Predicting the Thermodynamic Stabilities of Polymer/Carbon Nanotube Composites

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It is has been demonstrated that the addition of small quantities of carbon nanotubes (CNTs) can dramatically improve the thermal and mechanical properties of polymers. Polymer flammability, in particular, can be significantly reduced even at CNT loadings of 1 % or less. In many cases, however, this property enhancement is limited by the degree to which the CNTs can be uniformly dispersed within the polymer matrix. Unfortunately, CNTs do not spontaneously mix with most polymers and the composite materials made by mixing them are actually colloidal suspensions, which have a tendency to phase-separate over time. Thus, the properties of these materials may deteriorate with use even when good initial dispersion is achieved by high shear mixing. At the source of the problem are the very properties from which the benefits of CNTs derive. More specifically, CNTs reinforce the polymer matrix because they are inherently more rigid and less mobile than the polymer molecules they replace, but these attributes may also limit their miscibility. In this talk, we introduce a simple methodology, based on force field molecular mechanics, that can be used to estimate the free energy of nanoscale mixing and apply it to the prediction of the thermodynamic stability of polystyrene/graphene nanocomposites as a function of the structural characteristics of the graphene nanoadditive.