Designing Non-Traditional Materials Based on Geometrical Principles

Hanover, Germany

19-22 June 2005

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Book of Abstracts

Program

Sunday, 19.06.2005	
17:30 - 20:00	Registration and get together

Monday, 20.06.2005	
09:00 - 10:00	S1
10:00 - 10:30	Tea Break
10:30 - 11:30	S2
11:30 - 12:30	S3
12:30 - 14:00	Lunch Break
14:00 - 16:30	S4
16:30 – 17:00	Tea Break
17:00 - 19:00	Discussion

Tuesday, 21.06.2005	
09:00 - 10:00	S5
10:00 - 10:30	Tea Break
10:30 - 12:30	S6
12:30 - 14:00	Lunch Break
14:00 - 15:30	S7
15:30 - 16:00	Tea Break
16:00 - 18:00	Discussion

Wednesday, 22.06.2005	
09:00 - 10:30	S8
10:30 - 11:00	Tea Break
11:00 - 13:00	Discussion
13:00 - 14:00	Lunch Break
14:00 - 16:00	Final Discussion

Sessions	Topic	Speaker(s)
S1	Keynote Lecture	Prof. Ashby
S2	Materials Selection	Prof. Brechet, Dr. Paun
S3	Crystal-Level Engineering	Prof. Hollingsworth, Dr. Pasternak
S4	Molecular and Nano-Level Design	Prof. Yakobson, Prof. Harrowfield, Dr. Katz, Dr. Maguire, Ms. Tao
S5	Topological Interlocking I	Prof. Estrin
S6	Topological Interlocking II	Prof. Dyskin, Mr. Khor, Mr. Schaare, Dr. Kanel-Belov
S7	Composite Materials	Prof. Ziegmann, Dr. Hawkins
S8	Cellular Materials	Dr. Woesz, Dr. Nadler, Mr. Mamoud

Session 1: Keynote Lecture

TO BE ANNOUNCED

Prof. Ashby
The University of Cambridge, Department of Engineering, Cambridge, UK

Session 2: Materials Selection

MATERIALS SELECTION AND MATERIALS BY DESIGN

Yves Brechet
LTPCM-INPG, Grenoble, France
Michael Ashby
The University of Cambridge, Department of Engineering, Trumpington Street, Cambridge, CB2 1PZ, UK
Florin Paun
ONERA, Chatillon, France

Materials and process selection tools can be used not only to guide designers in selecting the most appropriate materials for an application, but also to guide materials producers to design a new material specially suited for this purpose. Some examples of this methodology will be provided.

ELASTIC BEHAVIOUR OF RANDOMLY PACKED HOLLOW SPHERES METALLIC FOAM BY FINITE-ELEMENT COMPUTER SIMULATION

F. Mamoud*, F. Paun*, Y. Bréchet**
** ONERA/DMMP, 29 Avenue de la division Leclerc, 92322 Châtillon Cedex, France*
***LTPCM/INPG, BP 75, Domaine Universitaire de Grenoble, 98402 St. Martin d'Hères Cedex, France*

One solution for decreasing the aircraft engines' noise is the use of a sound absorbing material. A new cellular material features both open and a closed porosity. Open porosity makes the material a good acoustic absorber, while its closed porosity gives good mechanical properties at high temperature.

To study its elastic behaviour, a model has been proposed to derive cellular material properties out of the constitutive material properties. In this model, spheres are connected together by a brazing meniscus.

Two major difficulties occur when simulating the mechanics of the meniscus using a finite-element method. Firstly, the meniscus geometry, meshed by using tetrahedral elements, exhibits sharp edges in spite of smooth curves. Secondly, making the mesh accurate enough in the meniscus zone drastically raises the elements' number and consequently, the calculation time.

This analysis was carried out on a perfect FCC arrangement of hollow spheres. Processing cost considerations lead to the additional study of random spheres arrangements.

The concept explored in this work is to compare the behaviour of two virtual models for two brazed spheres: a numerical sample meshed completely (including the meniscus) with 3D tetrahedral elements and a sample meshed with 2D shell elements where the equivalent meniscus has been numerically simulated by fusing neighbouring sphere nodes. This approach considerably reduced calculation time.

