Development of Ecological High-Performance Tire by Modeling of Nano-Particle Network Structure in Rubber

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Abstract

Structure of Filler (Nano-particle) has an important role on "reinforcement effect" for rubber compound. The structure of fillers affects on the microscopic friction during driving cars. This friction is related to the increase of hysteresis loss on stress-strain curve. However the molecular-level mechanism of reinforcement effects is now open problem. We consider that it is important to understand the molecular-level behavior of rubber composite because molecular-level behaviors have an important role to bridge between fillers' structure and macro properties. In order to understand them, we considered that coarse grained molecular dynamics simulation is a powerful tool to reproduce rubber composite in the wide scale range from nanometer to micrometer. Here, we used filler-structure information obtained by the combination of 2D Ultra-small-angle X-ray Scattering (2D-USAXS) experiments and 2D patterns reverse Monte Carlo (RMC) analysis. In our previous study, we have developed new simulation model of rubber composite with keeping relation among length of entangled polymer chains, size and structure of fillers, and non-uniform distribution of crosslink by using the Kremer-Grest model. We found that stress-strain curves estimated by applying a certain uniaxial deformation to the system in simulations are in good agreement with those in experiments. It is successful to show difference on the stress-strain curve between existence / absence of fillers and qualitative dependence of attractive force between polymer and filler. In this year, we tried to estimate two-dimensional scattering patterns from results of large-scale molecular dynamics simulations of

the coarse-grained model of tire rubber with 256 fillers. We found that characteristic behaviors of two-dimensional scattering patterns for different elongation rates can be seen. We also tried to estimate tangent of phase angle by simulations under oscillating deformations. The tangent of the phase angle is used as index for energy loss of tire rubber in experiments. When the strain is given by sinusoidal function in time with a certain frequency, observed stress will lag by the phase angle. As the preliminary results, it is found that behaviors of the tangent of the phase angle in the rubber like region corresponding to the frequency of grips and breakings can be estimated by coarse-grained MD simulation of our model of tire rubber. Therefore, our simulation model is a hopeful candidate of the developing method of new industrial materials of tire rubber in the viewpoint of molecules architectures of polymers, fillers and their interfaces.

Keywords: coarse-grained molecular dynamics simulation, polymer-filler system, tire rubber