Solid-State Physics and Biophysics

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The Austrian Academy of Sciences commits its institutions to fundamental science at the highest level. However, this does not preclude the resulting findings from being "good for something". Indeed, in our day and age, the seeking of knowledge – at least in the field of natural sciences – without regard for potential applications finds less and less favor in the eyes of the taxpaying public, with whom decisions about funding ultimately rest. In this sense, the four institutions combined under the topic of *Solid-State Physics and Biophysics* are fully committed to fundamental science, but the selected research topics – usually in agreement with evaluation recommendations – often have themes that are relevant to practical applications. Because of their size, the two research institutes – the Erich Schmid Institute for Materials Science and the Institute for Biophysics and X-Ray Structural Science – more easily achieve the balance between pure science and applications-related research, than the two Commissions. This also holds true with respect to collaborations with industrial partners.

A striking feature of both research institutes is their intensive collaboration with international synchrotron and neutron radiation sources. Neither of the two entities could maintain international standing in their respective fields of research without carrying out regular measurements at these radiation sources. For a long time, the Academy has played a dominant role in enabling access for Austrian scientists to large international research institutions. It currently maintains formal partnerships with the *Institut Laue Langevin* (ILL) in Grenoble and with the synchrotron radiation source ELETTRA in Trieste. An unavoidable step in the near future will have to be full Austrian membership at Europe's most capable synchrotron radiation source, the European Synchrotron Radiation Facility (ESRF) in Grenoble. Again, the Academy will have to play the leading role in these negotiations.

Erich Schmid Institute for Materials Science

The Erich Schmid Institute for Materials Science (ESI) was founded during the 1970s as a research institution for metal physics, with special focus on deformation and fracture of metals. Since then, close ties have existed between the ESI and the Institute of Metal Physics at the University of Leoben. This is also emphasized by the fact that the same individual heads both institutions. With the appointment of a new chair for both institutions in 1998, the research orientation of the ESI has changed significantly. It now includes investigations into the interactions between structure and mechanical characteristics of complex materials. The strengths of the ESI are based on the characterization, description and modeling of properties of materials.

In its research orientation, the Erich Schmid Institute for Materials Science is committed to fundamental research, but with special emphasis on topics that are relevant to potential applications. Therefore, research is carried out with special emphasis on subjects with relevance to industry and medicine. Topics that apply to the medical field include the investigation of compound, cellular, and biological materials. Research on deformation and fracture, on multi-phase alloys and phase transformations has applications in industry. All of these topics apply the resources of the institute in the field of micro- and nano-structure research, and in the developing area of computer modeling.

The three areas that point towards medical applicability – which are strongly interconnected and therefore not easily distinguished from one another – will form the main focus for fundamental research at the ESI in the future. Compound and cellular materials are highly relevant topics in current international research. ESI's contribution to this area is focused on the determination of mechanical properties of these materials, taking into account characterization and modeling in the smallest dimensions (micro- and nano-structure). The research area of "biological materials" has special significance, as a dual goal is being pursued. On the one hand, biological materials are investigated from the aspect of bionics. This means that studies of natural tissues such as wood or bones are used to derive generally valid principles for the development and production of materials. On the other hand, research on bone materials is carried out in collaboration with medical institutions in order to answer clinically relevant questions.

Research into deformation and fracture is inseparably related to the above topic at the ESI, as biological and cellular, as well as compound materials are also being investigated from this aspect. In addition, ESI's competence in the area of deformation and fracture is highly regarded by industry. Therefore, this area again covers the two aspects of fundamental research and cooperation with industry. The field of multi-phase alloys and phase transformations will continuously change its emphasis towards applications-oriented research over the coming years. A large project with emphasis on fundamental science of phase transformations (particularly of precipitate formation), using experiments and computer modeling, will be successfully completed in the immediate future. The experience gained from this project has already proved to be very valuable in cooperation with industry. This is particularly true for the cooperation with the Materials Center Leoben (MCL).

Parallel to all other research areas, the ESI emphasizes two methodological topics: micro- and nano-structure research and computer modeling. The characterization of the micro- and nano-structure of complex materials is one of the internationally acknowledged strengths of the ESI. The leading role in the localized determination of structural parameters in heterogeneous hierarchical materials, using in-house micro-focus x-ray diffraction methods or external synchrotron radiation sources, such as ELETTRA and ESRF, has to be maintained and even expanded in the future. The ESI has also attained eminent standing in the area of materials characterization with scanning electron microscopes through the development of orientation imaging microscopy for the local detection of deformations in the (sub-) micron range with simultaneous determination of crystal orientation. This particular strength will also be built on in the future. These methodological areas are complemented by scanning electron microscopy combined with nano-indentation to determine local mechanical properties. In general, increased emphasis will be placed on future *in situ* investigations, such as deformation measurements with scanning electron microscopes or in synchrotron beams. A second approach involves the systematic combination of several observation techniques for the same sample.

