Molecular dynamic simulation of mechanical properties of polymer particles

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Summary. Polymeric particles with controlled microstructure play an important role as constituents in many composite materials for a number of emerging applications. The mechanical properties of composite polymer particles have been investigated by classical molecular dynamic simulation with a combination of united-atom force fields. The effect of particle size, chain architecture and temperature on the mechanical response of polymer particles has been explored and compared with experimental results to guide the design and control of particles.

Key words: molecular dynamic simulation, polymer particles, chain structure, nanoindentation

Introduction

Ugelstad monodisperse polymer particles have been widely used in chemical industries and biotechnology. Recently there is a growing interest in polymer particles with potential application in new electronic packaging technologies, such as Anisotropic Conductive Adhesives (ACA) in Flat Panel Displays. The particles are conductive through deposition of nano-scale metal coating on the particle surface. The metallized particles usually consist of a micron sized polymer core for improving contact compliance, a nanoscale nickel inner layer for bonding to polymer core and obtaining electrical conductivity, and a nanoscale gold outer layer for protecting inner layer from oxidation and improving the reliability of electrical performance. The use of metallized polymer particles in ACA technology possesses many advantages in terms of being lead-free, reducing package size and achieving high-density interconnections. The electrical characteristics as well as the reliability of the interconnection are mainly determined by the mechanical performance of the conductive polymer particles. Therefore, the mechanical performance of particles is of crucial importance to a reliable connection. This motivates us to study the mechanical properties of composite polymer particles and explore the structure-properties relationship to better design polymer particles for specific applications.

Methods

Molecular dynamic simulation

A combination of united-atom force fields was used for the molecular dynamic (MD) models of polyethylene nanoparticles in which carbon contained unit groups CH, CH2 and CH3 groups were considered to be single spherical beads interacting with each other, resulting in great saving in terms of the total number of atoms in the simulated systems. The total potential energy can be expressed as:

$$E_{\text{total}} = E_{\text{nb}} + E_{\text{bond}} = E_{\text{nb}} + E_{b} + E_{\theta} + E_{\phi},$$

(1)
where the total potential energy ($E_{total}$) includes two components: non-bonded ($E_{nb}$) and bonded ($E_{bond}$) interaction terms. MD models of polyethylene nanoparticles were constructed with different sizes and different molecular architecture for bulk MD models. The prepared polyethylene particles were compressed by rigid plates placed at the top and bottom of particles, similar as nanoindentation-based flat punch test in experiment. During compression the real time force and displacement on particles were monitored and the contact force-displacement curves were obtained. To compare the particle behaviour, the stress-strain relationship was calculated as follows:

$$\sigma_N = \frac{P}{\pi R^2}$$  
$$\epsilon_N = \frac{D}{R}$$

where $P$ was the applied force, $D$ was the half displacement during compression and $R$ was the radius of undeformed particle.

*Experiment*

The mechanical test of single micron-sized polystyrene particles was performed by using a nanoindentation-based flat punch methodology. A diamond flat punch of 100µm in diameter was specially designed to compress individual particles. The results were compared with MD simulation.

*Results*

Molecular dynamic simulation has been utilized to understand the mechanical properties of polymeric particles. In agreement with experimental results, a strong size effect has been observed which states that the smaller particle sizes the stronger it behaves. It is attributed to the increase in surface to total energy ratio in smaller particles. The increasing crosslinking density significantly strengthens mechanical properties of particles. Based on the results, the polymeric particles can be tailor-made to realize the required mechanical properties in different applications.

*References*

