HIGHLIGHTS SIMaP 2011 : PM team

Hardening precipitation in Al-Li-Cu alloys: a new approach based on high resolution advanced electron microscopy and the crystallography of complex metallic alloys

In Al-Li-Cu alloys, the T_1 phase precipitates are well known for their beneficial effect on mechanical properties. A detailed characterization (morphology, size, density, composition, structure ..) of the precipitation is required to understand the interaction between precipitate and matrix dislocations and further model and predict the impact on mechanical properties. The global characterization is performed with small angle X-ray scattering (SAXS) methods using the synchrotron ESRF facilities. This allows for a quantitative study of the precipitate density and volume fraction including under *in situ* conditions (strain and/or heating) [1].
Of crucial importance is also the structure and stoechiometry of the T_1 precipitates, which are likely to deviate from those of the bulk T_1 phase. This structure has been determined using Z contrast imaging (HAADF-STEM) on Cs corrected microscope (double correction Titan cube - CCEM McMaster university). The Z contrast images allow to rule out the structures earlier suggested. In addition, we have shown that the T_1 precipitate structure corresponds to a complex arrangement involving high coordinance polyhedra as expected in complex metallic alloys [2]. The structural analysis based on the crystallography of complex phases can then be performed. It constitutes a brand new approach for the understanding of the formation of nanoscale precipitates.

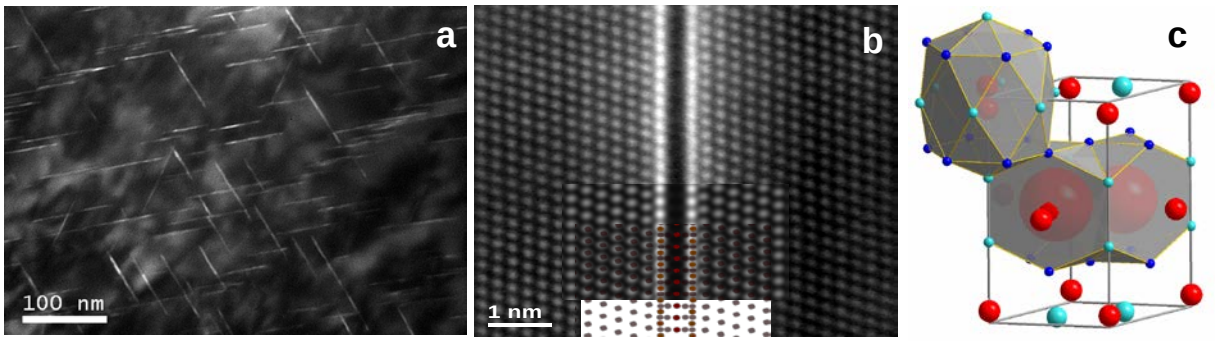

Figure 1: a) T1 phase precipitates forming thin platelets in the Aluminium matrix (conventional TEM DF image), b) High resolution STEM HAADF images showing the T1 phase precitate structure, in insert the model structure and its simulation, c) Complex coordinance polyhedra involved in the T1 phase.

[1] *Mapping the microstructure of a friction-stir welded (FSW) Al-Li-Cu alloy*. F. De Geuser, F. Bley, A. Denquin, A. Deschamps, Journal of Physics: Conference Series 247, 012034 (2010).
[2] *Atomic structure of T1 precipitates in Al-Li-Cu alloys revisited with HAADF-STEM imaging and small-angle X-ray scattering,* P. Donnadieu, Y. Shao, F. De Geuser, G.A. Botton, S. Lazar, M. Cheynet, M. de Boissieu, A. Deschamps, Acta Materialia,59, 2, 462 (2010).

National and international collaborations: ESRF, McMaster University, Canadian Center for Electron Microscopy, Alcan CRV
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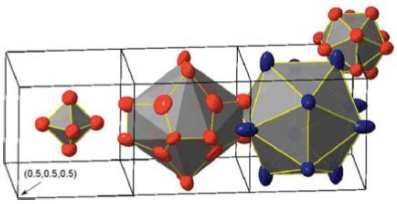
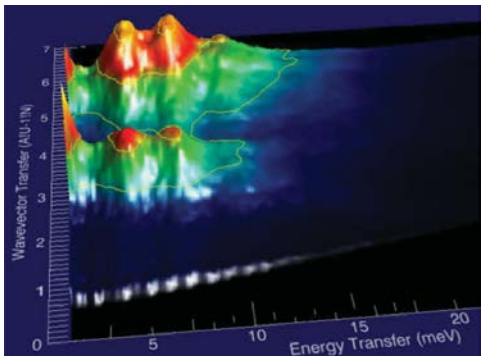
Anomalous vibrational dynamics in the Mg_2Zn_{11} phase by a Si single crystal surface

The Mg_2Zn_{11} phase presents an intermediate degree of complexity between more simple phases and quasicrystalline phases or approximants of these quasicrystals. Its can be described as a cubic packing of a triacontahedron whose centre is partially occupied by a Zn atom. The lattice dynamics of this phase, studied by X-ray and neutron inelastic scattering, presents low energy modes and a singularity around 4 meV, which is a unique feature for a nearly-close-packed metallic alloy. Simulations by ab-initio methods and using empirical EAM potentials describe well the experimental results and evidence the importance of the partially occupied site for the low energy modes. A detailed analysis of the vibration eigenmodes is presented, relating the characteristics of the vibrational spectrum to the atomic movements in the structural atomic blocs. This work has been accomplished in the framework of the European network CMAC (www.eucmac.eu).