The coming years will bring increased emphasis on computer modeling. While several specific activities exist already and have received positive attention, for instance simulations of crack propagation or separation processes, the capabilities for simulations of medically relevant topics (compound, cellular, and biological materials) remain to be developed.

Part of the activities in the areas of deformation and fracture, multi-phase alloys and phase transformations are primarily driven by the needs of industry. Therefore, the priority of these research projects will depend on the development of co-operation with industry. This is also true for those investigations in biological materials that are primarily focused on cooperation with medically oriented institutions.

The research programs of the ESI demand orientation towards intra- and interdisciplinary co-operation. The institute sees its main strengths in the characterization, description and modeling of the properties of materials. But since the ESI does not produce any new materials itself, many projects require substantial cooperation with producers of materials as part of their scientific work.

Intradisciplinary cooperation includes the Materials Center Leoben (MCL), established on the basis of the K+ program. The MCL carries out research projects together with several companies and with university institutes. The international involvement of the ESI is documented by extensive usage of large European research institutions for neutron scattering (HMI – Berlin, ILL – Grenoble, LLB – Saclay) and synchrotron radiation (ELETTRA – Trieste, ESRF – Grenoble). Interdisciplinary cooperation includes the on-going relationship with the Ludwig Boltzmann Institute for Osteology (LBIO) in Vienna, and a long-term collaboration with the Institute for Physics and Meteorology of the Universität für Bodenkultur (University of Agriculture, Forestry and the Environment) in Vienna in the area of the structure and properties of wood.

In order to reinforce research on micro- and nano-structure, existing collaboration with the European Synchrotron Radiation Facility (ESRF) in Grenoble should be intensified, and new cooperative efforts should be initiated, in particular for micro-tomography in order to obtain three-dimensional structural information in the sub-micron range, as well as for micro-fluorescence analysis. However, these plans make Austria's membership of the ESRF inevitable in the medium-term future.

Institute for Biophysics and X-Ray Structural Science

The research goals of the Institute for Biophysics and X-Ray Structural Science (IBX) lie in the field of macro- and supra-molecular nano-structures, their self-organization and dynamics. They emphasize biological agents of lipids, proteins and peptides, as they exist in the lipoproteins of blood and in cell membranes. Applications-related research is oriented towards the biomedical (fat metabolism, antibiotics) and also the nano-technological sector (nano-materials, supra-molecular switches, biosensors).

Research on these topics is closely related to measurement technology innovations in the area of x-ray structure analysis. They are mainly based on the usage of synchrotron x-ray sources. The IBX, with its branch at the synchrotron radiation source ELETTRA in Trieste, has access to internationally competitive institutions and equipment. The synergism between the institute's own x-ray laboratories, and synchrotron technology being advanced at ELETTRA, leads to the development of prototypes, which are applied to research itself, but are also used by industrial partners to produce marketable products. Increased cooperation with industrial partners is also at the forefront of the institute's long-term plans for a compact synchrotron (LITEC: Light-Based Technology) to be located in the Graz area.

Research will be focused on the following specific areas:

1. To make use of the dynamics of international developments in nano-biotechnology and to actively participate in it, vigorous initiatives are planned to advance research into model membranes and analogous mesomorphic systems on solid boundary layers. This in turn requires methodological advances in the area of surface x-ray diffraction with synchrotron radiation and classical x-ray equipment. Similarly, the biophysical area requires the design of functional supramolecular systems based on lipoprotein and lipopeptide complexes. They will have to be investigated with regard to their structural and functional interactions, using complementary physical and chemical methods, such as calorimetry and spectroscopy. The main goal in this respect is research into the structure and phase characteristics of mesoscopic systems in solid substrates.
2. High priority will continue to be given to research into high-resolution crystal structure analysis of natural lipoproteins, as well as of artificial protein, peptide and lipid systems. New techniques of crystallization on prefabricated boundary layers, such as cubic lipid phases, will help to lead to a complete structural analysis of lipoproteins, which can be crystallized by other means only with great difficulty.
3. The measurement technology aspects of x-ray analysis are to be developed with respect to automation and inclusion of artificial intelligence in data analysis. This will free the experimenter from issues of instrumental methodology and allow full concentration on the experiment itself. This is particularly relevant for the application of x-ray diffraction to high-throughput screening of heterogeneous phase systems, which has significant implications for industry.

The medium-term research program for 1996-2000 concentrated on the structural and dynamic characteristics of complex biological and biomimetic systems. In contrast, the next five years will see greater emphasis on functional interactions. This is a clear consequence of the institute's research goal to achieve concrete solutions in biomedical and technological areas. It also represents a way to increase the attractiveness of collaborations with new partners, including those from industry, in order to broaden the horizon of fundamental research. Particularly the combination of "soft" and "hard" systems – such as bio-membranes and semiconductors, or macromolecules and nano-particles – is expected to lead to completely new functionality that will be of great interest to both science and technology. The broad knowledge base from previous work forms the ideal prerequisite for this shift in emphasis towards functional interactions. It also uses the results from the high priority given to the development of synchrotron methodology in previous plans to optimal effect and leads to increased impact of these activities.

