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Coarse grained MD simulations of a fracture of filler-filled polymer nanocomposites under uniaxial elongation KATSUMI HAGITA, National Defense Academy of JAPAN, HIROSHI MORITA, AIST, HIROSHI TAKANO, Keio Univ. — We performed coarse grained molecular dynamics (MD) simulations based on Kremer-Grest model in order to investigate a fracture of polymer nanocomposites filled with spherical nanoparticles (NPs) under uniaxial elongation with a Poisson ratio of 0.4 [1]. In our model, the NP consists of 320 surface beads and one center bead. In order to make the NP spherical, a harmonic potential is applied to the surface particles from the center of the NP. Here, the initial volume fraction of the NPs is about 20%. The dependences of the fracture on the interactions between the NPs and polymers were examined. In order to observe the creation of nanovoids, the interaction among the polymers was set to be attractive. When the NP-polymer interaction is attractive, nanovoids appear in the bulk of polymers. On the other hand, for repulsive NP-polymer interaction, nanovoids are created at the surface between the polymers and NPs. At the same time, segregation of NPs is observed. We found that these behaviors depend on crosslink densities. [1] K. Hagita, H. Morita, H. Takano, Polymer, 99, 368-375 (2016).

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