Discovery at the Interface of Science and Engineering: **Science Matters!**

Materials Science and Technology
Nanocomposites

Rheology of Nanoparticle Suspensions

Diversity of nanoparticle interactions requires modeling at multiple length scales

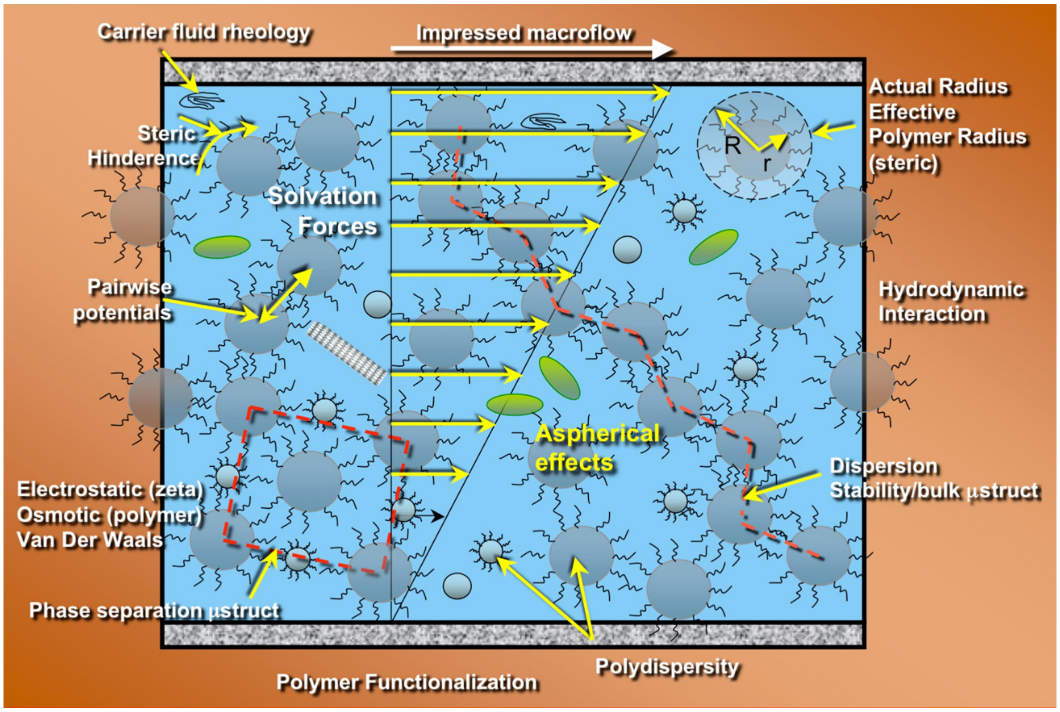

Figure 1: Illustration of the rich physical phenomena that control nanoparticle stability and rheology.

The growth of advanced nanoparticle fabrication techniques and analytical instrumentation has renewed the colloidal chemistry field and its application to nanoparticle composite manufacturing. Due to their small size, ranging from one to hundreds of nanometers, nanoparticles are mass efficient for modifying bulk and surface properties. They can now be made from a wide range of materials with unprecedented control of size and shape. There is also a rich set of possible nanoparticle coatings, particularly using the biochemistry of peptides and DNA, yielding new surface interactions. A distinct advantage of nanoparticles is that highly efficient and inexpensive polymer processing methods can be used to fabricate significant quantities of the composite material. Composites consisting of dispersed or ordered nanoparticle building blocks can be tailored to exhibit materials properties that have been unachievable with conventional materials, including increased strength and toughness of films and fibers to enhanced optical characteristics of coatings.

The most feasible way to disperse particles in a bulk material or control their packing at a substrate is through fluidization in a carrier that can be processed with well-known techniques such as spin, drip and spray coating, fiber drawing, or casting, followed by solidification via solvent evaporation, drying, curing, and sintering. Unfortunately, processing nanoparticles as concentrated, fluidized suspensions is a primary challenge and remains an art largely because of the extraordinary effect of particle shape and volume fraction on fluidic (rheological) properties. A second challenge is to create stable dispersions that can be processed into films, fibers, and other bulk structures. If the nanoparticles stick together and flocculate they cannot be processed. A schematic of the various interaction forces that are relevant on the nanoscale is shown in Figure 1. Clearly scientific under-