Subsequently, a numerical sample including large numbers of hollow spheres was simulated to determine the macroscopic mechanical behaviour.

Session 3: Crystal-Level Engineering

CRYSTAL ENGINEERING, CRYSTAL GROWTH AND MEMORY EFFECTS IN FERROELASTICS AND FERROELECTRICS

M. D. Hollingsworth, J. R. Rush, M. L. Peterson, M. J. Abel, A. A. Black, D. A. Kesselring, A. G. Butenhoff,
Chemistry Department, Kansas State University, Manhattan, KS 66506 U.S.A.

M. Dudley, B. Raghothamachar
Dept. of Material Science and Engineering, SUNY Stony Brook, Stony Brook, NY 11794 U.S.A.

In our efforts to better understand cooperative processes in crystalline solids, we have sought general strategies for developing series of ferroelastic and ferroelectric crystals, in which external anisotropic stresses or electric fields can be used to switch between orientation states. By using a variety of crystal engineering techniques to tailor the distortion from high symmetry in series of organic inclusion compounds, we have succeeded in preparing over forty new ferroelastic materials. A small fraction of these are also ferroelectric, as shown by videomicroscopy and electric field dependent NLO effects.

Although we have had great success in our efforts to generate new ferroelastic materials, developing general strategies for making new ferroelectrics is much more difficult; the requirements for ferroelectricity are much more stringent since the crystal should have a macroscopic dipole moment that can be reoriented in an electric field. This talk outlines our strategies for generating, aligning and optimizing the polar ordering of guests in ferroelastic inclusion compounds, thereby making them ferroelectric.

Much of this work has been on two classes of materials (urea inclusion compounds and calixarenes) that exhibit reversible "memory effects" upon release of the external stress. In these materials, the daughter formed under stress reverts to the orientation of the original mother domain when the coercive force is released. With synchrotron white beam X-ray topography of urea inclusion compounds, we have shown that the rubber-like behavior and memory effects can arise because crystal growth generates invisible, epitaxially matched twins that become mismatched in the stress-induced domain switching process. Our observation of electric field-induced poling of certain urea inclusion compounds is also consistent with metastable sites generated at the boundaries of mismatched domains. In the calixarenes, the mechanisms responsible for rubber-like behavior appear to be less straightforward.

MATERIALS WITH NEGATIVE POISSON'S RATIO AND NEGATIVE STIFFNESS

Elena Pasternak
School of Civil and Resource Engineering
University of Western Australia

Materials with negative Poisson's ratio and negative stiffness have outstanding engineering properties including increased effective stiffness and reduced thermal stress. There are a number of structures that produce the effect of macroscopic negative Poisson's ratio and stiffness. We develop a theoretical basis for designing such materials and predicting their properties based on microstructural approach and homogenisation procedures. We overview the previously proposed structures and demonstrate that simple arrangements of particles connected with elastic bonds can, depending upon the relation between the bond stiffnesses, produce structures with negative Poisson's ratio. We also examine the structures with negative stiffness and discuss their possible properties. Finally, we consider composites with inclusions with negative Poisson's ratio and negative stiffness imbedded in a conventional elastic matrix.

<u>Session 4: Molecular and Nano-Level Design</u>

MODELING OF NANOTUBES, THEIR ASSEMBLIES, AND TENSEGRITY STRUCTURES

B. I. Yakobson
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Quasi-one-dimensional solids – nanotubes and nanowires, promise a broad variety of applications and attract growing attention. We perform theoretical and computational modeling of carbon and boron-nitride nanotubes in order to evaluate the limits of their thermo-mechanical strength. This leads to a strength map, with symmetry, temperature, and load-rate present as parameters. We take into account two concurrent and competing mechanisms of structural yield: bond-rotation ("plastic") [1] and direct bond-breaking (brittle). Further, we investigate [2] possible nature of inter-tubular drag, resistance to shear, which appears to be a bottleneck for any nanotubes-based structural material performance. It can be done with quantum-mechanical calculations followed by statistical theory of energy dissipation, leading to toughness evaluation. We will also present recent results on structure, stability, and electronics of another class of 1D materials, Si wires [3]. Possibility of chemical binding of rigid beams into molecular tensegrity structures for materials applications will be discussed.