H. Euchner, M. Mihalkovic, F. Gahler, M. R. Johnson, H. Schober, S. Rols, E. Suard, A. Bosak, S. Ohhashi, A.-P. Tsai, S. Lidin, C. Pay Gomez, J. Custers, S. Paschen, and M. de Boissieu, PHYSICAL REVIEW B 83, 144202 (2011)



Structure of the Mg2Zn11, showing the successive layers in the atomic clusters



Measure of the inelastic scattering function S(Q, E) showing a peak around 4 meV

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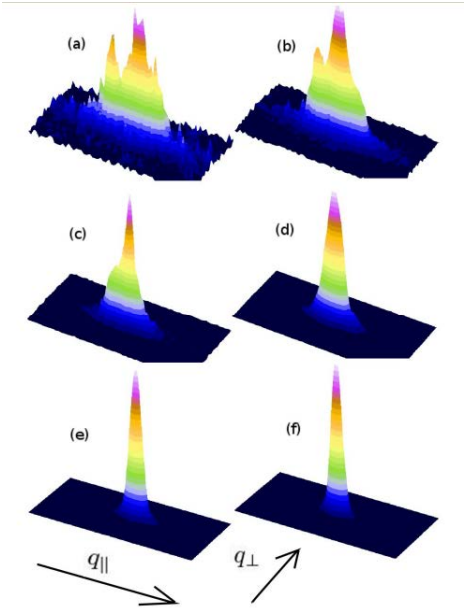
Coherent X-ray diffraction by a Si single crystal surface

Using coherent X-ray scattering, we evidence atomic step roughness at the (111) vicinal surface of a silicon monocrystal of 0.05° miscut. Close to the ½ ½ ½ anti-Bragg position of the reciprocal space which is particularly sensitive to the (111) surface, the truncation rod exhibits a contrasted speckle pattern that merges into a single peak closer to the (111) Bragg peak of the bulk. The elongated shape of the speckles along the (111) direction confirms the monoatomic step sensitivity of the technique. This experiment opens the way towards studies of step dynamics on crystalline surfaces.

F. Livet, G. Beutier, M. de Boissieu, S. Ravy, F. Picca, D. Le Bolloc'h, V. Jacques, Surface Science 605 (2011) 390–395



The transverse shape of the truncation rod for various (h,h,h) vectors at different successive distances between the anti-Bragg position (1/2,1/2,1/2) (a) and the Bragg peak (111). a : h=1/2, b : h=0.56, c : h=0.63, d : h=0.69, e : h=0.75, f : h=0.81.
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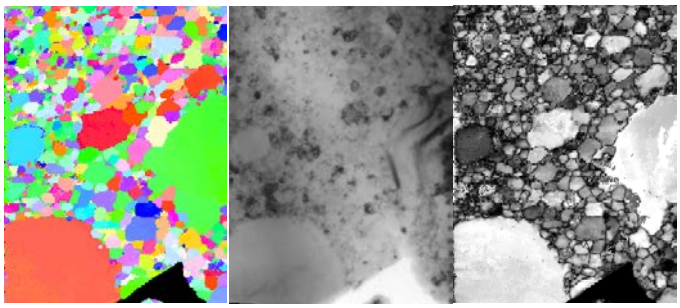
HIGHLIGHTS SIMaP 2011 : GPM2 team

EBSD for TEM: Automated Crystal Orientation Mapping (ACOM) package for Transmission Electron Microscopes

The ACOM/TEM package is an automatic crystallographic orientation indexing tool developed for transmission electron microscopes. The diffraction patterns are acquired thanks to a CCD camera. The crystal orientation is obtained by mapping the spot diffraction patterns with pre-calculated templates. Image matching techniques are used to select the template with the highest correlation index. The measurement of orientations of crystals in textured materials is generally performed in Scanning Electron Microscopy (SEM) by using Electron Back Scatter Diffraction (EBSD) technique. The main serious drawbacks of this technique are the sensitivity of Kikuchi's patterns to deformation and the limited spatial resolution. Non-conductive materials are also difficult to analyse by EBSD. Alternatively, orientation measurements can be done with TEM where image resolution below 1 nm can be reached if the microscope is equipped with a Fields Emission Gun. ACOM/TEM is a new approach based on the nano-beam electron diffraction (NBED) technique to extract the orientation from Bragg spot patterns. It allows the local orientations to be measured in nano-structured. Moreover the spot pattern is not critically sensitive to dislocation densities and severely deformed metals may be analysed without problem.



a b c

Application of the ACOM/TEM software to sintered nanocrystalline Al powder, step size 15 nm, maps measured on a JEOL 3010 equipped with a LaB_6 gun: a) bright field image, b) orientation map and c) reliability map.

