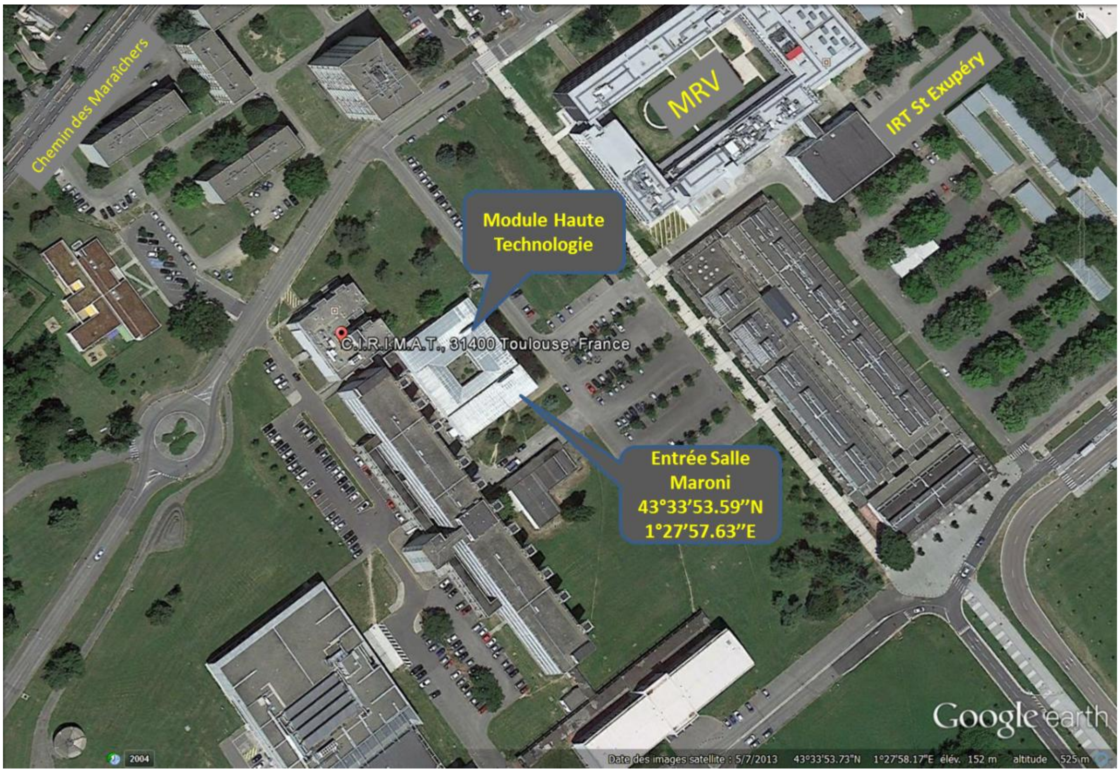
STAE TOULOUSE

Vieillissement des Matériaux Avancés

Le Chantier « Vieillissement des Matériaux Avancés » du Réseau thématique de recherche avancée Sciences et Technologies pour l'Aéronautique et l'Espace (RTRA STAE) organise un mini colloque en science et génie des matériaux (SGM). Structuré autour de deux interventions, assurées par deux Professeurs invités par le RTRA, il vise à établir des ponts entre les problématiques amont en SGM, et leurs pendants technologiques. A ce titre, le public concerné est tant les ingénieurs des bureaux d'études des sociétés industrielles du domaine AESE que les chercheurs et enseignants chercheurs des laboratoires académiques et des EPICS qui mènent des travaux dans ce domaine.

**Date : 04 juillet 2014, à partir de 08 :45**

**Lieu : Salle Maroni, Module Haute Technologie du CIRIMAT**
**Campus de l'Université Paul Sabatier à Rangueil**




**Programme :**

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| 08 :45 – 09 :00 | Accueil, café |
| 09 :00 – 09 :45 | ***Computer-aided Process Scale-up and Multiscale Analysis*** |
| | Andreas G. Boudouvis, Professor & Dean, School of Chemical Engineering, National Technical University of Athens, Greece |
| 09 :45 – 10 :00 | Discussion |
| 10 :00 – 10 :45 | ***Methods for Improving the Failure Resistance of Coatings and Thin Films*** |
| | Brian W. Sheldon, Professor, School of Engineering |
| | Brown University, Providence, Rhode Island USA |
| 10 :45 – 11 :00 | Discussion |
| 11 :00 | Fin du colloque |


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# Computer-aided process scale-up and multiscale analysis

Andreas G. Boudouvis
Professor & Dean, School of Chemical Engineering, National Technical University of Athens, Greece

Process scale-up amounts to connecting parameters/variables with the resulting product properties in the framework of a production procedure at a pilot plant-scale. The purpose to be served is to secure product conformity to market/end-user specifications, possibly high-throughput and economic efficiency – oftentimes conflicting objectives.

With the advent of computational power and powerful scientific software, process scale-up is effectively carried out at a process simulation level. This entails development of realistic models and employment of sophisticated numerical methods for the computer-aided solution of the associated complicated mathematical problems. The models account for all the important parameters of the process – ranging from operating, possibly manipulated, such as pressure, temperature and reactor geometry, to transport properties and reaction kinetic schemes. The parameters appear in the equations which are typically statements, in the form of partial differential equations, of the conservation laws of physical quantities – mass, energy and momentum. The process mechanisms are "hiding" in the equations and wait to be revealed by solving the latter and, especially, by examining the effect of the parameters on the solutions. So it is that the computations/experiments relationship is drastically revisited. On one hand, computations are superior in terms of save cost and labor savings; on the other, experiments are indispensable in providing input, guidance and validation to the former.

A process in point is Chemical Vapor Deposition (CVD), a popular one in the production of thin film coatings, usually for but not restricted to microelectronic applications. CVD is expected to be extensively implemented in aeronautics and space applications in view of new, binding specifications. A robust pathway towards process scale-up will be presented and the analysis will highlight the interplay of the physico-chemical mechanisms involved and the determination of advantageous process operating "windows". A key feature of the presentation will be the coupling of scales, that of conformal film growth in mm to μm size surface features, which are to be coated, with the macro-scale transport in the bulk of the CVD reactor. This so-called multiscale analysis enables predicting the effect of varying operational "macro"-parameters of the CVD process on the film growth rate inside micro-features on coated wafers.

## Methods for Improving the Failure Resistance of Coatings and Thin Films

Brian W. Sheldon
School of Engineering, Brown University, Providence, Rhode Island USA

Coatings and thin films are widely used to improve the performance of advanced materials in a variety of different applications. Thus, failure mechanisms in these surface layers are critically important. To avoid mechanical failures due to fracture and interfacial decohesion, several key properties of the material can be manipulated. The elastic properties of the materials are directly linked to the mechanical response, although these are often dictated by the choice of material. To control failure processes, the microstructure of the material can be manipulated to increase fracture energies of the coating material and at the coating/substrate interface. Failure can also be mitigated by controlling residual stresses that occur during processing. Examples where these strategies have been used successfully will be presented. These include ceramics with improved fracture toughness (for aerospace applications), improved diamond / metal interface adhesion (for machining applications), stress reductions in electrodeposited metal coatings, and several recent efforts involving electrochemically induced stresses in energy storage materials (used in both automotive and medical systems).