Work supported by the AFRL Materials Directorate, the ONR (DURINT), and NASA (URETI).

[1] Dumitrica and Yakobson, *Appl. Phys. Lett.* v. **84**, 2775 (2004).
[2] Lin, Zhao, and Yakobson, in progress; Zhao, Yakobson, Smalley, *Phys. Rev. Lett.* v. **88**, 185501 (2002).
[3] Zhao and Yakobson, *Phys. Rev. Lett.* v. **91**, 035501 (2003).

SUPRAMOLECULAR CHEMISTRY OF GRIDS AND HELICES - WAYS OF USING MESSAGES IN MOLECULES

Jack Harrowfield
Universite Loius Pasteur, harrowfield@chimie.u-strasbg.fr

Polytopic metal-ion-binding molecules (ligands) can be used to to create metal aggregates with particular geometries which determine their properties such as magnetism and both the absorption and emission of light. This talk will summarise work in Strasbourg concerned specifically with metallo-grids and -helices constructed using polypyridine ligands, outlining some of the problems and the prospects in this area.

FULLERENE-LIKE STRUCTURES IN CARBON MOLECULES AND NANOMATERIALS, LIVING ORGANISMS AND ARCHITECTURE: A HISTORICAL VIEW

Eugene A. Katz
Department of Solar Energy and Environmental Physics, J. Blaustein Institute for Desert Research, Ben-Gurion University of the Negev, Sede Boqer, 84990 Israel

The discovery of C_{60}, a third variety of carbon, in addition to the more familiar diamond and graphite forms, has generated enormous interest in many areas of physics, chemistry and material science. Furthermore, it turns out that C_{60} is only the first of an entire class of closed-cage polyhedral molecules consisting of only carbon atoms - the fullerenes (C_{20}, C_{24}, C_{26}, … C_{60}, …C_{70}, … $C_{1000000}$-carbon nanotubes). This talk presents main geometrical principles of engineering of fullerene-like structure of molecules, viruses, living organisms and buildings. The story of the fullerene discovery, together with a long history of exploration of polyhedra by science and fine art, is also reviewed briefly.

TO BE ANNOUNCED

Dr. Maguire
AFRL/MLBP, USA

SHAPING METAL NANOCRYSTALS

Jiaxing Huang, Franklin Kim, Andrea Tao, Susan Habas, Stephen Connor, Hyunjoon Song and Peidong Yang
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Systematic shape evolution of metal nanocrystals with sizes between 100 and 300 nm was observed in a modified polyol process. Careful regulation of the growth rate along different crystallographic directions allows exquisite shape control over metal nanocrystals. For example, platonic shapes of gold nanocrystals including tetrahedron, cube, octahedron, and icosahedron (dubbed platonic nanocrystals, see picture) with high yield and good uniformity are readily prepared by adding a surface-regulating polymer and foreign ions. Shaping the metal nanocrystals enables the studies on their shape-dependent properties and potential applications such as in catalysis (Pt) and Surface Enhanced Raman Scattering (SERS) spectroscopy (Ag). With the nanoscale building blocks of different size, shape and materials available, it would also be possible to construct complex superstructures.

Session 5: Topological Interlocking I

INTERLOCKING STRUCTURES: GEOMETRY AND POTENTIAL FOR STRUCTURAL APPLICATIONS

Y. Estrin
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We found geometrical shapes and arrangements of building blocks that permit fabrication of structures in which the blocks are held together by mutual interlocking. Three classes of the element geometries are possible: (i) convex polyhedra (platonic bodies), (ii) osteomorphic blocks with concave-convex interfaces and (iii) tubular elements derived from tetrahedron geometry.

These geometries give rise to a new principle of material design based on interlocking elements. The fact that the blocks are held together within a structure (e.g. a layer) without a binder or connectors provides interesting mechanical properties of such an assembly. For instance, any crack propagating within a block will be arrested at the block interfaces. Furthermore, many of these structures are extremely tolerant to local failure.

In the talk, mechanical properties of prototype structures made from topologically interlocking elements will be discussed along with possible applications of a design principle based on topological interlocking.

