

International Conference and Exhibition on onference[®]s Nanotechnology & Nanomedicine

March 12-14, 2012 Omaha Marriott, USA

TITLE

Molecular simulations to predict the properties of polymer nano composite: Effect of shape of particles

Sudip K. Pattanayek and Sunil Kumar

Indian Institute of Technology, India

Dolymer nano-composites, blend of a polymer and nano- particles have attracted researcher because of its wide range of application from aerospace material to biomedical applications. In general, the polymer used is semi-crystalline, which is semi flexible in nature. Properties of the nano-materials depend on the arrangement of the polymers near the particles. We have employed both Monte-Carlo (MC) method and Molecular Dynamics (MD) to the effect of particle size and shape effect on arrangement of polymers on it. We simulate both flexible chain and semiflexible chains in the presence of following particles: (i) zero size nano-particle (ii) variable spherical particles (iii) cubical particles (iv) flaky particles. In all these simulations favorable interaction between polymer and nano-particles are considered. The semiflexibility is considered through the bending energy penalty.

We found that dispersion and agglomeration of zero size nanoparticle is depend on its surface energy of nano particles. The nano-particles agglomerates to a big particle due to its attraction. A long flexible polymer chain covers the agglomerated particle while a semiflexible chain depending on its bending constant may cover the particle or displace the nano particles depending on the initial random number. A flexible chain adsorbs on the surfaces of all the particles with favorable polymer-surface interaction. Because of random structure flexible chain the chain covers all the particles. But a semi-flexible chain forms arranged structure far away from the particles. The order parameter of the semilexible polymer is much higher on the cubical particle. We will also present the ongoing work on the mechanical properties of the composite material obtained in these simulations.

Keywords:

Mr. Sunil Kumar has been doing his PhD on this topic. Dr. Sudip K. Pattanayek has completed his Ph.D from IIT Bombay and postdoctoral studies from Sydney University and Monash University, Australia. He has published more than 12 papers in reputed journals.