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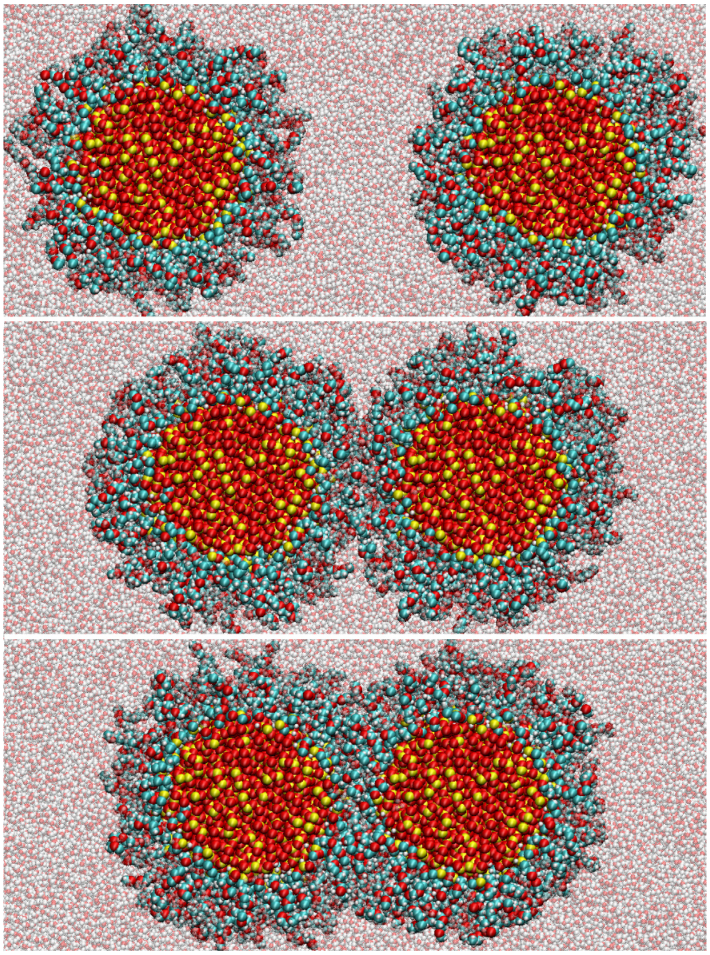

Figure 2: Polyethylene coated silica nanoparticles in water at three separations. Silica core of nanoparticle is 5 nm in diameter. Courtesy of J. Matthew Lane.

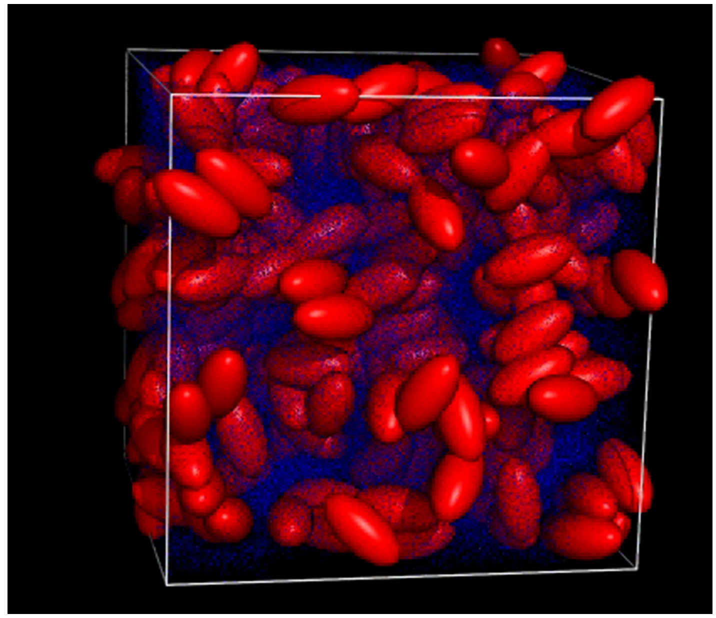

Figure 3: Snapshot of ellipsoidal nanoparticles (red) at 20% volume fraction in solvent (blue). Courtesy of W. M. Brown.

standing at multiple length scales, from atomistic to continuum, is crucial to surmounting these challenges in designing and manufacturing nanocomposite materials.

To achieve a stronger scientific understanding of the factors that control nanoparticle dispersion and rheology we are developing a multiscale modeling approach which will bridge scales between atomistic and molecular-level forces active in dense nanoparticle suspensions. At the atomic scale, we are carrying our molecular dynamics simulations with full atomistic detail to determine the interparticle forces between nanoparticles of various sizes and coatings. The solvation (velocity independent) and hydrodynamic (velocity dependent) forces are determined by moving two nanoparticles together at a given velocity as illustrated in Figure 2 for two polyethylene coated silica nanoparticles in water. To study the effect of particle shape on rheology we are simulating ellipsoid nanoparticles as shown in Figure 3.

At the meso-scale, a coarse-grained solvent model is being used to capture hydrodynamic effects. The interparticle forces determined from these simulations will be used in large-scale continuum flow solvers to model the rheological response and dispersion characteristics typical in a processing flow. The aim of our research and development is to achieve a unique meso-scale modeling and simulation tool-set designed to predict the key underpinning phenomena of nanoparticle suspension rheology and stability.

Sandia National Laboratories

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