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Mesoscopic Simulation for the Prediction of Macroscopic Properties of Nanostructured Systems

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Abstract: One of the major goals of computational material science is the rapid and accurate prediction of properties of new materials. In order to develop new materials and compositions with designed new properties, it is essential that these properties can be predicted before preparation, processing, and characterization. Despite the tremendous advances made in the modeling of structural, thermal, mechanical and transport properties of materials at the macroscopic level (finite element (FE) analysis of complicated structures), there remains a tremendous uncertainty about how to predict many critical properties related to performance. The fundamental problem here is that these properties depend on the structure that the material exhibits at a length scale ranging from few to some dozens of nanometers, and this structure depends strongly on the interactions at atomistic scale. In order to substantially advance the ability to design useful high performance materials, it is essential that we insert the chemistry into the mesoscopic (MS) modeling. Currently, atomistic level simulations such as molecular dynamics (MD) or Monte Carlo (MC) techniques allows to predict the structure and properties for systems of considerably large number of atoms and time scales of the order of microseconds. Although this can lead to many relevant results in material design, many critical issues in materials design still require time and length scales far too large for practical MD/MC simulations. Given these concepts, it is than necessary to carry out calculations for realistic time scales fast enough to be useful in design. This requires developing techniques useful to design engineers, by incorporating the methods and results of the lower scales (e.g., MD) to mesoscale simulations [1]. To this aim, we have developed a multiscale molecular modeling protocol, based on the combination of different techniques each of them suitable for the simulation at a given time and length scale. The protocol is able to predict macroscopic properties taking into account the nanostructure and the effect of the interphases/interfaces at nanoscale, thus resulting in a powerful tool for designing nanostructured systems [2]. The talk will describe the details of the multiscale molecular simulation framework, and will focus on some examples of industrial relevance involving nanostructured systems [3].

References:

[1] Fermeglia M., Pricl S., Multiscale molecular modeling in nanostructured material design and process system engineering, Computers & Chem.Eng, 33:1701-1710 (2009).

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