Poster Session | E. Deformation and Fracture Mechanism of Materials

## [PO-E1]Poster Session 1 Symposium E Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

## [P1-25]Fracture behavior of multi-walled carbon nanotube under biaxial loading condition

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One-dimensional carbon materials such as Carbon Fibers (CFs) and Carbon nanotubes (CNTs) are applied in a wide range of areas. For example, carbon fiber reinforced plastics are put to practical use for bodyworks of cars and airplanes. Though carbon materials in composites are subjected to complex deformation by multiaxial loading, the fracture mechanism of them is not clarified under multiaxial stress conditions. In this study, we have performed deformation simulations on multi-walled CNTs under biaxial loadings in order to clarify the fracture criterion of one-dimensional carbon materials from nanometer scale viewpoints. CNTs in simulation cell are compressed in a radial direction, and extended in a longitudinal direction by molecular dynamics simulation using the adaptive intermolecular reactive empirical bond order (AIREBO) potential. Fracture of CNTs originates from a bond breaking by the tensile loading for longitudinal direction, under small compressive stresses for the radial direction. On the other hand, high compressive stresses for the radial direction trigger a collapse of six-membered ring structures before the bond breaking by the longitudinal tension. The collapse occurs in the neighborhood of the innermost layer in highly compressed CNTs.

In addition, we have also performed biaxial deformations of composite models which are made by filling amorphous polyethylene structure in the space between MWCNTs. As a result, fracture behavior varies with stress conditions, as in the case of models without polyethylene. A collapse of six-membered ring structures under high compressive stresses occurs not from the innermost layer but from the outermost layer by the interaction between polyethylene and CNTs.