Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Mechanical Properties of Graphene-Polymer Nanocomposites

ASANKA WEERASINGHE, Department of Physics, University of Massachusetts, Amherst, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst, ASHWIN RAMASUBRAMANIAM, Department of Mechanical and Industrial Engineering, University of Massachusetts, Amherst — We report results from molecular-dynamics simulations of straining of polymer (high-density polyethylene) nanocomposites reinforced by graphene and fullerenes with the aim of elucidating the underlying mechanisms that govern the mechanical response of these composite materials. Using a united-atom-based model of the glassy polymer matrix, we show systematic trends in the enhancement of the mechanical stiffness of the composite as a function of filler concentration, size, and morphology, as well as matrix-filler interfacial interaction strength. From systematic studies of mechanical behavior, we find that the stiffness reinforcement is only weakly dependent on the filler size for fullerenes but shows an appreciable size dependence for graphene fillers. We explain the filler-size dependent elastic response of the graphene-reinforced polymer composites through detailed atomic-scale characterization in conjunction with a modified shear-lag continuum-mechanics model. In addition to capturing the nanocomposites' elastic response accurately, the modified shear-lag model also provides a quantitative estimate for a critical graphene flake size beyond which these 2D fillers can provide effective mechanical reinforcement through interfacial stress transfer.

Asanka Weerasinghe
Department of Physics, University of Massachusetts, Amherst

Date submitted: 02 Nov 2016 Electronic form version 1.4