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Glass transition temperature of polymer nano-composites with polymer and filler interactions KATSUMI HAGITA, National Defense Academy, HIROSHI TAKANO, KEIO University, MASAO DOI, University of Tokyo, HIROSHI MORITA, AIST — We systematically studied versatile coarse-grained model (bead spring model) to describe filled polymer nano-composites for coarse-grained (Kremer-Grest model) molecular dynamics simulations. This model consists of long polymers, crosslink, and fillers. We used the hollow structure as the filler to describe rigid spherical fillers with small computing costs. Our filler model consists of surface particles of icosahedra fullerene structure C320 and a repulsive force from the center of the filler is applied to the surface particles in order to make a sphere and rigid. The filler's diameter is 12 times of beads of the polymers. As the first test of our model, we study temperature dependence of volumes of periodic boundary conditions under constant pressures through NPT constant Andersen algorithm. It is found that Glass transition temperature (Tg) decrease with increasing filler's volume fraction for the case of repulsive interaction between polymer and fillers and Tg weakly increase for attractive interaction.

[X] Prefer Oral Session
[ ] Prefer Poster Session

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