Session 6: Topological Interlocking II

TOWARDS FRACTURE MECHANICS OF FRAGMENTED SOLIDS

A.V. Dyskin
School of Civil and Resource Engineering, The University of Western Australia, Australia

A prospective method of constructing new materials is based on assembling the material from separate non-connected elements hold together by external constraint. The advantages of such materials include the possibility of combining elements made of different not-necessarily compatible materials, high fracture toughness, a possibility of capitalising on the inverse scale effect, etc. Form the mechanics point of view, such a material can be regarded as a representative of the class of *fragmented solids*. Important natural representatives of this class are the blocky and heavily fractured rock masses and fractured ice. Engineering examples are fractured but still stable coatings and mortar-free structures ranging from ancient structures (pyramids, dry stone walls) to modern interlocking structures.

As far as the crack propagation in fragmented solids is concerned the main feature is the presence of multiple interfaces intersecting the crack path. It is important that these interfaces can be locally delaminated and opened by the tensile stress concentration at the crack tip even if the ambient stress is compressive, Fig. 1a. The delamination zone arrests the crack such that the continuation of the crack growth can only happen by initiation of a new crack at the end of delamination zone, Fig. 1b. Subsequently, further crack propagation is characterised by a zigzag trajectory. The present paper analyses the propagation of such cracks and develops a macroscopic model that refers to the scale larger than the characteristic size of the zigzag elements.

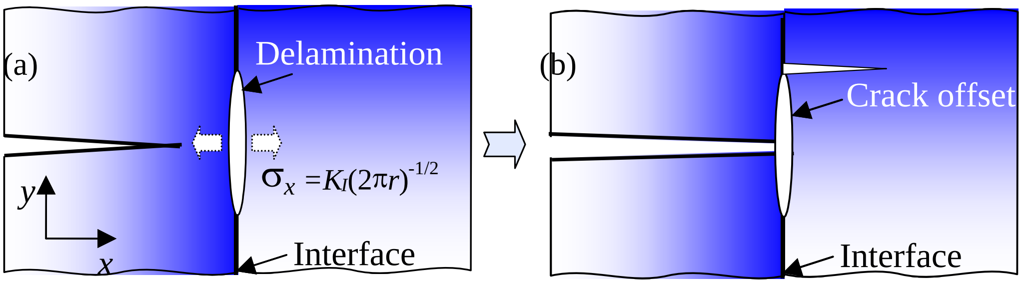


Fig. 1. Schematics of deflection of the crack path by an interface.

TOPOLOGICAL INTERLOCKING IN CIVIL ENGINEERING

H. C. Khor
School of Civil & Resources Engineering, University of Western Australia, Australia

The principle of interlocking has been playing a key role in Civil Engineering for centuries, dry stone walling being a classic example. The general idea of the construction method in dry stone walling is to use small stones to fill in the big stones' gaps and thus producing a sort of interlocking. Recently this technique was refined by utilizing blocks with specially engineered shapes that ensure interlocking without connectors or keys, i.e. without stress concentrators. Two classes of interlocking shapes were identified. The first is interlocking by special arrangements of convex elements such as tetrahedron, cube etc, which provides interlocking in a plane. The second is interlocking by non-planar surfaces providing interlocking in all directions. A representative of this class is the osteomorphic block, Fig. 1.

This paper discusses the types of structures that can be constructed from osteomorphic blocks, as well as the properties of assemblies of these blocks: enhanced fracture toughness and tolerance to missing blocks and to roughness of the contact surfaces. In addition, preliminary experiments on vibration of columns of osteomorphic blocks will be reported.

