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After a PhD in solid state physics (1979) at the Ecole Polytechnique Fédérale de Lausanne (EPFL) and a post-doc at Oak Ridge National Laboratory, Michel Rappaz joined the Laboratory of Physical Metallurgy of EPFL to start an activity on simulation of solidification in 1984. He was nominated Adjunct Professor in 1990 and Full Professor in 2003, time at which he took the lead of the laboratory, renamed then Computational Materials Laboratory.

The main axis of his research is the connection between macroscopic aspects of solidification and microscopic aspects related to microstructure and defect formation. Beside experimental investigations and validations, his group has developed several new physical modelling tools (in particular cellular automata for grain structure formation and granular model for hot tearing). Many of these developments are commercialised by a spin-off company founded by the laboratory in 1991 and now part of the ESI-group (Calcom-ESI). He initiated in 1992 an annual postgraduate course on solidification which has been attended by more than 700 participants from all over the world. Michel Rappaz has received several awards: the Latsis price in 1990, the Mathewson co-author and author award of TMS in 1994 and 1997, the Koerber foundation award with Profs Y. Bréchet and M. Ashby in 1996, the Sainte-Claire Deville medal of the French Metallurgical Society in 1996, the Bruce Chalmers Award of TMS in 2002, the Mc Donald Memorial Lecture award of Canada in 2005, the Grand Medal of the French Metallurgical Society in 2011. He is a highly-cited author of ISI, a fellow of ASM and IOP, and has co-authored about 300 papers, two books and several proceedings.

Multi-twinned nanoparticles, quasicrystals and twinned dendrites: What is the link?

In the 1960's, it was shown that nanoparticles of metals can be multi-twinned: in order to minimize their surface energy, they are typically made of $\{111\}$ tetrahedra arranged in a five-fold symmetry (e.g., icosahedron), but with some distortion (and elastic energy) involved to compensate for the closure defect. In the 1980's, five-fold symmetry quasicrystals (QC) were discovered in Al-alloys: they inherit the local arrangement of atoms in the liquid already predicted by Frank in the 1950's, without exhibiting translation invariance. On the other hand, twinned dendrites have been observed in Al-alloys under certain solidification conditions for more than 60 years: they are made of $\langle 110 \rangle$ trunks split in their center by coherent $\{111\}$ twin planes. While their growth mechanism is now better understood, nucleation of the twins still remains unclear. Very recently, we have shown that minute Cr additions (typically 0.1 wt%) to Al-Zn alloys solidified in a uniform temperature field spontaneously lead to the formation of fine equiaxed grains. Furthermore, these grains exhibit an unexpectedly large number of twin relationships and some of them are even in a five-fold symmetry twin relationship with a common $\langle 110 \rangle$ direction. These results become fully consistent when one considers that the primary fcc phase forms on facets of QC's, or alternatively on nuclei of the parent stable phase having several five-fold symmetry building blocks in its unit cell. This nucleation mechanism is most probably responsible of twinned dendrite formation, but more important, it could be exploited as a new grain-refining technique in Al alloys and maybe in other fcc metals.



Johan A. Martens

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Johan Martens received his PhD (1985) and his habilitation (1988) in applied biological sciences at the KU Leuven. He started his academic career 1982 at the Research Foundation Flanders; from 1988 on he was lecturer, later senior lecturer at KU Leuven. 1997 he became a professor at this university, being the Head of the Department of Microbial and Molecular Systems (2005-2010) and also the Head of Centre of Excellence in Catalytic Science (2005-2009).

Professor Martens' core expertise is in synthesis and application of functionalized nanoporous materials in catalysis, adsorption, molecular separation and controlled release. He contributed substantially to the understanding of molecular mechanisms of formation of structured nanoparticles, zeolites, ordered mesoporous materials and porous materials in general. He performed experiments under microgravity in the International Space Station, and combined advanced physico-chemical techniques to reveal the supramolecular assembly mechanisms of inorganic structures on organic sacrificial templates. Professor Martens has never been constrained to a single area of research and has always been attracted by real-world problems, seeking collaboration with colleagues from other disciplines and especially physics and pharmaceutical and biomedical sciences to tackle scientific challenges of high societal relevance. Quite unique is that he has contributed to very fundamental studies as well as to the implementation of fundamental knowledge into practical solutions. In this sense he is a pioneer of translational research.

45 patent families were granted to Professor Martens. Several of these basic research inventions are being implemented in commercial applications or commercialized in spin-off companies founded by him. Johan Martens received several awards: the Exxon Chemical Biannual European Science and Engineering Biannual Award in 1995, the ESA Certificate of Merit in 2002, the "Enterprize 2005" – a contest for innovation and entrepreneurship in Belgium. 2009 he received the Methusalem funding – the highest level of structural funding in Flanders granted in regard to proven excellence. Since 2012 he is an active member of the Royal Flemish Academy of Belgium for Sciences and the Arts.

