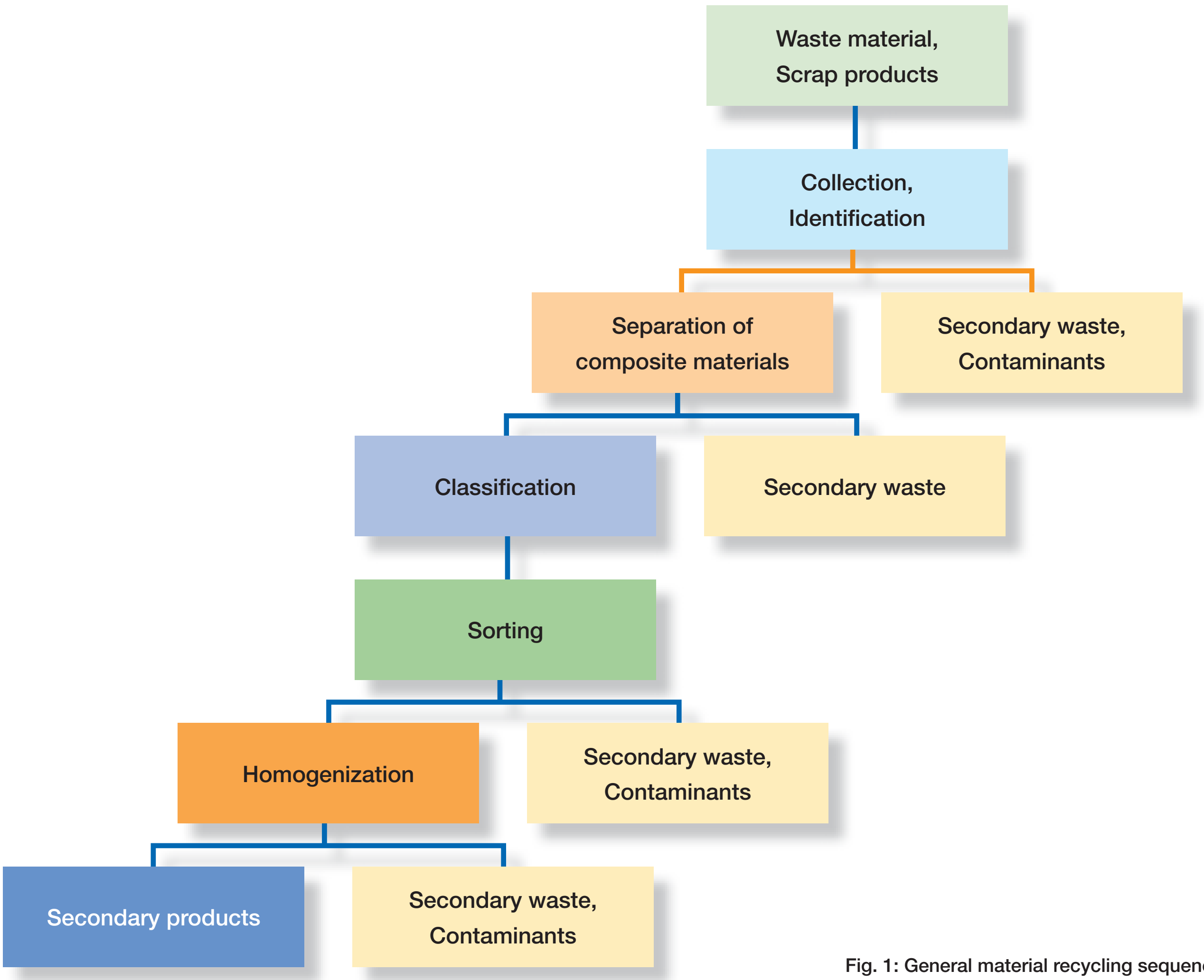


Fig. 1: General material recycling sequence

5.2. Relevance

As technology continues to advance, a wider range of raw materials is being used to manufacture products. The following examples from everyday life give an idea of the complex raw material issues involved. The emphasis is on materials generally regarded as critical because reserves are limited and the materials are very important for the manufacturing industry rather than on bulk commodities such as iron, steel and chromium. A study by the Fraunhofer ISI and IZT Institutes contains a detailed analysis of the raw materials requirements for tomorrow's technologies.[23]

Information and Communications Technology (ICT)

Cellphones and laptops are typical products in the ICT sector. They essentially consist of an enclosure, display and battery along with several printed circuit boards (PCBs) which are populated with a diverse range of electronic components. Leaving the batteries aside, cellphones are made primarily of plastic (more than 50% by weight) followed by copper, iron and glass.[24] The total content of gold, silver and palladium by weight is only tenths of a percent but these metals account for 93% of the scrap value.[25]