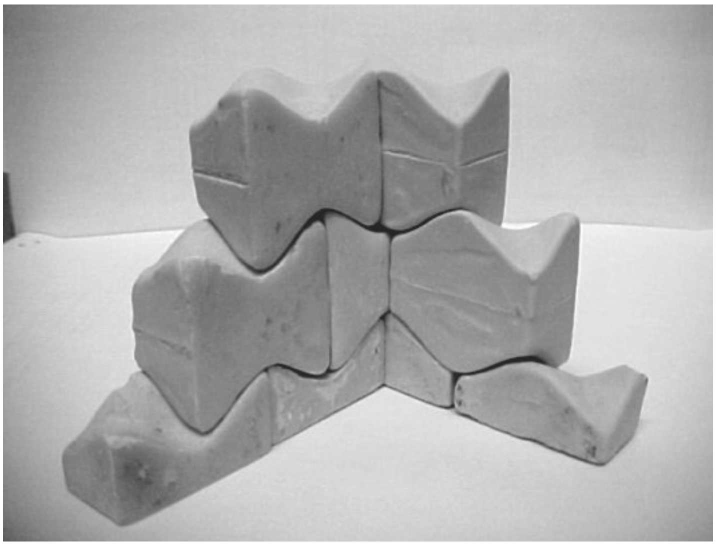


Fig. 1. A corner wall built from osteomorphic blocks.

COMPOSITES BASED ON TOPOLOGICAL INTERLOCKING OF CUBES

S. Schaare
Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal, D-38678 Clausthal-Zellerfeld, Germany

Topological Interlocking is a new method of assembling identical building blocks, e.g. those having the geometrical shape of one of the platonic bodies, into structures. The building blocks are stacked together in such a way that they support each other preventing disintegration of the structure, particularly a layer. No connectors or a binder phase are thus required. Only on the periphery of such a structure a support is necessary to take up the function of the neighboring blocks.

We shall demonstrate how Topological Interlocking works in the case of cubes and discuss basic properties found in structures assembled from cubes. Special attention will be put on structures made from combinations of different materials. Combining different materials is easily achieved by Topological Interlocking, as only the geometry of the individual elements is of relevance. Thus, using this method it would be relatively easy to assemble non-conventional functional composites.

ESSENTIALLY NON-PLANAR INTERLOCKING STRUCTURES

A. J. Kanel-Belov
Einstein Institute of Mathematics, Hebrew University, 91904 Jerusalem, Israel

In recent works, some interlocking structures were constructed. These structures were based on periodic tailings in a plane and were quasiplanar. In addition, they were unstable in the following sense. After removing a finite set of elements, they can de disassembled one by one.

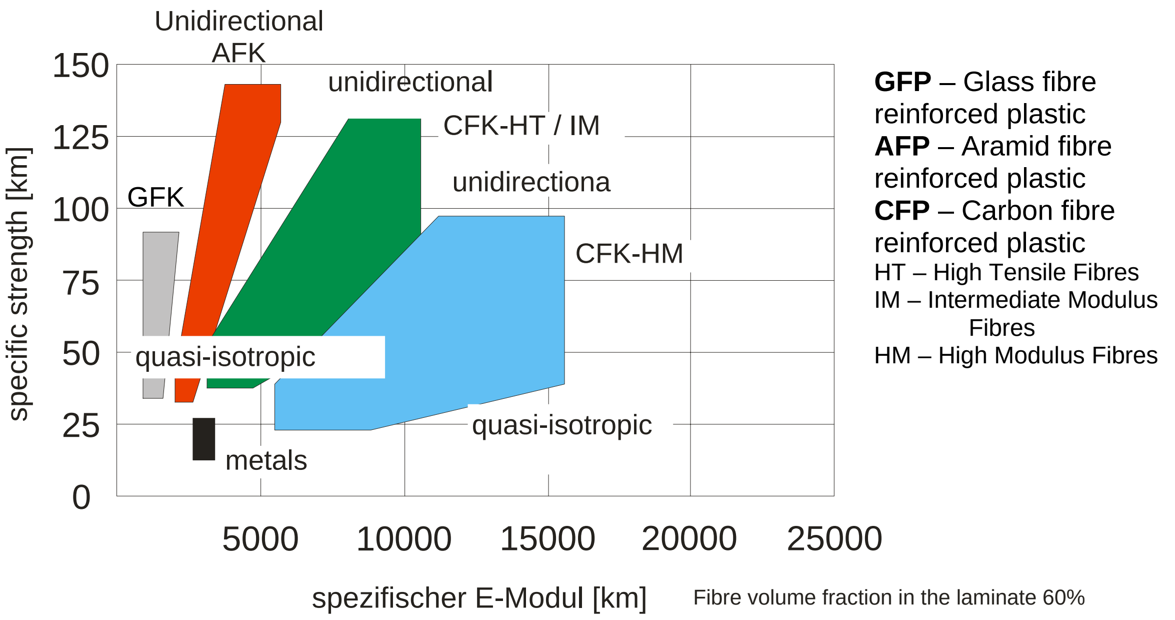
Here we present spatial structures that are interlocking in several planes simultaneously. There is also another spatial effect. If a plane is divided into convex figures, there always one such that it has common edges with no more then 6 its neighbours. However, in 3D space it is not so. For any *n* there is a division of space into congruent convex bodies such that any one of them has a common face with more than *n* its neighbours. This construction allows us to have interlocking in any number of layers. In addition, we discuss a way to generate interlocking structures and their possible properties. Finally, we present a review of different interlocking structures and formulate some open problems.

