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

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Abstract

Rubber compounds filled with carbon black and silica particles are known to exhibit a significant reinforcement effect, which are increases in mechanical strength and in energy dissipation under cyclic deformation. The energy dissipation affects the performance of tire products such as mileage performance and wet traction. This performance is evaluated by rheological indexes such as loss tangent (tanδ) in the field of product developments. Fortunately, regions of the frequency of the cyclic deformation for the mileage performance and the wet traction are different. Thus, it is considered that we can improve the balance between the decrease of the energy dissipation for the mileage performance and the increase for the wet traction. We considered that coarse-grained molecular dynamics (MD) simulation of filled rubber compounds is a one of reliable approaches to understand its dynamical behavior from molecular level behaviors. Thus, we performed preliminary study to estimate mechanical behaviors by the coarse grained MD simulation. We considered that coarse gained MD simulation is an effective method to estimate a value of loss tanδ under sinuous strain with the frequency region for wet traction. In the last year, we studied frequency dependence of tanδ in the range of the frequency related to the wet traction for the both cases with repulsive and attractive interaction between filler surface and polymer in order to model the difference between silica- and carbon black- filled rubber compounds. It is found that the slope of tanδ along frequency estimated by using a model containing 32 filler particles for the repulsive case becomes steeper than that for the attractive case. In this year, we examined effects of the modified filler by grafted polymers to the frequency dependence of tanδ. We performed material experiments to estimate number of chains connected on a silica filler particle

as effective number of the bonds per a filler particle. We obtained preliminary results that the slope of frequency dependence of tanδ increased with an increase of number the bonds around the number based on the experimental results. Although this explorative joint study had stopped due to company's decision from viewpoints of managements, to complete this study we should treat larger simulation system and longer simulation time to improve precision in the future.

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