Developing models of disordered surfaces for “real world” materials applications

A8. Advanced Materials for Aerospace

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Introduction/Purpose

Our group specializes in the development of tailored thin films and coatings through metalorganic chemical vapour deposition, and in surface reactivity and gas/surface interactions. For the last 8 years, we have conducted researches dedicated to the development of light and durable components for new generation satellites. Our industrial partners have developed carbon reinforced epoxy parts, such as waveguides, startrackers or antennas. And we developed the processes for coating their inner surfaces in order to recover functional properties (conductivity, light absorbance). In the course of these above-mentioned studies, we figured out that very few studies are dedicated to the modeling of the epoxy surfaces, although the need is great. Hence, we decided to fill that void and contribute to a more generic knowledge. We can now synthesize model samples that are suitable for fine surface science experiments, suitable for calculations/experiments comparison, but that are still well representative of the industrial material. In this example, we will show how DFT and classical MD calculations are used to model the epoxy surface, to simulate XPS spectra, and to explain Cu chemisorption which correspond to the first step of satellites components metallization. It is noticeable that our methodology also applies to many other disordered systems for which a need exist. For instance, we have recently started to model organosilicon membranes and their interactions with BTEX gases.

Methods

Results

Conclusions

Selected references