Coarse grained MD simulation for fracture and reinforcement of polymer materials

Katsumi HAGITA

Department of Applied Physics, National Defense Academy, Yokosuka, Kanagawa 239-8655

We investigated fracture behaviors of polymers such as morphology changes and chain breaking by uniaxial elongations. Understanding of fracture mechanisms with molecular level is considered to be important on reinforcement of polymer materials. We performed coarse grained (CG) molecular dynamics (MD) simulations of polymer materials. Here, we considered Kremer-Grest (KG) model, united atom (UA) model and reactive force field (ReaxFF) MD. KG is bead spring model. UA and ReaxFF can be regarded as CG of all atomistic MD simulations and DFT simulations, respectively. These simulation methods can be performed by LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), which was used in the present studies. We also studied Dissipative particle dynamics (DPD) which is a stochastic simulation method that can handle larger time scales than the KG model. This year, we focused on ABA tri-block copolymers (BPCs) and crystallized polyethylene (PE).

For ABA tri-BCPs, we studied morphology changes via two-dimensional scattering patterns (2DSPs) for correspondences between simulations and experiments. Recently, we proposed Thinning Approximation (TA) to calculate 2DSPs under shear flows for KG model [1]. We performed CGMD simulations of KG model of ABA tri-BCPs for various fractions. Systematic changes of 2DSPs under uniaxial elongations were observed by using TA [2]. Also, we performed CGMD simulations of KG model to examine filler-filled systems such NC-clay nanocomposites [3], and nano-particle (NP) filled rubbers [4]. On the study of NC-clay nanocomposites, we could reproduce the stress-strain curve and the change of 2DSPs during elongation at the same time. For the NP-filled rubbers, we found that effect of polymer-NP interactions and nanostructures on glass transition temperature.

In order to investigate the fracture behaviors from the equilibrium structure of phase separated ABA tri-BPCs by elongations, we considered an improvement of segmental repulsive potential (SRP) of DPD simulations. To reduce bond crossing probabilities and keep the equilibrium structure before and after introducing of SRP, we proposed multipoint SRP [5].

As studies behaviors of 2DSPs of NP-filled rubbers, we proposed filler network model of

filled rubber materials in order to study system size dependence of 2DSPs and obtain a rough model to reproduce structure-property relationship for machine learning studies [6].

To study fracture of realistic materials, we considered crystallization of PE chains. As produces in our usual life, branched PE chains such as high- and low-density PE (HDPE and LDPE) are used. We found that branched junctions are mainly localized in amorphous layer. To study formations of amorphous layers, we compared ring and linear PE polymers. Here, amorphous layers have important role on fractures of PE materials. We found that crystallization of ring PE polymers is faster than that of linear PE polymers [7]. In addition, we also investigated the topological effect of a knot of a ring on crystallization of ring PE polymers [8]. To reproduce chain breaking, we used ReaxFF MD simulations. In our study, UAMD was used to prepare crystallized PE and ReaxFF MD was used to study chain breaking under stretching.

To enhance material researches including developments of real materials, we examined AI based information analysis methods. As the first example, we studied image classification of images of NPs in rubbers [9]. As the second example, we considered super resolution for asymmetric resolution of FIB-SEM (focused ion beam scanning electron microscopy) 3D imaging of NPs in rubbers [10].

References

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