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

Project Representative

Hiroyuki Kishimoto

Sumitomo Rubber Industries Ltd.

Authors

Hiroyuki Kishimoto[*1], Toshio Tada[*1], Yasumasa Bito[*1], Shinichi Ueno[*1], Masaki Shiraishi[*1], Hiroya Suno[*2], Hitoshi Uehara[*2], Yoshinari Fukui[*2], Misako Iwasawa[*2], Satoru Shingu[*2], Manabu Omiya[*3], Hiroshi Takano[*4], Masao Doi[*5], Hiroshi Morita[*6], Katsumi Hagita[*7]

＊1 Sumitomo Rubber Industries Ltd.

＊2 Japan Agency for Marine-Earth Science and Technology

＊3 Hokkaido University

＊4 Keio University

＊5 The University of Tokyo

＊6 National Institute of Advanced Industrial Science and Technology

＊7 National Defense Academy

Abstract

Rubber compounds filled with carbon black and silica particles are known to exhibit a significant reinforcement effect, that is, the increases in mechanical strength and in energy dissipation under cyclic deformation. The reinforcement effect is considered to originate from the hierarchical aggregate structure constructed by the filler particles in the matrix of rubber compounds. 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 ($\tan\delta$). 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. The collapse and reconstruction of the network structure in the rubber matrix under deformation is considered to play a role in the energy dissipation. In order to clarify the mechanism of the reinforcement effect, understanding of dispersing structure of the filler particles in the rubber matrix is required at least, although detailed picture of the reinforcement effect of the commercial filled rubber compounds does not exist. Coarse-grained molecular dynamics (MD) simulation of filled rubber compounds is considered as one of the reliable approaches to understand the reinforcement effects from molecular level behaviors. Thus, we have tried to estimate the mechanical behaviors by the coarse-grained MD simulation. As a preparation of the

simulation, the aggregated structure of filler particles ranging from the nanometer to micrometer scales has been estimated by two-dimensional pattern reverse Monte Carlo method for a two-dimensional scattering pattern obtained by time-resolved two-dimensional Ultra Small-angle X-ray scattering (2D-USAXS) measurements exploited at SPring-8. In FY 2009, we confirmed that coarse gained MD simulation is an effective method to estimate the value of loss $\tan\delta$ under sinuous strain with the frequency region for wet traction. Here, the value of $\tan\delta$ is an important factor used to evaluate the mileage performance and wet traction of tire in the field of product developments. In FY 2010, we studied the frequency dependence of $\tan\delta$ in the range relevant to the wet traction for the both cases with repulsive and attractive interaction between filler surface and polymer. This aims to explain the difference of performance on wet traction between silica- and carbon black- filled rubber compounds. It is found that the frequency dependence of $\tan\delta$ estimated using a model containing 32 filler particles for the repulsive case is steeper than that for the attractive case. This behavior is consistent with the results observed in the experiments.

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