Opportunities in Synthesis and Application of Nanoporous Materials

Many applications take advantage of the large accessible pore volume, uniform pore size and pore walls with unique adsorptive and catalytic functions offered by nanoporous materials. Over 5 million tons of synthetic zeolites are yearly produced in industry for three main applications: detergents, molecular separation and catalysis. In the past two decades several new generations of nanoporous materials have been discovered holding great promise for many more applications, but industrial breakthrough of the new nanoporous materials often is hampered by high manufacturing cost and upscaling difficulties. In this lecture two new synthesis approaches are presented overcoming these difficulties.

We have developed a facile method of creating ordered mesoporous silica (OMS) materials with potential application in drug delivery and chemical sensing. OMS usually is synthesized either in strongly acidic or basic synthesis mixture under hydrothermal conditions maintained for hours. We discovered a synthesis protocol at neutral pH and ambient temperature using cheap reagents producing OMS within seconds. The synthesis can be carried out in a continuous

process by combining a stream of sodium silicate with buffered P123 triblock copolymer solution in a receptacle. The obtained OMS platelets with short identical channels and thick pore walls are sufficiently robust for applications in drug delivery and chemical sensing. In a recent phase 1 clinical study the use of OMS carrier material for enhancing the bioavailability of fenofibrate, a drug to reduce cholesterol levels in patients at risk of cardiovascular disease, was demonstrated. In another application OMS film applied on silicon photonic micro-ring resonator enables selective and reversible ammonia gas detection at ppm concentration level.

A potentially attractive development is the use of relatively weak permanent magnetic fields to assist materials synthesis. Magnetic fields applied on circulating liquid mixtures previously have been demonstrated to assist formation of monodisperse emulsions, to facilitate nano-aggregate breakup, and to be beneficial in Mo-V-Sb mixed oxide catalyst synthesis. Our latest discovery is that weak external magnetic fields facilitate formation of materials containing antiferromagnetically coupled paramagnetic ions. This magnetohydrodynamic effect is demonstrated for three different, technologically relevant materials: HKUST-1 type metal-organic framework encapsulating $\text{Cu}_{1.5}[\text{PW}_{12}\text{O}_{40}]$ polyoxometallate, manganese oxide nanotubes and mixed valence vanadium oxide gels, the precursor of vanadium oxide nano-scrolls used as cathode material in a rechargeable lithium battery. Although the detailed mechanism of the observed magnetic field effect is yet to be discovered, this simple, practical and versatile strategy could innovate crystallization of a wide variety of materials with technologic and economic relevance. Besides increasing efficiency of their synthesis, the magnetic field permanently and drastically improves magnetic order in the material. The systematic observations for different materials allow prediction which chemical systems can benefit from magnetically enhanced synthesis.

To be presented at EUROMAT 2013, Seville, Spain

**Michel Perez**

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Michel Perez received his engineer degree and his master degree in Materials Science from the University Lyon / INSA Lyon. 2000 he received his PhD with honours at INP Grenoble with a thesis on contactless viscosity measurement by gas film levitation technique. In the next two years he was a post doc at INSA Lyon with the GEMPPM; at this time he got involved with modeling of precipitation phenomena. Dr. Perez was nominated 2001 assistant professor at INSA Lyon with the MATEIS group; 2007 he defended his habilitation thesis "Multi-scale approach of precipitation" and was nominated 2010 full professor at the same institute.

Precipitation phenomena in metallic systems are a central area of interest of Prof. Perez; he developed activities with ferrous systems (martensite tempering, precipitation of copper in steels and of carbonitrides in steels) and aluminium alloys. On the basis of these activities he is currently working in atomic scale techniques to model precipitation phenomena, coupling Molecular Dynamics and Kinetic Monte-Carlo tools. Further areas of interest of Prof. Perez are the mechanical properties of block copolymers and of entangled materials, building up from 3D tomography to discrete element methods.

Prof. Perez received 2012 the Jean Morlet Prize of the Société Française de Métaux et Matériaux (SF2M).

Multiscale approach to steel design

We present here a multi-scale modelling approach to steel design: from *ab initio* to Finite Element Methods. This approach will be illustrated on far-from-equilibrium phases, obtained after FeC coatings on a steel sheet. *Ab initio* techniques are used to construct an interatomic FeC potential for Molecular Dynamics simulations. Resulting potential energy landscapes serve as entry parameters for Atomic Kinetic Monte-Carlo, which, itself, predicts long-term microstructure evolution kinetics. Then, Mean Field precipitation and diffusion models provide solute content and phase fractions evolutions at different location of the component. Finally, this information is used to get the constitutive relation at each node of a Finite Element mechanical calculation. Modelling results are validated with various experimental techniques from the atomic scale (Tomographic Atom Probe) to the specimen scale (tensile tests).

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