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

Project Representative

Yasuhisa Minagawa

Sumitomo Rubber Industries Ltd.

Authors

Katsumi Hagita [*1], Yasuhisa Minagawa [*2], Yasumasa Bito [*2], Hiroshi Yoshinaga [*2], Hiroya Suno [*3], Hitoshi Uehara [*3], Satoru Shingu [*3], Manabu Omiya [*4], Hiroshi Morita [*5], Hiroshi Takano [*6], Masao Doi [*7]

＊1 National Defense Academy

＊2 Sumitomo Rubber Industries Ltd.

＊3 Japan Agency for Marine-Earth Science and Technology

＊4 Hokkaido University

＊5 National Institute of Advanced Industrial Science and Technology

＊6 Keio University

＊7 The University of Tokyo

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 under cyclic stretching. However the mechanism of reinforcement effects is now open problem. In order to understand the detail mechanism of the reinforcement effect, we considered that coarse-grained molecular dynamics simulation that reproduces rubber composite using filler network structure information which is observed in the wide scale range from nano-meter to micro-meter is a powerful tool. In our previous study, we examine the structural changes of fillers in the elongating rubbers by the combination of 2D Ultra-small-angle X-ray Scattering (2D-USAXS) experiments and 2D patterns reverse Monte Carlo (RMC) analysis. In addition, we confirmed qualitative agreement among experiment result and simulation one by the large-scale simulation of finite element method and obtained important information related to “reinforcement effect”. We consider that it is important to understand molecular level behavior of rubber composite because molecular level behavior has an important role to bridge between filler-structure and macro physical properties. Especially, filler, polymer and interaction between them have a very important role. Therefore, as our strategy we consider that coarse-grained molecular dynamics simulation is most suitable in order to clarify the role of filler, polymer and interaction between them with the wide

scale ranging. In this study, we 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. Here, we used a purely massive parallel code, which has been developed in the last year, of coarse-grained molecular dynamics simulation for a large-scale (from nano-meter to micro-meter) system. We obtained a preliminary result of large scale coarse-grained Molecular Dynamics simulation of filled polymer melts with sulfur-crosslink under a uniaxial deformation. Here, we use the subset of filler positions obtained by 2D pattern RMC analysis for 2D-USAXS experimental results using SPring-8. It is 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. Thus, the expectations of the present simulation model for developing new industrial materials become larger.

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