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Computer-Assisted Design of Materials

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In the future, materials research will rely on computers for assistance – for the selection of suitable materials and for simulating their properties. The 1996 Körber Prizewinners' aim is to further improve these computer processes.

Yves Bréchet
(Photo: Friedrun Reinhold)

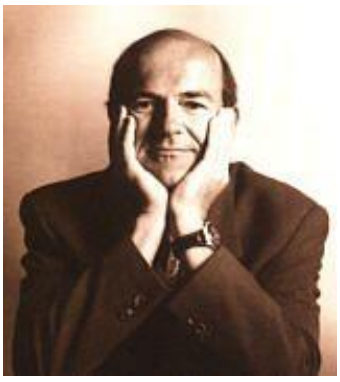
Depending on how they are counted, there are between 50,000 and 80,000 materials on earth. Materials, not chemical substances: "A material is matter with a function," explains Prof. Yves Bréchet, who along with Prof. Michael Ashby and Prof. Michel Rappaz, has won this year's Körber Foundation prize of 500,000 DM to support their work. This represents a formidable wealth of materials available to the engineers, subdivided into six classes: metals, polymers (covering natural materials such as wood and leather as well as plastics), elastomers, ceramic materials, glasses and composite materials. Materials research addresses the properties of these substances. It is an undervalued discipline. The very title highlights this: normally 'materials research', as opposed to 'material science'. Their colleagues in the theoretical disciplines look down condescendingly on researchers getting their hands dirty dealing with concrete problems on the ground. "In the land of Descartes where the illusion prevails that a complex reality can only be understood by calling on the deductive skills of the human mind and applying axiomatic methods, materials research is something of a Cinderella discipline," sighs Bréchet.

The 35-year-old professor at the Institut National Polytechnique (INP) in the French city of Grenoble is the epitome of the multi-disciplinary high-flyer: even as a student at the famous Ecole Polytechnique in Paris he had developed an interest in both abstract science and concrete applications alike – his diploma thesis was in mathematics and materials research which, as he saw it, bridged the artificially created gulf between theoretical and applied research. "In the French tradition, you have to work with useless things to be recognized as a ground-breaking researcher," he complains. He does not want to align himself with this tradition, but rather with the Renaissance, which saw the combination of theory and practice still representing the norm. He likes to trace back material science to Galileo who as early as the 17th century published two articles on the stability of substances. Materials research draws together knowledge from a wide variety of research fields and is by its nature interdisciplinary," explains Bréchet: "For mechanics, we are physicists, for chemists we are mechanics, and for physicists we are chemists." In centuries past the use of materials was an empirical matter, passed down from generation to generation. It is only since the 1930s that we can really talk about any systematic approach to materials research. And until the 1960s had arrived, in practical terms "material" equated to "metal". It was only then that the dominance of metals was broken by new plastics and composite materials. Since then, it has become possible to speak of a genuinely comparative science – with the possibility of quite different materials being suitable for one and the same purpose. The next change set in around ten years ago: with the

development of ever more powerful computers there are entirely new opportunities being opened up for materials research. However, materials researchers cannot simply adopt computer processes from other disciplines. The aim of the Europe-wide project supported by the Körber Foundation funds is to develop specific methods for use in this field. Apart from Bréchet, the leading lights are the British researcher Michael Ashby at Cambridge University and Michel Rappaz at the Ecole Polytechnique Fédérale in Lausanne (EPFL).

A nickel-based superalloy under the electron microscope.
(Photo: Friedrun Reinhold)

Chemists now have a number of software tools available for 'designing' new materials at the level of the atom and the molecule. Even at macroscopic level (i.e. the range at which we can identify items with the naked eye), there is a wide variety of computer processes providing assistance for engineers, such as CAD software, for example. Materials researchers are interested in an intermediate range labeled by Yves Bréchet as the 'mesoscopic' level – and to date there have been very few computer models in existence here. There are hardly any materials for which it is possible to reach conclusions about their physical properties directly from their atomic structure, and these are not necessarily the most interesting anyway. For example, materials displaying a perfect crystal lattice are extremely brittle. Plasticity does not appear until there are what are termed 'dislocations' in the crystal structure, i.e. points at which the lattice is broken. "Most material properties are derived from defects – just as with people," says Bréchet. While the elementary building blocks of material, atoms and molecules are quite universally and unambiguously determined, at the mesoscopic level the 'units' look quite different: depending on the material and the questions asked, this might amount to instances of dislocation, but may can also relate to grains in metals, the inclusion of other materials or what are termed 'dendrites', i.e. branching structures created when liquid metal is cooled. Michel Rappaz in Lausanne is working on how the creation of such structures can be influenced so as to obtain the best possible materials for the job.



