

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Mechanical Properties of Cross-linked Epoxy - Carbon Nanotube
Nanocomposites: Effect of Interfacial Interactions and Nanoconfinement**

KETAN KHARE, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — The effect of fillers on polymer nanocomposites is conceptually analogous to the effect of nanoconfinement of polymers by solid substrates. This assertion is tested in our work by studying the volumetric, structural, dynamic, and mechanical properties of nanocomposites of cross-linked epoxy and carbon nanotubes (CNTs) using molecular simulations. We use atomistically detailed models in our simulations, which allow us to explicitly account for the specific chemical interactions between the filler and the matrix. Our results show that the poor interfacial interactions between the filler and the matrix lead to a tendency for depression in the glass transition temperature (T_g) of the nanocomposite compared to the neat cross-linked epoxy. Functionalization of CNTs is expected to strengthen interfacial interactions between the filler and the polymer matrix, and thus can have a strong impact on the properties of the nanocomposite. The relationship between the T_g , molecular dynamics, and the mechanical properties of the nanocomposites can be non-intuitive. Results will be presented for the relationship between mechanical properties, molecular dynamics, and the T_g of nanocomposites of cross-linked epoxy containing both, pristine and functionalized CNTs.

Ketan Khare
Department of Chemical Engineering, Texas Tech University

Date submitted: 04 Dec 2012

Electronic form version 1.4