Nano tools for macro problems: multiscale molecular modeling of life and material sciences

Maurizio Fermeglia

Molecular Simulation Engineering Laboratory,
Department of Industrial Engineering and Information Technology,
University of Trieste

Abstract

A current challenge of sciences is to develop theoretical tools for predicting structures and bio-physical properties of complex systems at nano-scale from the knowledge of a few input parameters.

A current challenge of physical, chemical and engineering sciences is to develop theoretical tools for predicting structure and physical properties of complex systems at nano-scale from the knowledge of a few input parameters. However, despite all efforts, progress in the prediction of macroscopic physical properties from structure has been slow. Major difficulties relate to the fact that (a) the micro-structural elements in multiphase material are not shaped or oriented as in the idealizations of computer simulations, and more than one type can coexist; (b) multiple length and time scales are generally involved and must be taken into account, when overall thermodynamic and mechanical properties wish to be determined, and finally (c) the effect of the inter-phases/interfaces on the physical properties is often not well understood and characterized. As a consequence, their role is often neglected in the development of new theoretical tools or they are treated in a very empirical way. In this work, we focused on issues (b) and (c) in a multi-scale molecular simulation framework, with the ultimate goal of developing a computationally-based nano-composite designing tool to be applied to a large number of systems. In particular, we apply a general multi-scale simulation methodology to some examples of industrial relevance both in material science and in life science.

The first example is of general importance for the polymer industry and is related to the enhancement of mechanical and barrier properties if a nanofiller is dispersed into a polymer matrix: the role of multiscale modeling for the development of the material in the stage of screening the best design is evidenced.

The second example, important for the opto-electronic industry, is related to the prediction of the dispersion of gold nano-particles into a diblock co-polymer system forming different nanostructures (lamelles, cylinders,...). In this case it is relevant to understand how it is possible to influence the self-assembly of the nanoparticles in different regions of the diblock co-polymer structure.