# Coarse grained MD simulation for fracture and reinforcement of polymer materials

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We have studied polymer materials through coarse grained MD simulations for their fracture and reinforcement. We focused on the following three subjects.

1) Fractures of polymer materials such as polyethylene including scission of main chains. Understanding of molecular mechanism and model development using various simulations.

2) Relationships between reinforcement and structure, and fracture and structure through coarse grained (CG) MD simulations.

3) Reinforcements and fractures of filler-filled rubber materials through CGMD simulations.

Especially, this year, we focused on the following research topics.

a) Crystallizations of polyethylene (PE) [1,2]. Comparison between ring and linear melts [1]. Structure formation of a quenched single polyethylene chain [2] to compare force fields.

b) Nanovoids (early fractures) in elongated polymer networks with crosslink [3] and with crosslink and nanoparticles [4].

c) Two-dimensional scattering patterns (2DSPs) in CGMD simulations. [3-9]

d) Reinforcements of filler-filled polymer materials. [3-6, 10]

e) Developments of simulation methods of coarse-grained models [11-13]

f) Visualization methods of material systems [14,15]

Regarding the subject 1), crystallization-behaviors of PE chains were studied through the topic a) in order to obtain a crystallized structure quickly. For PE, we found that united atom (UA) model with Deriding force fields provided acceleration of the crystallization process due to distribution of torsional angles [1,2]. Here, UA model can be regarded as a coarse-grained model of all-atomic simulations. LAMMPS was used for massive parallel simulations. We also investigated ReaxFF simulations using LAMMPS for continuing works from initial structure created by UAMD. Here, ReaxFF can be regarded as a coarse-grained model of DFT calculations.

Concerning the subject 2), 2DSPs originated from structure were investigated for the cases of phase-separation of ABA block copolymer [7] and nanovoids of crosslinked polymers [3] under stretching. For these topics, LAMMPS was used for massive parallel simulations. The analysis code to compute 2DSPs was developed

from scratch. As forthcoming works, studies of machine/deep learning for relationship between 2DPSs and stress-strain curves are in progress.

On the subject 3), CGMD simulations of polymer materials filled with nanoparticles [4, 6, 8] and clay (disc) [5]. Behaviors of 2DSPS were examined. For these topics, LAMMPS was used for massive parallel simulations. In addition, SMP parallelized version of OCTA/cognac was used for continuing researches. The analysis code to compute 2DSPs was developed from scratch. Moreover, particle-mesh version of two-dimensional pattern reverse Monte Carlo modeling was developed, modelling from 2DSPs of NPs in gels by CGMD simulations [8] were compared with reference NP-structure, and several verifications of actual experimental were carried.

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