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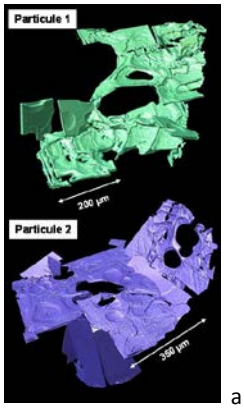
In-situ x-ray microtomography applied to alloys in the semi-solid state

X-ray microtomography has been extensively developed during the last few years particularly in terms of spatial and temporal resolutions owing to the use of synchrotron radiations. SIMAP has contributed to these developments in relation with the staff of the ID19 and ID15 beamlines of ESRF. SIMAP has studied in-situ the formation of solidification structures in aluminium alloys, their evolution during a thermal treatment in the semi-solid state and the deformation mechanisms of these alloys when they are deformed in tension in the solidification interval. Microtomography has therefore allowed observing in-situ the nucleation and growth of Fe-based intermetallics (Al_5FeSi) in Al-Si-Cu-Fe alloys [1], visualising in 3-D the evolution mechanisms of Al-rich dendrites in binary Al-Cu alloys [2,3] and characterising the liquid flow and the formation of pores and hot tears during the tensile deformation of a semi-solid alloy [4]. These studies allow better understanding the formation of microstructures end defects during the elaboration processes of alloys by solidification thus contributing to the optimisation and improvement of the resulting properties.



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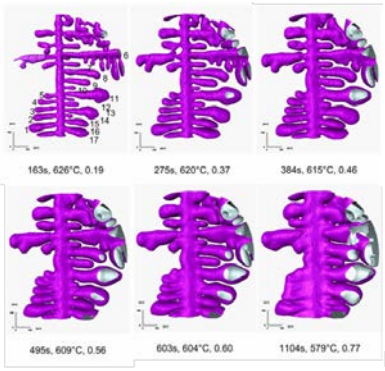

b

a. 3D image of intermetallic particles after solidification of an Al-Si-Cu-Fe alloy

b. Evolution of a dendrite during solidification of an Al-Cu alloy

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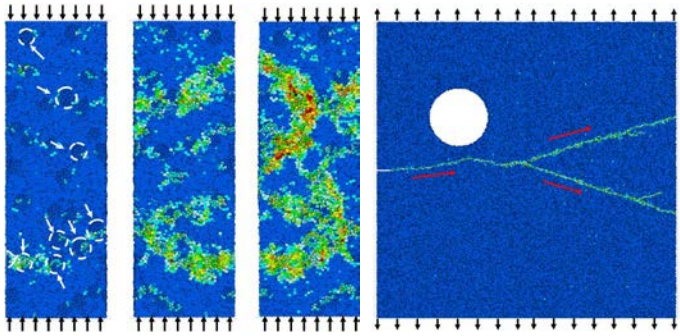
Discrete element simulations: simulation of materials strength

Originally designed for geomaterials, the Discrete Element Method (DEM) is now also a powerful simulation tool in materials science applications. The dp3D code, developed at SIMaP, allows complex three-dimensional microstructures originating from ceramic or metallic powders to be reproduced at the length scale of individual particles. Thanks to the use of realistic contact laws, the mechanical and conductive behavior of these microstructures can then be quantitatively obtained. Partially sintered porous electrodes used in SOFCs (Solid Oxide Fuel Cells) are a good application example. These electrodes may be compositionally graded, multi-layered or fabricated with large pore formers (fig. a). Another particularly interesting feature of DEM is that fracture is simply coded at the length scale of particles. Thus, strength and toughness can be readily obtained, with microstructure optimization as the final goal of the simulations (figure b). The last developments are directed toward the use of dp3D to represent fully dense material with an emphasis again on the fracture behavior.



a b

a) Damage evolution during compression of a SOFC porous electrode sintered with large (white) pore formers

b) Crack evolution in a pre-notched sample under tension. Note how the crack is deflected by the hole

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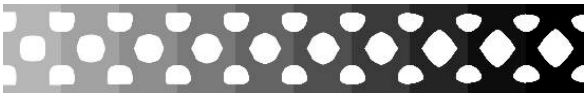
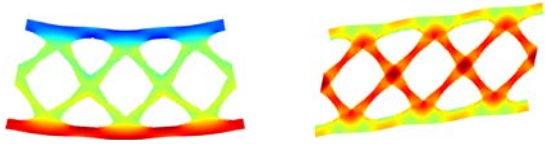
Topological optimization of architectured materials

Architectured materials are especially interesting when multiple functionalities (*e.g.* stiffness and thermal insulation) are required. Finding the architecture that combines in the most efficient way a given set of conflicting properties is a key issue. In particular, the infinite number of possible shapes leads to non-trivial optimization problems. In such a context of "material by design", we have developed a numerical approach based on topological optimization techniques. The distribution of matter is defined thanks to a level-set function, and the convergence toward the optimized pattern is performed through the evolution of this function. An application is presented here for the optimal design of a periodic architectured core material implemented in a lightweight flexural panel. It consists in finding the distribution of matter in the unit cell that gives the best compromise between the conflicting shear and flexural stiffness. Fig. (a) shows different iterations of the optimized solutions, for a given weight given to shear and flexural stiffness. Evolution of matter depends on stress state calculated by finite element method, fig (b). Prototypes of the optimized solutions have been fabricated by selective laser sintering of PA6 powder and an experimental validation has been completed by four-point bending.

