Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Controllable Reconfiguration of Polymer-grafted Nanoparticle Networks Under Torsion TAO ZHANG, BADEL MBANGA, VICTOR YASHIN, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh, Pennsylvania 15261, USA — We use 3D computational modeling to study mechanically-induced changes in the structure of networks formed from polymer-grafted nanoparticles (PGNs). The nanoparticles rigid cores are decorated with a corona of grafted polymers, which contain reactive functional groups at the chain ends. With the overlap of the grafted polymers, these reactive groups can form labile bonds, which can reform after breakage. These PGN networks consist of two types of nanoparticles, which differ in the reactive functional groups at the chain ends. The energy of the labile bonds that are formed depends on the nature of these reactive groups. We demonstrate that the application of a rotational deformation results in a controllable reconfiguration of the network. Depending on the labile bond energies, the PGN networks are shown to exhibit a deformation-induced phase separation. The restructuring process can be controlled by boundary conditions. We can create complicated morphology such as spiral, with enhanced mechanical properties. Our results provide guidelines for designing mechano-mutable PGN-based materials whose nanoscale structures can be controllably changed under an applied mechanical action.

Tao Zhang
Univ of Pittsburgh

Date submitted: 11 Nov 2016 Electronic form version 1.4