Session 7: Composite Materials

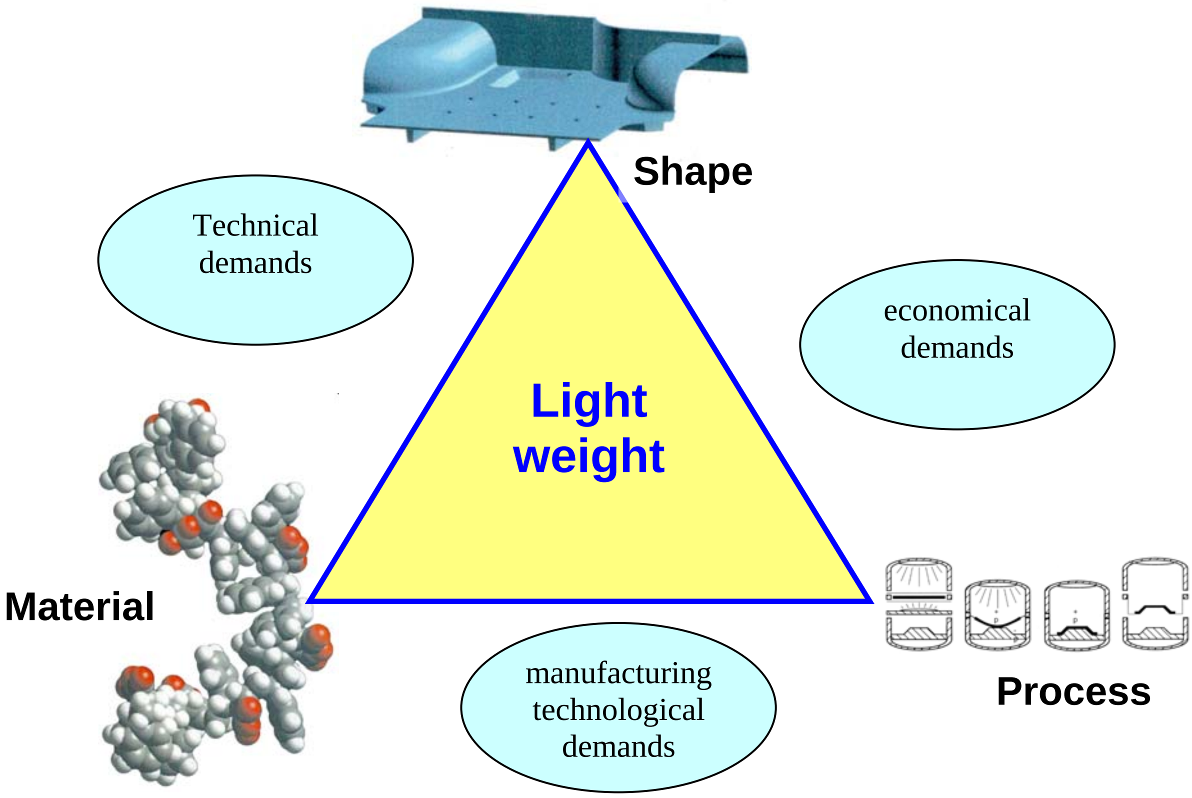
THE CHALLENGE OF COMPOSITE STRUCTURES

Prof. Dr.-Ing. G. Ziegmann, Dipl.-Ing. P. Fideu, Dipl.-Math. F. Klunker
TU Clausthal, Germany

In the field of high loaded structures for advanced applications in aircraft or transport industry, mechanical or civil engineering as well as in sports application polymer composites are well established. Those materials are defined by the matrix, acting as an embedding system and by the reinforcing fibres which take the load in advanced structures. Due to the extreme mechanical/physical properties at low density composites are offering a very interesting weight gain in comparison to lightweight metals (fig. 1).



