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**Multiscale atomistic and coarse-grained-particle analysis of fracture of graphene sheet** RYO KOBAYASHI, TAKAHIDE NAKAMURA, SHUJI OGATA, Nagoya Institute of Technology — The problems related to material strength such as crack propagation, dislocation motion, and response to nano-indentation involve multiscale phenomena which atomistic or non-linear events occur at a certain confined region and elastic or linear deformation takes place at surrounding wide-spread region. In order to tackle these multiscale problems, we have developed the hybrid molecular-dynamics/coarse-grained-particle (MD-CGP) method which eliminates the artificial effects often occurred at the interface of atomistic and coarse regions by using extra atoms and particles at the interface and applying the Langevin thermostat for the extra atoms and particles. The method allows us to perform multiscale simulations of any materials such as metals, semiconductors, and insulators and of dynamic phenomena at finite-temperatures. We have performed the multiscale simulation of fracture of defect-free graphene membrane by nano-indentation and clarified that decrease of the fracture strength with respect to temperature is almost same as that by existence of a vacancy. We will discuss detail about the computational efficiency of this method and simulation results.

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