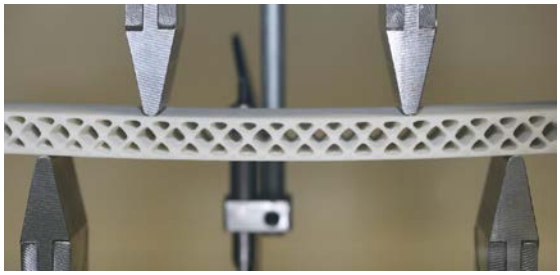
a.



b.



c.



a) Geometry evolution of the unit cell from starting geometry (left) to optimized (right) architecture. The volume fraction is given and remains fixed all along the optimisation procedure.

b) FEM simulation for respectively bending and transverse shear.

c) Four-point bending test on a specimen elaborated by selective laser sintering

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HIGHLIGHTS SIMaP 2011 : SIR team

Behavior of ferritic stainless steels stabilized during the annealing and pickling stages

During the industrial processing line of stainless steel flat product, a **short annealing** (approximately 60 s) at high temperature under an oxidizing atmosphere ($O_2/H_2O/CO_2/N_2$) is carried out after cold rolling. This annealing leads to the formation of a thin oxide layer (chromia) removed by pickling. In order to control the product quality, the phenomena occurring during these stages must be understood. The metal/oxide interface of oxidized samples was **three dimensional reconstructed** using a scanning electron microscope coupled with a focused ion probe: **MEB-FEG/FIB**. At the metal/oxide interface, metallic protrusions (in blue) are localized in the chromia layer (in red) through a discontinuous silica film (in green).

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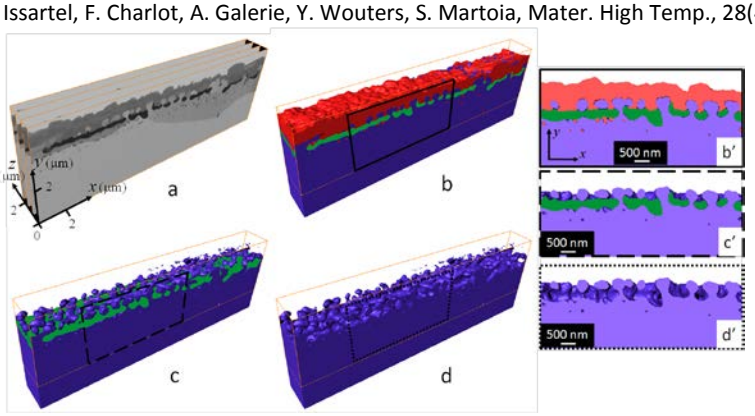
J. Issartel, F. Charlot, A. Galerie, Y. Wouters, S. Martoia, Mater. High Temp., 28(4), in press



Three dimensional reconstruction of the metal/oxide interface.

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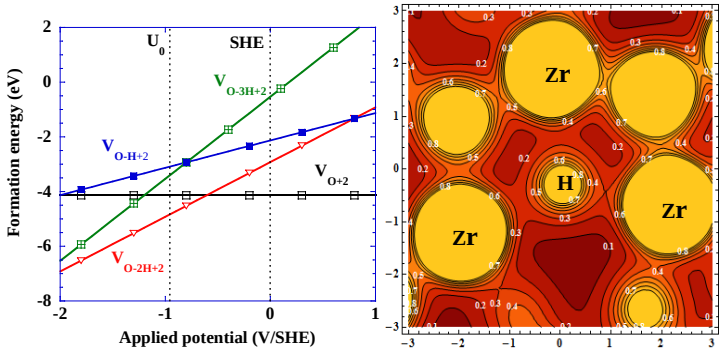
This work has been carried out during the thesis of Jérôme Issartel in collaboration with the technical centre of APERAM Isbergues (France)

Density Functional Theory study of corrosion of Zirconium alloys

Modelling the corrosion process from scratch is a formidable task due to the different length and time scales involving in this process. DFT based calculations can be combined with thermodynamic and kinetic concepts to develop a multi-scale modelling approach of corrosion. As an illustrative example, we study corrosion properties of zirconium alloys used as fuel cladding in nuclear reactors. We investigate the hydrogen effect on the stability of oxygen vacancies in ZrO_2 oxide in aqueous environment. We found that the nature of the medium (gaseous or aqueous, considered at various pH) appears to be a key factor in controlling the predominant defect at the oxidizing interface. In particular, we show that in a reducing environment, a complex defect consisting of an oxygen vacancy and a hydrogen atom (V_{OH}, see contours plots beside) is more stable than any other form of hydrogen in ZrO_2. The nature of this is determinant to explain the enhanced oxidation kinetics observed for zirconium alloys in aqueous conditions.

References

B. Malki, O. Le Bacq and A. Pasturel, J. Nucl. Mater., 416, (2011) 362.
A. Janotti and C. G. Van De Walle, nature materials, 6, (2007) 44.



Left: Calculated defect formation energies for various $V_{O\text{-}nH}$ complexes as function of the potential (U/SHE) for pH 7 and in reducing aqueous environments.

Right: Contour plots of the electrons charge densities ($e/Å^3$) for the V_{OH} complex in the plane of the three nearest Zr atoms.