The application in high loaded structures is driven by the material/material combinations, the geometrical concept as well as by the processes (i.e. autoclave technique, pressforming, RTM etc.) and secondary processes like bonding, welding, riveting etc. Especially with thermoset resins material and structure are created in one step what requires a special focus on the possibilites and limitations for different applications.



The varieties of textile structures-UD-rovings, woven fabrics, knitted braided textiles, noncrimped fabrics etc. - and the freedom in fibreorientation are offering numerous possibilities for optimizing the anisotropic structure regarding optimized structural solutions. Especially the RTM-technique allows optimization strategies by positioning dry textile structures in a mould with applied fibre orientations and by impregnation of the textile with low viscous resin and curing in the mould.

In this presentation some principles on composites, their mechanical/physical properties, some processing technologies and manufacturing principles are discussed, regarding applications in aircraft, transport and sporting goods industry.

OBTAINING NEW MATERIAL PROPERTIES BY EMBEDDING SMALL SIMPLE MACHINES

Gary F. Hawkins and Michael J. O'Brien
The Aerospace Corporation

We have demonstrated that materials with unique properties can be manufactured by embedding many small, simple machines in a matrix. We have been referring to these as Machine Augmented Composites (MAC). The simple machines modify the forces inside the material in a manner chosen by the material designer. When these machines are densely packed, the MAC takes on the properties of the machines just as a fiber-reinforced composite takes on the properties of the fibers. Much of our research has involved small, extruded, nylon machines that are very inexpensive to manufacture yet yield properties not easily obtained in any other manner. We have extended this concept in quite a few different directions. We began this effort by embedding many small '4-bar linkages' in a matrix material to convert compressive stresses into shear stresses. Since then we have put small liquid filled ‘shock absorbers’ into a matrix and measured the resulting damping properties. Currently, we are integrating slightly more complicated machines in the core of a honeycomb material to modify the sound transmission properties. Finally, we are developing a material where we change the pressure in the embedded machines causing the material to change shape.

During this talk, I will review the experiments we have performed, the analytical tools we have developed and some of the potential applications of the material.

Session 8: Cellular Materials

MECHANICAL PROPERTIES OF UNIT-CELL BASED CELLULAR SOLIDS

Alex Woesz
Max-Planck-Institute of Colloids and Interfaces
Department of Biomaterials, woesz@mpikg.mpg.de

Rapid Prototyping was used for the production of cellular solids, which have been designed using computer aided design methods. In a first set of experiments, five structures with constant apparent density but different architecture have been produced from polyamide and tested in compression, revealing that changes in architecture result in variations of strength and stiffness as well as defect tolerance independently from each other by a factor of three. In a continuation, we investigated the influence of the loading direction as well as the influence of an increasing degree of irregularity on strength, stiffness and defect tolerance of structures produced by a digital light processing based rapid prototyping method. In addition, the results were compared with results of finite element simulations, which were performed using beam as well as continuum elements.

THERMOCHEMICAL PROCESSING OF CELLULAR ARCHITECTURES FOR MULTIFUNTIONAL APPLICATIONS

Jason H. Nadler
ONERA, Chatillon, France

Metallic cellular structures require unique processing routes and benefit from a multidiscipinary approach. Some of the processing routes investigated and elaborated include direct reduction, enhanced sintering, electroless, electrochemical and vapour deposition and slurry rheology. Applications include structural acoustic and thermal management as well as impact resistance.

Elastic behaviour of randomly packed hollow spheres metallic foam by finite-element computer simulation

F. Mamoud*, F. Paun*, Y. Bréchet**

** ONERA/DMMP, 29 Avenue de la division Leclerc, 92322 Châtillon Cedex, France*
***LTPCM/INPG, BP 75, Domaine Universitaire de Grenoble, 98402 St. Martin d'Hères Cedex, France*

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