Recycling is primarily concentrated on recovery of the precious metals. Pyrometallurgical techniques are currently state-of-the-art. The combustible parts are used as fuel to produce energy and as reduction agents. The contaminants are filtered out of the off-gas or are immobilized in the slag.[26] Precious metal-copper alloys are extracted and purified through hydro- or electro-metallurgical recovery. Special metals such as indium, tellurium and selenium are recovered from slag which contains lead.[27] Precious metal purity and yield are conflicting goals. A combination of manual and mechanical pre-processing is needed to arrive at the best compromise.[28]

Besides optimization of these techniques, the use of bio(hydro)metallurgy[29] is also being considered. This technology could also provide an attractive alternative beyond the realm of ICT. This includes bioleaching by iron and sulfur oxidizing bacteria which have been used for years for beneficiation of low-grade copper ore. Biosorption (passive) and bioaccumulation (active) are other techniques which can be used to concentrate metals biomass or microorganisms.[30] They could augment the existing processes, e.g. during processing of the fine particle and dust fraction from the mechanical operations to increase the metals yield.

23 Angerer, Gerhard; Erdmann, Lorenz; Marscheider-Weidemann, Frank; Scharp, Michael; Lüllmann, Arne; Handke, Volker; Marwede, Max (2009): Rohstoffe für Zukunftstechnologien. Einfluss des branchenspezifischen Rohstoffbedarfs in rohstoffintensiven Zukunftstechnologien auf die zukünftige Rohstoffnachfrage. Stuttgart: Fraunhofer-IRB-Verl.

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25 Hagelüken, Christian (2006): Improving metal returns and eco-efficiency in electronics recycling. A holistic approach for interface optimisation between pre-processing and integrated metals smelting and refining. In: Proceedings of the 2006 IEEE International Symposium on Electronics and the Environment.

26 Hagelüken, Christian (2006b): Recycling of Electronic Scrap at Umicore's Integrated Metals Smelter and Refinery. In: World of Metallurgy - ERZMETALL 59 (3), S. 152–161.

27 United Nations Environment Programme (UNEP) (Hg.) (2009): Recycling - From E-waste To Resources.

28 Meskers, Christina E. M.; Hagelüken, Christian; Salhofer, Stefan; Spitzbart, Markus (2009): Impact of pre-processing routes on precious metal recovery from PCs. In: Jens Harre (Hg.): European Metallurgical Conference EMC 2009. June 28 - July 1, Innsbruck, Austria : proceedings. Clausthal-Zellerfeld: GDMB

29 Cui, Jirang; Zhang, Lifeng (2008): Metallurgical recovery of metals from electronic waste: A review. In: J HAZARD MATER 158, S. 228–256.

30 Velasquez, Lina; Dussan, Jenny (2009): Biosorption and bioaccumulation of heavy metals on dead and living biomass of Bacillus sphaericus. In: J HAZARD MATER 167 (1-3), S. 713–716.
Vijayaraghavan, K.; Yun, Yeoung-Sang (2008): Bacterial biosorbents and biosorption. In: BIOTECHNOL ADV 26 (3), S. 266–291.

Waste electronic equipment

The increasing popularity of electrical and electronic household appliances and the proliferation of instrumentation and control devices and ICT equipment for business and home use are creating mountains of defective equipment and scrap. All of this is a significant potential environmental hazard. On the other hand, all of this is a readily available source of many types of metal and plastic which need to be collected, recycled or properly disposed of to avoid incineration or dumping at landfill sites.

E-waste contains many contaminants such as:

- Mercury in switches, fluorescent tubes, batteries and LCD background lighting
- Lead and cadmium in batteries and display screen glass
- Chromium compounds

There are also many materials that are worth recycling:

- Steel in enclosures and functional parts (washing machines, refrigerators, electrical tools)
- Aluminum in chassis and cooling elements
- Gold, palladium and silver in contacts, bonding wires and batteries
- Tin, lead, silver and bismuth in solder
- Zinc, nickel, cobalt and manganese in batteries
- Tantalum in capacitors
- Indium in LCD screens, cellphones, LEDs and thin-film solar cells
- Ruthenium in hard disks
- Rare earth elements in luminescent substances and batteries

Electromobility

Technology for the generation, storage and conversion of electrical energy will be needed to support widespread rollout of electric drive systems. The feasibility of electromobility will depend on the availability of a large number of generators, batteries and electric motors designed for mobile use.

Permanent magnets with high coercive field strength and remanence are essential for power generation and conversion. The same applies to miniaturization of electronic ICT devices.[31] A neodymium-iron-boron alloy ($Nd_2Fe_{14}B$) is currently the best material available. The somewhat weaker samarium-cobalt alloys $SmCo_5$ and Sm_2Co_{17} are also still being used because they have better thermal and corrosion properties. While demand for these alloys continues to increase, the recycling rate for rare earth metals is extremely low (estimated to be less than 1% in current study).[32]

Equally relevant is the use of permanent magnets containing other rare earth metals such as dysprosium. According to a study[33] carried out by the Fraunhofer ISI and IZT Institutes in 2009, an estimated 0.5 - 1 kg of neodymium is needed to produce a hybrid vehicle. This means that as this technology becomes more widespread, demand for neodymium will increase to tens of thousands of tonnes.