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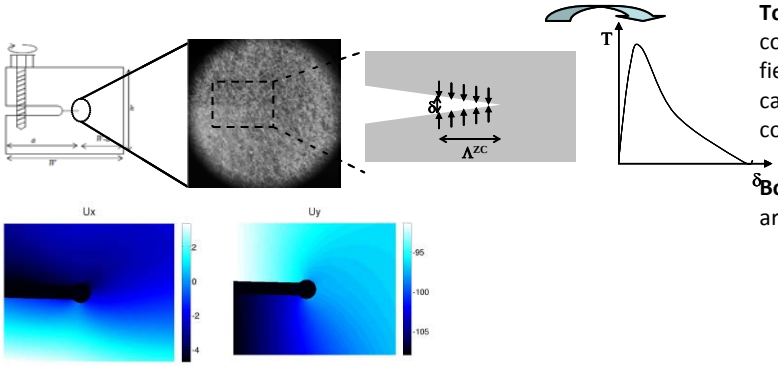
Identification of Cohesive Zone models

Cohesive zone models are used to mimic mechanically the materials fracture or adhesion mechanism. Within a local approach of fracture, this description incorporates intrinsically a length scale that enables the investigation of size effects explicitly. Except in specific cases in which a direct observation of the fracture/adhesion process zone is possible, cohesive models are calibrated from macroscopic measurements and motivated on available physics. At SIMaP (R. Estevez, M. Braccini, G. Parry) and in collaboration with LaMCoS (J Réthoré, INSA Lyon), we attempt to observe the local displacement fields from DIC in order to extract the local stress intensity factors and position of an equivalent elastic crack during the loading. These inputs are used to identify a representative cohesive zone in a finite element calculation. The methodology is exemplified in the fracture of PMMA and is currently under development for the characterization interface mechanics with a blister test available at the laboratory.

References

Estevez R., Réthoré J., 2011, "Identification expérimentale d'une zone cohésive par traitement d'images, Exemple pour une rupture par craquelage dans un polymère amorphe ", 10e colloque national en calcul des structures, CSMA, Giens.



Top: description for the identification of cohesive zone model. Local displacement fields are extracted from DIC and FE calculations are used to identify the cohesive zone model

Bottom: Extracted displacement fields around the crack tip.

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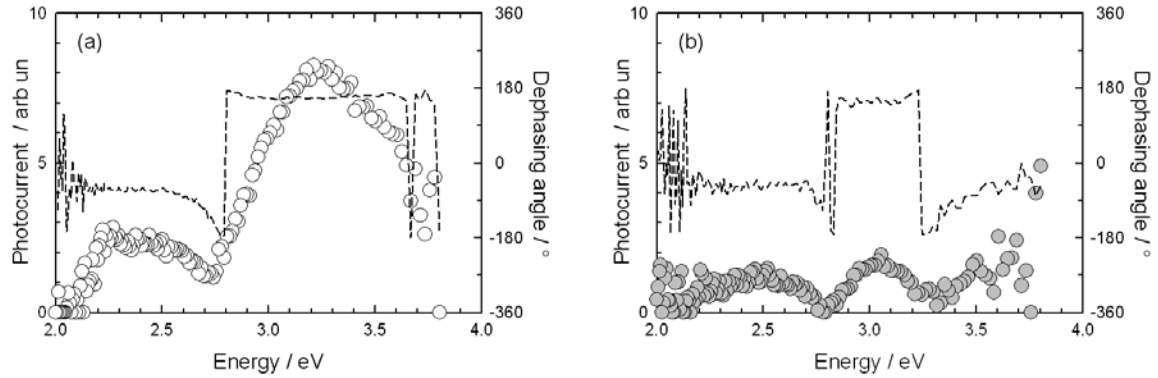
Towards multiscale photoelectrochemical characterizations

A first multiscale photoelectrochemical characterization of oxide layers was performed, by adding the mesoscopic scale (ca 30 µm) to the microscopic (ca 1µm) and macroscopic ones. For the first time, indeed, photocurrent energy spectra could be recorded, on individual ferritic and austenitic grains of an unique 2205 duplex stainless steel oxidized sample. These spectra allowed to explain contrasts issues in the photoelectrochemical images obtained from the oxidized sample. Moreover, the bandgap energies obtained by fitting these individual mesoscopic photocurrent energy spectra, with a novel approach developed in our team, showed that all oxide scales were constituted of Fe_2O_3 and Cr_2O_3 and of a $Fe_{2-x}Cr_xO_3$ solid solution, but that the x-value of the latter was different depending on the metallurgic phase of the oxidized substrate.

References

A. Srisrual, J.-P. Petit, Y. Wouters, C. Pascal, A. Galerie, Mat. High Temp. 28(4), in press.



Photocurrents vs. energy spectra and its dephasing angle obtained on an individual grain of (a) austenitic grain and (b) ferritic grain

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This work is part of the PhD thesis of Anusara Srisrual, lecturer at the University of Bangkok (Thailand

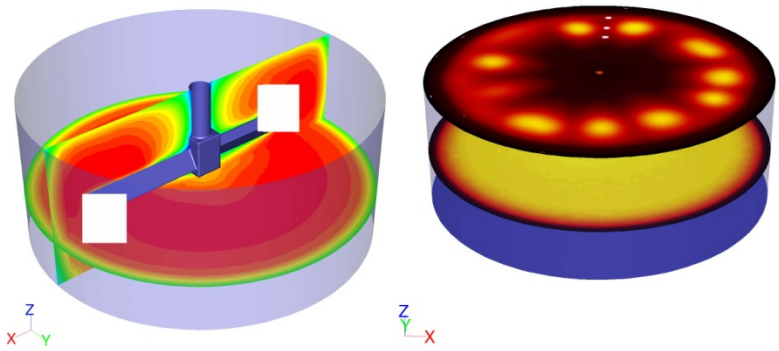
HIGHLIGHTS SIMaP 2011 : EPM team

Cold crucible for nuclear waste vitrification

scientific leaders : Annie Gagnoud, Yves Fautrelle

On April 17, 2010, at nuclear fuel reprocessing plant in La Hague, the first container of vitrified waste was processed using a cold crucible technology. Due to a collaboration between CEA-Marcoule and AREVA, this process reduces by a factor of 2-3 the volume of the technologic waste, thanks to the increase of the life of molten glass pots, moreover, by increasing the concentration of waste in the glass, it decreases approximately 25% of the volume of produced glass.