The already existing orientation towards European cooperation will be strengthened. Over the coming years, specific project collaborations in the area of light-based technology (LITEC) will be elevated to the level of a center of excellence. This strategy conforms structurally to the policies of the European science community, and is also consistent with the need for an expansive positioning in the field of nanotechnology. The increased inclusion of industrial partners will be of particular importance in this context. The building infrastructure in the new AAS Research Center at Graz provides ideal conditions for the described activities.

Commission for Geophysical Research

The science program of the Commission for Geophysical Research consists of the following projects: *Deep Reflection Seismology Rechnitz – Lithosphere Research in the East-Alpine Pannonic Transition Region, Inventory of Austrian Glaciers – Areas and Volumes, and A Gravity Map of Austria.*

The project CELEBRATION 2000 derives its importance from the combination of a totally new measurement methodology with the well-known geophysical technique of refraction seismology. This allows not only greater depth penetration into the Earth's mantle and/or the asthenosphere, but also the possibility of obtaining a three-dimensional image of important deep geological structures. Even at this early stage of data acquisition, the applicability of this method to a young, geologically complex orogenic area has been tested successfully for the first time. It is planned to extend these tests to the Ligurian Sea and the Slovenian Dinarides.

The *Deep Reflection Seismology at the Eastern Edge of the Alps* project allowed clear statements about the meaningfulness of explosion seismology with regard to structures in the upper and lower crust in important geological formations. Almost always a well-reflecting lower crust exists, in which a closely spaced sequence of reflecting elements hints at strong vertical changes in the reflective impedance. The Mohorovicic discontinuity is characterized by reflections of less than ten seconds, declining slightly towards the west, and also by the lack of definite, coherent reflections below. Similarly, the upper crust (above three seconds) appears to exhibit a reflection-free zone of about six kilometers. In contrast, the uppermost kilometers of the crust – clearly the Rechnitz Pennine unit – show reflection characteristics leading to the assumption that this area is similar to the Bündner Schiefer in eastern Switzerland, and that it can be resolved satisfactorily by appropriate imaging geometry.

Assuming realistic average speeds in the crust yields a depth for the Mohorovicic discontinuity of about thirty kilometers at the Hungarian border, with a slight westward decline. In combination with the *Deep Reflection Seismology of North-East Styria* project funded by the Austrian Foundation for the Support of Scientific Research, a profile of over seventy kilometers was characterized. It is representative for the depth structure of the easternmost part of the Alps and allows a comparison with the western Carpathians. With respect to the large-scale structure of the crust, it also benefits from the link to the detailed network of measurements in Hungary.

In spite of the short profile lengths of only ten kilometers, test measurements around Eisenerz have yielded good results in terms of the reflexivity of the Grauwacke Zone, as charges of up to 1300 kg could be used. A core result is the fact that reflections of up to sixteen seconds, and therefore already from the upper mantle, were obtained.

As part of the project *A Gravity Map of Austria* project more than 32,000 measurements from various sources were analyzed uniformly, laying the groundwork for future work on Bouguer gravity and geoid research, in coordination with the networks of measurements in neighboring countries. The group of Austrian scientists was also able to gain substantial experience with the issues of gravity measurements in the area of the Alps.

Geophysical research depends a priori on international cooperation in many areas, particularly with cross-border projects. However, cooperation is also necessary for national projects, due to the subcritical size of individual institutions. Interdisciplinary collaboration is a necessity for the interpretation of geophysical phenomena, and is therefore part of all projects of the commission. The *Gravity Map of Austria* project is expected to be complete by 2002, and no doubts exist about its successful conclusion.

Commission for Basic Research on Mineral Raw Materials

Over the coming years the commission will concentrate on the issues of completing the published metallogenetic map of Austria with data on not yet included mineral deposits and their geological development. Zeolite studies will also be supported, as they become a more important field of international research.

The planned projects will investigate the mobilization and migration of matter in the Eastern Alps, which led to the formation of mineral raw materials during the alpine orogeny cycle, in combination with endogenous processes. Building on combined regional deposit information, such as the metallogenetic map of Austria, the enrichment and formation mechanisms of select groups of mineral deposits during the main phases of the alpine orogeny cycle are to be investigated. The CD-ROM version of the metallogenetic map will provide valuable assistance in the interdisciplinary regional analysis of all available deposit-related data. Further research goals include the generation of technologically interesting zeolites and the determination of their structure.

It must be emphasized that in some cases these relatively minimally funded projects have led to much larger, successful proposals to the Austrian Foundation for the Support of Scientific Research. Thus, the relatively modest Commission budget can serve as seed money and may ultimately lead to a positive multiplicative effect.