

## MD simulation of structural change of polyethylene induced by high energy ion bombardment

Chansoo Kim<sup>1</sup>, Sk. Faruque Ahmed<sup>2</sup>, Myoung-Woon Moon<sup>2</sup>, Kwang-Ryeol Lee<sup>1</sup>

<sup>1</sup>Computational Science Center, Korea Institute of Science and Technology (KIST), Korea

<sup>2</sup>Future Convergence Laboratory, Korea Institute of Science and Technology (KIST), Korea

Ion beam bombardment at low energy forms nanosize patterns such as ripples, dots or wrinkles on the surface of polymers in ambient temperature and pressure. It has been known that the ion beam can alter the polymer surface that induces skins stiffer or the density higher by higher compressive stress or strain energies associated with chain scissions and crosslinks of the polymer. Atomic scale structure evolution in polymers is essential to understand a stress generation mechanism during the ion beam bombardment, which governs the nanoscale surface structure evolution.

In this work, Molecular Dynamics (MD) simulations are employed to characterize the phenomenon occurred in bombardment between the ion beam and polymers that forms nanosize patterns. We investigate the structure evolution of Low Density Polyethylene (LDPE) at 300 K as the polymer is bombarded with Argon ions having various kinetic energies ranging from 100 eV to 1 KeV with 50 eV intervals having the fluence of  $1.45 \times 10^{14}$  #/cm<sup>2</sup>. These simulations use the Reactive Force Field (ReaxFF), which can mimic chemical covalent bonds and includes van der Waals potentials for describing the intermolecular interactions.

The results show the details of the structural evolution of LDPE by the low energy Ar ion bombardment. Analyses through kinetic and potential energy, number of crosslinks and chain scissions, level of local densification and motions of atoms support that the residual strain energies on the surface is strongly associated with the number of crosslinks or scissored chains. Also, we could find an optimal Ar ion beam energy to make crosslinks well.