Evaluation of dispersion state of silica particles in rubber during elongation using RMC modelling

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Since reverse Monte Carlo (RMC) method can construct a three-dimensional atomic configuration that reproduces the scattering profile by randomly moving particles in the simulation box, it has been widely used for the modelling of glass, liquid, and amorphous materials [1]. Recently time-resolved small angle X-ray scattering measurement (SAXS) using synchrotron radiation has been carried out on polymer materials with a hierarchical structure, in a large spatial scale (several nm to several μm). It is necessary to develop a high-throughput RMC code to model a large simulation box with millions of particles to understand huge amount of experimental data at multi-scale.

In this research, we developed a high throughput RMC code dedicated to time-resolved measurement that can handle millions of particles. They were applied to SAXS data and the dispersion state of the silica particles in the rubber during elongation was evaluated.

An elastomer filled with 15 vol% silica particles with a particle size of 110 nm was performed elongation SAXS measurement using a bulge tester. RMC simulation was carried out using the data of the obtained distortion rate 0% and 2.7%. An RMC simulation with 60,000 particles in a large simulation box (side length of the box is 3000 nm) was performed. From the three-dimensional particles arrangement, the dispersion state of the silica particles was evaluated by using the pair distribution function, the coordination number distribution and the distribution of the voids. From the pair distribution function, the distance between particles increased with elongation, and the coordination number tended to increase with elongation. It can be confirmed from the voids between the particles (void distributions) that number of large voids decrease with elongation (Fig. 1). This suggests that the dispersion of particles became a uniform state from a nonuniform state by elongation. In present, we are analyzing how the arrangement of particles influences the physical properties from these results. In the presentation, we will report details of analysis method and result by RMC.

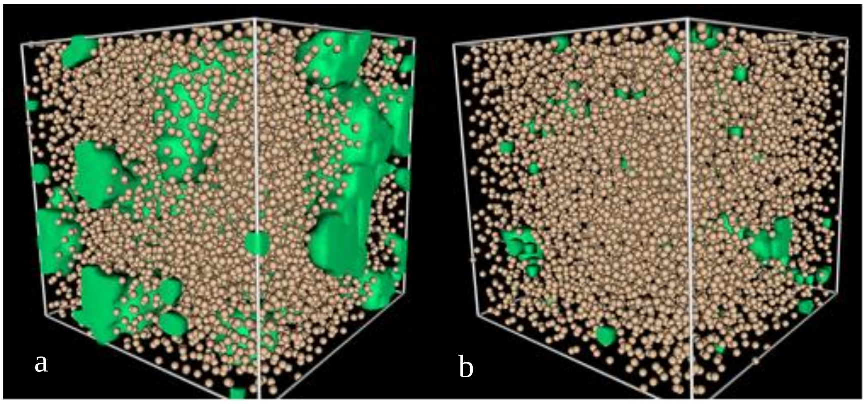

Figure 1: a: Dispersion of particles and distribution of voids at strain 0%. b: Dispersion of particles and distribution of voids at strain 2.7%. Ivory color is particle and green color shows void distribution, respectively

References

[1] R. L. McGreeby and L. Pusztai, Mol. Simulat. **1**, 359 (1988).