

Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Mechanics of Graphene and CNT-polystyrene nanocomposites

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ABSTRACT

We performed molecular dynamics simulation to investigate the mechanics of graphene and CNT-polystyrene nanocomposites. First, we studied the different mechanical properties of polystyrene and matched with experimental data. Then, we have investigated the interfacial and adhesive strength of graphene and CNT with polystyrene. For graphene, we considered the effect of hydrogen functionalization and different defects: stone-wales, vacancy. For CNT, we considered different chirality. Our simulation supported with analytical model give comprehensive insight into mechanism of graphene and CNT-nanocomposite.