115b Experimental and Computer Simulation Studies of the Mechanical Behavior of Nanoparticle Chain Aggregates

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ABSTRACT

Nanoparticle chain aggregates (NCA) are branched structures composed of primary particles with diameters ranging from 1 to 50 nm. They are a frequently observed state of matter that can form during nanoparticle synthesis in industrial or laboratory aerosol reactors, in many natural processes or in the combustion of carbonaceous fuels. Interest in NCAs stems from their importance in the manufacture of nanocomposite materials such as reinforced rubber, their use as planarization agents and their role in air pollution. The presence of aggregates may also affect transport across cell membranes. The use of NCAs as reinforcing fillers in rubber and other polymeric materials results in improved mechanical properties including increased tensile strength and Young's modulus. Although fillers constitute a significant volume fraction (30-40%) of the nanocomposite, the mechanism of interaction between NCA and the polymer chains is not well understood.

Previous experimental studies in our laboratory have shown that NCAs made of various materials, can be strained up to 100%; after breaking they contract to more compact structures. We have observed the behavior of NCA under strain in the transmission electron microscope (TEM) where they can be stretched (i) across holes that appear in carbon/formvar films on TEM grids, (ii) in a specially designed nanostructure manipulation device and (iii) using an AFM to measure force displacement curves (force spectroscopy) for aggregates stretched between a cantilever tip and an aggregate-coated substrate. The characteristic sawtooth pattern observed with the AFM was interpreted as a series of stretching/breaking events of the aggregates. Calculated tensile strength (4.5 ± 2.5 MPa) based on the sawtooth events compared well with the literature value for bulk material. Estimated values of Young's modulus (3.0 to 8.8 MPa) of single aggregates were significantly lower than bulk values. AFM measurements show special promise for determining the nanoscale properties of single NCAs.

Using atomistic computer simulations, the behavior of small copper nanoparticle aggregates under strain was investigated and force estimated. The copper interatomic interaction potential was obtained with the embedded atom method. Aggregates were strained to breaking using molecular dynamics and energy minimization straining. Although simulation strain rates were orders of magnitude higher than experimental values, different strain rates has little effect on aggregate behavior. Two seven-nanoparticle aggregates were studied, one linear and the other kinked. The linear aggregate yield strain was about 0.1. The kinked aggregate elastic limit was also about 0.1, but only one third of the stress developed compared to the linear aggregate. The kinked aggregate broke at a strain of about 0.5, five times higher than the breaking strain of the linear aggregate. The ability of the kinked aggregate to straighten through combined nanoparticle interface sliding and rotation accounts for the extra strain accommodation.

Applications of the experimental and computer simulation studies are to the behavior of nanocomposite materials, aggregate sampling by high speed impactors and the formation of flexible coatings of nanoparticles for sensors and deformable electronic surfaces.

References:

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