31 Du, Xiaoyue; Graedel, T. E. (2011): Global Rare Earth In-Use Stocks in NdFeB Permanent Magnets. In: J IND ECOL 15 (6), S. 836–843.

32 Graedel, T. E.; Allwood, Julian; Birat, Jean-Pierre; Buchert, Matthias; Hagelueken, Christian; Reck, Barbara K. et al. (2011): What Do We Know About Metal Recycling Rates? In: J IND ECOL 15, S. 355–366.

33 Angerer, G., Erdmann, L., Marscheider-Weidemann, F., Scharp, M., Lüllmann, A., Handke, V., Marwede, M. (2009) Rohstoffe für Zukunftstechnologien, Fraunhofer ISI und IZT gGmbH, S. 38

Lithium-ion batteries have a high energy density to weight ratio, making them ideal for electric vehicles. A number of systems are currently under development which use different anode and cathode materials. At the cathodes, most of the versions currently in use have lithium metal oxides along with a certain amount of cobalt, nickel and manganese. When these batteries are recycled, the main emphasis is on recovery of cobalt, nickel and copper using metallurgical techniques. The principle behind these techniques was described for PCBs in the ICT section above. During development of new recycling techniques, recovery of lithium should also be a priority because it plays such a large role in battery technology.

5.3. Technological/scientific challenges

It is clear from the examples listed above that a lot of research will be needed in organic chemistry (plastics, lightweight design and composites), solid-state chemistry (inorganic materials, lightweight design and composites) and industrial chemistry (process engineering). Interdisciplinary information sharing will be essential to identify the need for new recycling technologies at an early stage and to ensure that recycling is part of the materials development roadmap.

The incessant increase in complexity at the materials and component level (micro and nano structuring) creates a particular challenge. State-of-the-art high-performance materials contain a variety of chemical substances, some of which are only present in very small quantities and are finely distributed (dissipative) but represent the major portion of the recycling value. Laminates, thin coatings, fibers and particles make it even more difficult to cleanly separate the materials.

In many electronic devices, the concentrations of high-value materials are so small that it is generally not economically viable to recover them. Besides trying to recycle or reuse nearly all of the different high-value materials, it may well make sense to recover the existing compounds or components rather than attempting to extract the chemical elements in pure form. This could eliminate the need for expensive purification steps which create large amounts of waste. The components should be returned to a state where they can be re-used for the intended purpose.

Composites are also difficult to recycle. This category includes hybrid materials which are found to an increasing extent in lightweight design. At the current state of technology, recycling usually consists of wet chemical separation followed by filtration (laminates), shredding and molten-state filtration (metal/plastic particle composites). To enhance the quality of the various fractions, dry recovery should be used where possible, because this improves separation of the matrix from the filler or separation of the layers depending on the type of material. This poses significant challenges for process engineering.

Energy and resource conservation is another priority, because it creates opportunities to further reduce costs and reduce the environmental impact to a reasonable level. The goal is to develop low-energy processes which can handle several tonnes of material an hour and to deploy the technology on an industrial scale. An Effort should be made to avoid the use of process auxiliaries (fluids, gases, etc.) or at least return them to the process where they can be re-used multiple times.

5.4. Need for further research

Despite the fact that Germany already has a highly developed recycling infrastructure for raw materials and scrap materials, there is still room for optimization and innovation at all levels. The existing economic and ecological potential is not sufficiently understood, and it is not being effectively exploited. A holistic approach is needed, and recycling must be a major priority right from the product development stage. The right design, material selection and material concentration choices greatly enhance the efficiency of the recycling process. Holistic, cross-industry strategies must be developed to maximize recycling and re-use of valuable raw materials.

To come as close as possible to complete realization of closed-loop recycling along the entire process chain from the starting material to the end product, the following fundamental strategies have been identified:

- Systematic collection of recycling materials flows based on materials flow analysis
- (determine the actual status, develop action plans based on status information)
- Combine existing techniques to increase efficiency (process analysis)
- Include recyclability as a material and product design goal
- Develop new technologies for materials that will be recycled in the future, e.g. functional materials for energy and electronics applications, construction materials (lightweight design and composites)

There is a particular need to:

- Expand existing collection systems / devise new collection systems for consumer products
- Develop techniques to specifically recover high-value materials from the material mix
- Expand the use of “dry” processing to selectively recover specific materials fractions
- Continue development of recycling techniques for composites, emphasizing re-use for the production of new materials
- Develop single-stage final chemical treatment for materials fractions which have recovered with dry sorting

Substitution of critical materials and the development of sensible long-term strategies to manage the worldwide natural resource base must be clear priorities for research and government policy.

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