The numerical models that have allowed the scaling up of the cold crucible have been achieved through ongoing collaboration between the EPM group and CEA-Marcoule, in the form of four theses (Denis Saumabère (1994), Laetitia Jacoutot (2006), Emilien Sauvage (2009) and Marcio Da Silva (current)).

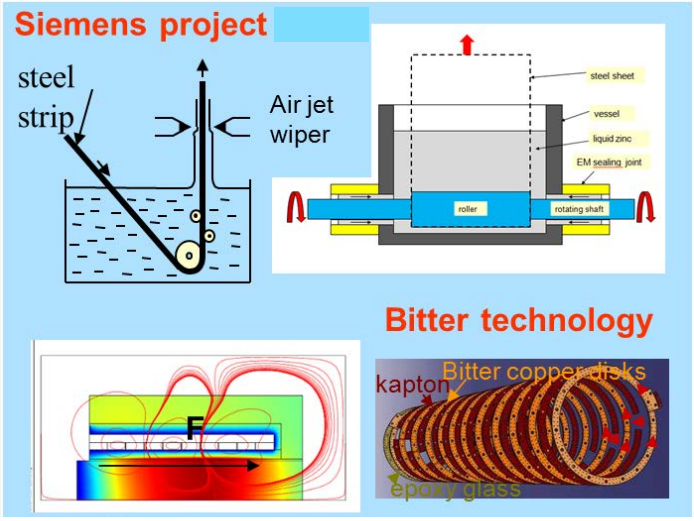


Validation of an electromagnetic seal on the industrial galvanizing pot at CRM Belgium

scientific leaders : Roland Ernst, Mikaël Dumont

Since 2005, a collaboration is committed with Siemens SVAI (subsidiary specializing in equipment for galvanizing lines-zinc deposit liquid steel plates) on innovation aspects including a set of electromagnetic systems.

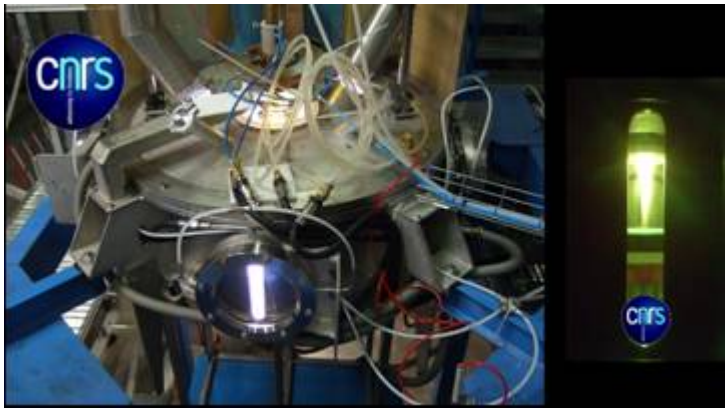
The first part had been focused on the achievement of a device (electromagnetic seal) in collaboration with IPUL (Latvia). Using electromagnetic forces that offset the effects of gravity, this device holds the liquid zinc in the electroplating tanks at the bearings of the rollers that immerse the plate in the tank of molten zinc. This reduces maintenance costs. The project was to design, to scale (analytical computation, modeling) and to built a prototype to be integrated into an industrial plant. Based on a traveling magnetic field produced thanks to a "Bitter" technology -50Hz-100kW. The system was successfully tested on site for a week long in September 2010 on a tank (about 9t) filled with 1m high of liquid zinc.



Startup of the "SUSI" platform at INES Chambery

scientific leaders : Yves Delannoy, Guy Chichignoud

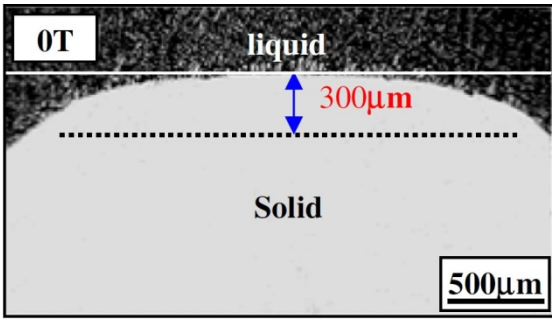
The use of inductively coupled plasma can promote the formation of volatile species and thus obtain purified material. The experimental facility SUSI, started in June 2011, is dedicated to the study by spectroscopy of active species formed in situ by the plasma. Large windows (200mm diameter) combined with a spectrometer equipped with a CCD camera allow a full and rapid qualification of the plasma. Compared to the “Maia” platform based at SIMAP, this facility has a higher plasma power (60kW instead of 40kW), a more accurate and complete instrumentation (flow rates, gas, temperature, frequency ...) for the achievement of balance sheets, an effective system to minimize suction fouling of the enclosure and security conditions suitable for the injection of reactants (H2) at the highest concentrations. It will soon be equipped with a silicon furnace of a 20kg capacity.

