Chemical Engineering Spring 2023 Seminar Series

Lewis Lecture Technical Seminar: Multiscale Modeling of Polymers at Interfaces and Polymer-Matrix Nanocomposites

Doros N. Theodorou SM '83, PhD '85

Professor of Chemical Engineering
National Technical University of Athens, Greece

March 23, 2023
66-110
4:00-5:00pm
3:45pm Reception

The properties of a polymer may change dramatically upon dispersion of nanoparticles in it. Two basic questions one faces in trying to design nanocomposites with tailored properties are: (a) How does the dispersion of nanoparticles in a polymer matrix depend on the molecular parameters (concentration, shape, size, chemical constitution, surface treatment of the nanoparticles; constitution, architecture, molar mass distribution of matrix chains and of chains that may be chemically grafted on the nanoparticle surfaces; areal density of grafting) and on the processing conditions? (b) How do properties (e.g. thermal, mechanical) depend on the dispersion and on the molecular parameters?

Molecular modeling and simulation can help address these questions. Because of the broad range of length and time scales governing structure and molecular motion in polymeric materials, one must resort to hierarchical modeling strategies involving many interconnected levels, each level addressing phenomena over a specific window of length and time scales.

In this lecture we will discuss some examples of such multiscale modeling efforts. We will start with atomistic simulations of flat polymer melt surfaces and polymer melt/solid interfaces aiming at the prediction of surface thermodynamic properties, such as surface tension and work of adhesion. In systems of spherical nanoparticles (fullerenes, silica) dispersed in an amorphous polymer matrix (polystyrene) we will quantify changes in the segmental dynamics, glass transition temperature, and local elastic constants in the glassy state in dependence of the molecular parameters. We will also see how the local shear strength of graphene/epoxy interfaces can be probed with atomistic simulations. We will then discuss systems of polymer-grafted surfaces and spherical nanoparticles immersed in a polymer melt of the same chemical constitution as the grafted chains. Here, self-consistent field theory, invoking a realistic free energy functional for nonbonded interactions and combined with a new finite element scheme for solving the governing integrodifferential equations in three dimensions, is valuable for exploring structure and interparticle interactions. We will present predictions of density profiles for grafted and free chain segments and compare them against neutron scattering measurements. We will also calculate potentials of mean force between grafted nanoparticles as functions of their center-to-center distance and explore the conditions for a stable dispersion. The three-dimensional formulation allows addressing the effects of nonuniform grafting scenarios on structure and interparticle interactions.

http://cheme.mit.edu/seminar-series/