# 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 on the stress-strain curves. However the mechanism of the reinforcement effects is now open problem. In our previous study, we examine the structure changes of fillers in the elongated rubbers by the combination of the Ultra Small Angle X-ray Scattering experiments and 2D patterns reverse Monte Carlo analysis. In order to understand the detail mechanism of the reinforcement effect, we develop a purely massive parallel code for a large scale (from nm to micro-meter) molecular dynamic (MD) simulation of filler reinforced rubber. For a few hundred nm scale system with the full atomistic MD simulation, we have to treat a few hundred million particles in the box of periodic boundary conditions. Such a huge data is impossible to handle on the single node of the preset fastest computer. Thus, we must apply the spatial decomposition method to the calculation of the force along polymers in addition to that of the non-bonding force among the neighbor particles. We confirmed the one hundred thirty million particles with the coarse-grained MD simulation using 512 nodes (4096CPUs).



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