Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Computational modeling of mechanical response of dual cross-linked polymer grafted nanoparticle networks BALAJI IYER V S, VICTOR YASHIN, University of Pittsburgh, ISAAC SALIB, Intel, TOMASZ KOWALEWSKI, KRZYSTOF MATYJASZEWSKI, Carnegie Mellon University, ANNA BALAZS, University of Pittsburgh, ANNA BALAZS COLLABORATION, KRZYSTOF MATYJASZEWSKI COLLABORATION — We develop a hybrid computational model for the behavior of a network of cross-linked polymer-grafted nanoparticles (PGNs). The individual nanoparticles are composed of a rigid core and a corona of grafted polymers that encompass reactive end groups. With the overlap of the coronas on adjacent particles, the reactive end groups can form permanent or labile bonds, which lead to the formation of a "dual cross-linked" network. To capture these multi-scale interactions, our approach integrates the essential structural features of the polymer grafted nanoparticles, the interactions between the overlapping coronas, and the kinetics of bond formation and rupture between the reactive groups on the chain ends. We investigate the mechanical response of the dual-cross linked network to an applied tensile deformation. We find that the response depends on the bond energies of the labile bonds, the fraction of permanent bonds in the network, and thickness of the corona. This model provides a powerful tool for the computational design of dual cross-linked PGN's by predicting how the structural features of the system affect the mechanical performance.

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Date submitted: 08 Nov 2012 Electronic form version 1.4