Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Stress-Strain Relation of Tire Rubber Consist of Entangled Polymers, Fillers and Crosslink KATSUMI HAGITA, National Defense Academy of Japan, Y. BITO, Y. MINAGAWA, SRI, M. OMIYA, Hokkaido Univ., H. MORITA, AIST, M. DOI, Univ. of Tokyo, H. TAKANO, Keio Univ. — We presented a preliminary result of large scale coarse-grained Molecular Dynamics simulation of filled polymer melts with Sulfur-crosslink under an uni-axial deformation by using the Kremer-Grest Model. The size of simulation box under periodic boundary conditions (PBC) is set to about 66nm to consider length of entangled polymer chains, size and structure of fillers, and non-uniform distribution of crosslink. We put 640 polymer chains of 1024 particles and 32 fillers into the PBC box. Each 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. Here, the particles of the fillers are chosen to be the same as the particles of the polymers and the diameter of the filler is about 15nm. The distribution of the fillers used in this simulation is provided by the result of 2d pattern RMC analysis for 2D-USAXS experiments at SPring-8. Sulfur crosslink are randomly distributed in the system. It is found that stress-strain curves estimated by applying a certain uni-axial deformation to the system in simulations are in good agreement with those in experiments. It is successful to show difference on the S-S curve between existence / absence of fillers and qualitative dependence of attractive force between polymer and filler.

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Date submitted: 18 Dec 2008 Electronic form version 1.4