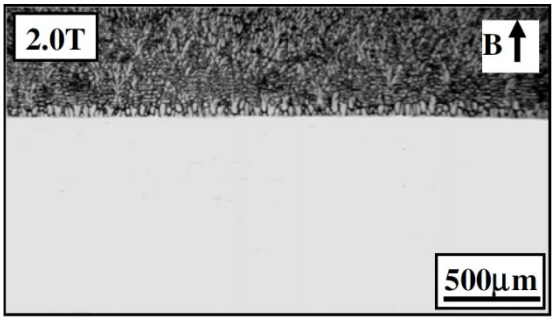


Influence of an axial uniform magnetic field on the solid/liquid interface curvature and macrosegregation in directionally solidified the Al-0.85 wt% Cu alloy

scientific leaders : Yves Fautrelle, Annie Gagnoud, Xi Li

The effect of a uniform magnetic field on both the shape of the solid / liquid interface and the solutal concentration in the solid has been studied experimentally and numerically. The shape of the liquid / solid interface and segregation in the solid are strongly influenced. These results suggest that the thermoelectric convection plays an important role in the directional solidification under a magnetic field. (X. Li et al. / Materials Letters 65 (2011) 3340–3343)





HIGHLIGHTS SIMaP 2011 : TOP team

Throwing light on the undercooling puzzle

Undercooling was discovered in 1724 by Fahrenheit while observing that water droplets stay liquid below 0°C. However numerous questions about the underlying mechanisms remain nowadays still open. In the 1950's, theoricians postulated the structure at the atomic level to be incompatible with crystallization. This led to the speculation that the atoms in the liquid could locally arrange in icoahedra characterized by a five-fold symmetry. Fifty years after, *ab initio* molecular dynamics simulations revealed for the first time five-fold coordinated clusters (pentagons) in pure liquid metals as well as liquid alloys, some of them being known to form quasicrystalline phases upon rapid solidification [1, 2].
Using *ab initio* molecular dynamics simulations, a new remarkable undercooling phenomenon has been explained [3], namely an undercooling as deep as 350°C for Gold-Silicon eutectic alloy in contact with a specially decorated silicon (111) surface where the outermost layer of the solid featured pentagonal atomic arrangements. Such a five-fold coordinated surface influences the short-range order and the metastability of the liquid, favoring the existence of pentagons in this phase. This result has wide. For instance it should lead to important technological applications in the field of nanowire growth for which the eutectic alloy act as a catalyst. It is also speculated that the containerless techniques required today to obtain undercooling could be in the future be replaced by icosahedrally coated solid containers.

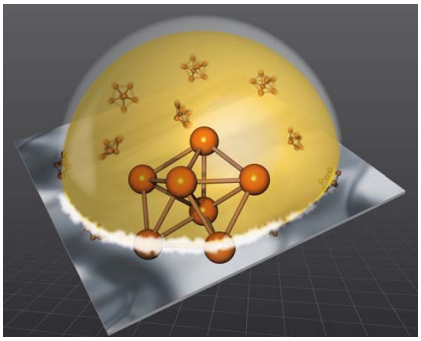


Figure 1: Pentagonal arrangements in the gold-silicon eutectic droplets are stabilized by a decorated silicon (111) surface.

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National and international collaborations: ESRF, RTRA Nanosciences, TU Wien
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The electromagnetic phase separation technique in the determination of solid / liquid equilibria in multicomponent systems

The knowledge of liquid/solid equilibria is of particular interest in the development of special materials with high characteristics, or in solidification process applications. The electromagnetic phase separation (EPS) technique, developed at the laboratory a few years ago, constitutes a powerful and viable technique to establish phase relationships in the solid/liquid range of a large variety of metallic systems, by maintaining long time annealing at high temperature, and thus to achieve the constitution of solid and liquid phases in equilibrium at selected temperatures and compositions. The method is appropriate for systems with volatile and reactive components to be studied at relatively high temperature.
Fe-W-C and Fe-Ti-B ternary systems and Al-based systems have been investigated successfully to determine equilibria involving a liquid phase. In the case of the Fe-W-C system, the link between DTA- determined temperatures and micrographs is not direct and the settling effect of WC carbides has to be taken into account. The EPS technique allows to determining the equilibrium states involving the liquid phase between 1423 K and 1543 K and to specifying the position of the liq./ WC+gamma and liq./WC+M_6C univariant lines.

