

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Dynamics of Coarse-grained Model of Filled Rubber Composite under Deformation** KATSUMI HAGITA, National Defense Academy, SHINICHI UENO, YASUMASA BITO, Sumitomo Rubber Industries, Ltd, HIROSHI TAKANO, Keio Univ., MASAO DOI, Univ. of Tokyo, HIROSHI MORITA, AIST — 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. Because all polymer chains are connected to one network gel, the size of simulation box under periodic boundary conditions (PBC) is set to about 33nm. We put 4 fillers, 80 polymer chains of 1024 particles, and many crosslink into the PBC box. One filler consists of 1280 particles of the  $C_{1280}$  fullerene structure. A repulsive force from the center of the filler is applied to the particles of  $C_{1280}$  in order to make a sphere whose diameter is about 15nm. Some patterns of distribution of the fillers are examined. The stress-strain curves estimated by applying a deformation to the system in simulations qualitatively agree with those in experiments. It is successful to show hysteresis on the S-S curve between elongation / release of the filled rubber.

Katsumi Hagita  
National Defense Academy

Date submitted: 20 Nov 2009

Electronic form version 1.4