Surface and interface chemistry applied to composite metallization

Laboratory : CIRIMAT–ENSIACET, Toulouse, Group Surfaces : Reactivity & Protection (SURF)

Supervisors : Corinne Lacaze-Dufaure (Dir.) et Thomas Duguet (Co-advisor)

Contact : by email to Thomas.Duguet@ensiacet.fr and corinne.dufaure@ensiacet.fr

Fundings (not yet funded) : Apllied for MESR grant, and ANR grant

PhD project

The present project will serve as fundamental knowledge for the understanding of surface mechanisms involved in the treatment by chemical vapor deposition of composite parts for the space industry. This field has been reinforced recently in the group by the creation of a joint laboratory with a SME partner of the aerospace domain. Scientific aspects involve surface reactivity, gas/solid interactions, nucleation and growth of thin films, and adhesion mechanisms, that impact our coatings activities, including metallization.

The PhD project is focused on the experimental and theoretical study of the surface of a poly-epoxy polymer. Once synthesized and modeled, it will be used as a template for reactivity studies, e.g. reactivity towards metallic film formation from CVD precursors. Nowadays, there is no model available for such study, most likely because of the bottleneck posed by the intrinsic structural disorder of polymers. Treatment methods are thus empirical and far from being generic. In order to circumvent this issue, we propose to define a methodology, both experimental and theoretical, that will end up with a robust model of the surface and its properties. With this aim, theoretical calculations will be confronted to "model" experiments, meaning that the physical and chemical features of our samples will be mastered in order to introduce a minimum of errors (defects, topological difference, heterogeneity, etc.). Actually, defects are not included in theory, and therefore they would render the experiment/theory comparison impossible.

The first step of the work is to synthesize clean surfaces, homogeneous in composition, without defects at the nanoscale, and compare characterization results with DFT and MD calculations results, obtained on a model macromolecules network. Preliminary experiments in the group showed that it is indeed feasible, but the student will have to consolidate these results and perform the calculation part.

In a second stage, the knowledge acquired above about the surface itself will be used for the study of surface functionalization. For instance, AFM experiments on a submonolayer metallic film can determine nucleation density, which in turns can be compared to the calculated adsorption energy map.

The present topic belongs to two complementary disciplines: surface science and theoretical chemistry. With the aid of his/her supervisors, the PhD student will share its work between experiments and calculations, giving him/her the possibility to adjust the experimental design efficiently.