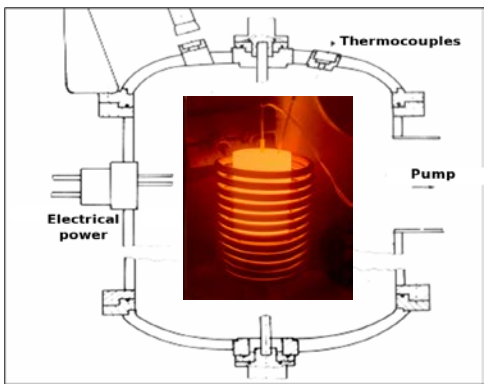


Figure 1. Medium frequency induction furnace (10 kHz

National collaborations: ANR ADRERA project
Contacts: A. Antoni-Zdziobek, TOP

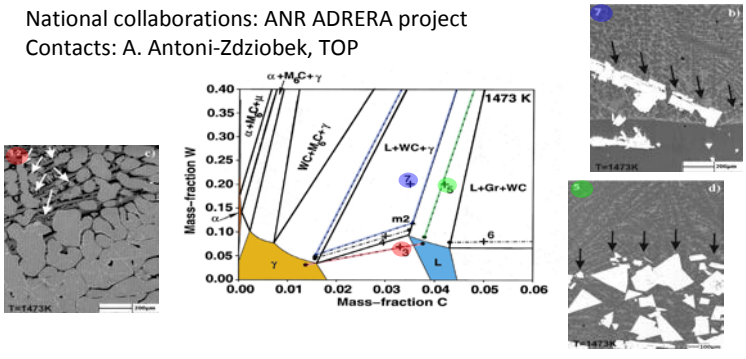
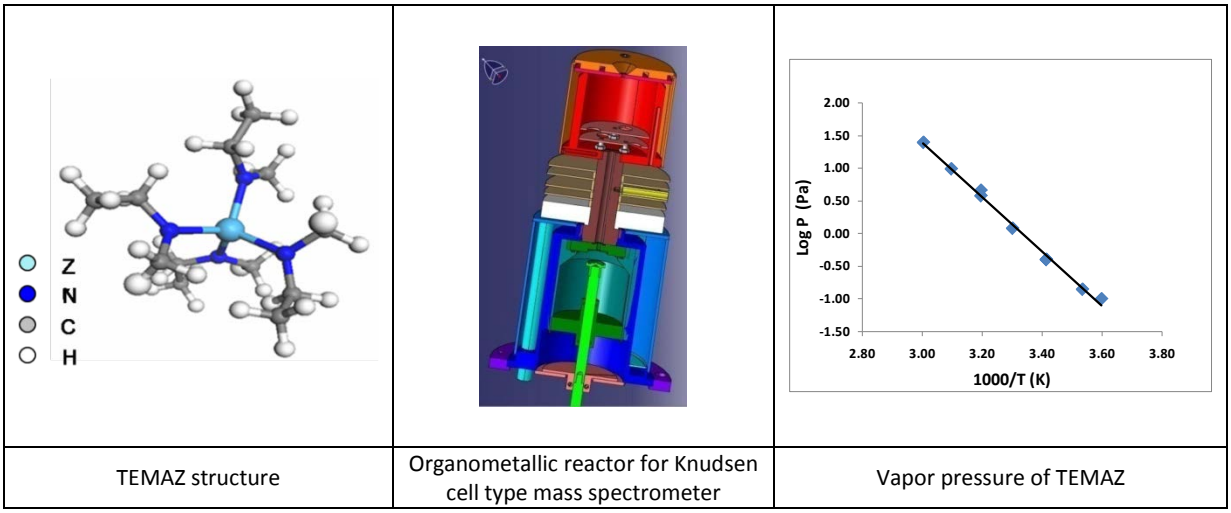


Figure 2. Composition of phases in equilibria corresponding to tie-lines and tie-triangles on the isothermal section at 1473 K of the C-Fe-W system. The arrows indicate a boundary limiting a liquid area. The coarse solid phases are located below this boundary.

Gaseous phase study of the ALD organometallic precursors

Organometallic molecules are commonly used as gaseous precursors in Atomic Layer Deposition/ Chemical Vapor Deposition (ALD/CVD) processes. However, the use of these molecules, which are generally thermally unstable at temperatures close to the deposition one, require an understanding of their gas-phase chemical behavior. The thermal cracking of the gaseous precursor as pentakis dimethylamino tantalum (PDMAT), tetrakis(ethylmethylamino)zirconium (TEMAZ), new in the ALD/CVD TaN deposition processes, has been studied in the temperature range from 343 to 723K and 278-333 K, respectively. To study these two precursors a specific reactor coupled with our Knudsen cell type mass spectrometer has been built in the laboratory. The reactor could work either as a conventional Knudsen evaporation cell - where the organometallic sample is evaporated using the only lower (or first) Knudsen cell and the mass spectrometric analysis is thus performed on saturated vapors - or like tandem cells (the evaporation cell linked to the cracking cell) in order to analyze the non-saturated gas phase issued from the thermal decomposition. The first effusion cell reproduces conditions existing in the bubbler of an ALD system and the cracking cell that of the transport lines and the ALD oven.

The study of thermal cracking of PDMAT from 343 to 723K showed that the precursor was a minor component of the gas phase, meanwhile $Ta(NC_2H_6)_4$(g), and HNC_2H_6 (g), were the major gaseous species that decompose at higher temperatures. Oxygen containing molecules were also observed in all temperature ranges. The final decomposition of the amine branch occurred at relatively high temperatures compared to those of any ALD process and at that time the deposited solid phases in the cracking cell could have reacted with cracked gaseous species to produce water. For better ALD process understanding, the obtained results suggest to use a low deposition temperature to avoid PDMAT decomposition and add a reducing molecule such as hydrogen to reduce the oxygen contamination.
For TEMAZ in the 278-333 K temperature range, no decomposition was observed.



TEMAZ structure	Organometallic reactor for Knudsen cell type mass spectrometer	Vapor pressure of TEMAZ

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