Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Deformation and fracture of Coarse-grained Model of Filled Rubber Composites KATSUMI HAGITA, National Defense Academy, HIROSHI MORITA, AIST, MASAO DOI, University of Tokyo, HIROSHI TAKANO, Keio University — We presented a result of coarse-grained Molecular Dynamics simulation of filled polymer melts with Sulfur-crosslink under deformation based on the Kremer-Grest Model. Under uni-axial deformation (extension) by setting Poisson's ratio to less than 0.5, facture of this polymer nanocomoposites occurs due to volume increase for increasing the strain. In order to study facture behavior, we use the original Lennard Jones potential formula (with attractive part) as interaction between polymers. The size of simulation box under periodic boundary conditions (PBC) is set to about 133nm. We put 2048 fillers, 5120 polymer chains of 1024 particles, and many crosslink into the PBC box. Due to the crosslink, all polymer chains are connected to one network gel. One filler consists of 320 particles of the C320 fullerene structure. A repulsive force from the center of the filler is applied to the particles of C320 in order to make a sphere whose diameter is about 7nm. We can observe the fracture occurs due to void created near surface of fillers for the case that interaction between polymer and filler is relatively non- attractive. Various cases of Poisson's ratio and interaction between polymer and filler are examined.

Katsumi Hagita
National Defense Academy

Date submitted: 07 Dec 2010 Electronic form version 1.4