



# CHALLENGES AND OPPORTUNITIES IN NANOCOMPOSITES

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## Abstract

In recent years, as various nanomaterials have been developed with advancement in nanoscience and nanotechnology, applications of nanomaterials to reinforce polymeric materials have been attempted and have also attracted the interest of many researchers. Increased specific surface area is one of the nano effects that makes nanomaterials significantly distinct from other bulk materials. Nanoparticles are now added in polymer matrices as fillers in order to take advantage of increased reactive surface area to molecules in polymeric materials. The mechanical properties of particulate composites are mainly dependent on the volume fraction, the size of the particle, and the interfacial behavior between particles and polymeric matrix. They have been studied with micron size particles for many years. However, because of the extreme size of nanomaterials, there are numerous challenges in the development of nanocomposites including processing, characterization, and modeling of these new materials. In this presentation, some of the major challenges (and opportunities) that we face today will be discussed.

**Processing** – Dispersion of nano particles in a polymer matrix has been a major hurdle in making good quality nanocomposites. Because of their inherent mutual attractive forces, nano particles agglomerate and form clusters in the composite forming effectively defects in the composite. Because of these agglomerations the resulting nanocomposite may suffer reductions in strength and fracture toughness. Various processing methods have been proposed and investigated. Process has been slow. The new in-situ formation of nano particles in solutions using the sol-gel method seems to be able to produce good results.

**Intrinsic size effect** – Although many nano materials have superior mechanical and physical properties due in part to their nano meter size, these properties may or may not translate to bulk composite properties. This is a paramount issue concerning nanocomposite. At the nano scale level, the interaction between molecules of the polymer matrix and the nanoparticle that is supposed to enhance the mechanical or physical properties of the polymer has been studied. The effects of increased particle/matrix interfaces are mixed. In other words, the increase in surface area provided by nano particles is not always desirable. For example, the increased interface thermal resistance resulting from the increased interfaces can negate the superior heat conduction property of nanoparticles in nanocomposites. Similarly, the effect of particle size on the mechanical properties of nanocomposites has multiple facets and needs to be understood.

**Modeling** – Nanocomposites are materials of multiple scales. Molecular Dynamics simulation is usually employed to interpret the interaction behavior between the nano particle and the surrounding molecules of the polymer matrix. However, MD simulations are computationally prohibitive at this stage. Moreover, the nanoscale property needs to be translated into the bulk property of the composite for engineering designs and analyses and the MD alone is not suitable for performing this task. There are multiscale modeling methods for nanocomposites, among which most are numerical. Alternatively, Cosserat type of continuum mechanics has been developed to extend the continuum theory to account for the multiscale effects. Many of these efforts are still in progress.