Michel Rappaz
(Photo: Friedrun Reinhold)

Rappaz invokes a graphic comparison in explanation of his work: "Look at frozen water, for example. Depending on the environmental conditions, you can have clear ice or snow in any of its many variants." Here, the hexagonal structure of the snowflakes originates in the crystalline structure of the ice. Branching structures also form in the cooling metal in a quite similar fashion. For the most part they grow in from the cooled periphery of the mould towards the middle, however frequently they also spontaneously form 'germs' at the centre of the mould, with such a 'treelet' starting to grow there. When two of these what is known as 'dendrites' meet each other, a grain boundary is formed. Depending on the technical requirements, what the engineers desire varies widely: for many applications the need is for the grain size to be as small as possible, while for others it is all about having the work piece made up of one single 'grain'

as far as possible, to obtain the most homogeneous properties possible. This is the case, for example, for the rotor blades in aircraft engines or power station turbines. So for Rappaz and his colleagues, it is all about simulating the growth in these metal trees as exactly as possible. The mathematical tool for this is what is known as 'cellular automata'. With these, the volume of the casting mould is divided up into tiny cube-shaped cells, each of which has a specified status. From the known physical laws of the influence of heat, it is now possible to calculate – over discrete time steps – how the status of each cell changes from generation to generation, depending on the status of the neighboring cells. The advantage of this method is that it is possible not only to simulate the structure (and therefore the material properties) of known metal alloys, but one can also experiment with new combinations within the computer. And the possible applications are not restricted solely to metals: Michel Rappaz's team is also simulating the solidification process for cacao butter on behalf of a foodstuffs group.

Simulation of grain structure in cooled metal (top) and section of metal rod cast under real conditions (bottom).
(Photo: Friedrun Reinhold)

The fact that selection of the right material for a specific product can represent a problem, and a mathematical one at that, does not immediately occur to the layperson. If, for example, the job is to construct the forks of a racing cycle, it is clear that materials such as glass, polystyrene and rubber cannot be considered. But are aluminum alloys better suited for this purpose than titanium alloys? What about carbon fibre composites? Engineers have traditionally relied on their empirical experience to make the right choice from the thousands of alternatives available. This is the wrong approach, according to Michael Ashby, the third member of the group of Körber Prizewinners. People tend to think conservatively ("we've always used aluminum for this, so we'll use aluminum again"), and the optimum solution for a material problem is often a very unconventional one. To simplify the engineer's tortuous selection task and to place the procedure on a more objective basis, Ashby has developed a process which he is also marketing as commercial software, under the name "Cambridge Materials Selector" (CMS).

"A good designer does not say: 'I need a metal' or 'I need a polymer'," states Ashby in setting out the problem. "What is required is not a material, but a properties profile." In the case of a bicycle forks, for example, it is all about identifying a material providing the greatest possible strength at the lowest possible weight – as after all the forks must not give way under the load imposed by the cyclist. In Ashby's procedure, all materials are now entered in a system of coordinates in which the specific weight is entered on the one axis, with the rigidity value on the other. It is now a simple mathematical matter to determine the optimum material classes. In the present case there are four candidates: an aluminum and a titanium alloy, a special steel and most carbon fiber composite materials. The process of selecting from these can then continue with reference to other criteria: for a recreational bike the less expensive steel option may be preferred, but with the carbon fiber material reserved for a professional racing cycle.

With the Körber Prize funding of 500,000 DM, Yves Bréchet and Michael Ashby are intending to further refine this computerized process, as selection is not always as simple as in the example of the bicycle.

Michael Ashby
(Photo: Friedrun Reinhold)

Sandwich structures (as are used in the manufacture of skis, for example) consist of three layers, and even for the professionals the number of possible combinations of materials practically defines comprehension. Within this context, Bréchet has already been experimenting with the use of modern artificial intelligence (AI) processes. Fuzzy logic is a useful tool for making a choice when the criteria are not quite clear and may even be contradictory – a kind of formal representation of the human's 'common sense'. Bréchet has then optimized the candidates selected in this way with the assistance of what are termed genetic algorithms: with the mechanisms of mutation, recombination and selection found in the natural world, some solutions are developed on within a process of artificial evolution, while the poor solutions fall away. "The most interesting aspect of our results is that the process comes up with all of the known sandwich materials for skis, but also a few fresh solutions which may be even better," reports Bréchet.

None of the computer models currently in existence takes time as a dimension adequately into consideration. But changes take place in materials: signs of fatigue appear, along with wear and oxidization. Environmental requirements mean that recycling must be possible. The objective pursued by Bréchet and Ashby is the development of integrated expert systems into which criteria like these are fed, similarly to the various manufacturing processes for the material or the wide range of possibilities for combining materials. At present, the use of computerized methods in materials research remains underdeveloped, in comparison with other disciplines. Yves Bréchet is determined to change this, and sees himself as a pioneer in the field: "There are currently many problems to be solved, and this is the interesting aspect. The main solutions in this field will be developed over the next ten years." And one can certainly assume that the name of Yves Bréchet will be prominent in this connection. However, there is no danger of himself and his colleagues turning into pure computer geeks in the process: "In the field of materials research it is inconceivable that models can be produced without a background of experimentation. If we were to allow a theoretician to work away on his own, it is fairly certain that he would come up with nonsense."

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