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Molecular dynamics simulation on the formation and annihilation behaviors of radiation defects in Li2O (P4-H-354)

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The influence of radiation defects is one of the main factors that determine tritium release behavior from blanket breeding materials in fusion reactors. Classical molecular dynamics simulation (MD) is a powerful technique to investigate the radiation damage processes, because it can provide atomic-scale information on the defects. In this study, we conducted radiation simulation for Li2O using MD and analyzed formation and annihilation behaviors of radiation defects, as a fundamental research for radiation response of Li-containing oxides.

Buckingham type two-body potential model was used. In order to remove the unphysical impulsive force at short inter-ionic distances in Buckingham model, each potential function was connected to that of the ZBL potential models at around 0.8 A. NEV ensemble was employed with the initial simulation temperature of 0 K. 10x10x10 supercell consisting of 4000 Li2O was used as a unit cell under 3D periodic boundary conditions. Radiation simulation was initiated by introducing an energy of a certain direction to an ion, as a displacement energy. The lowest displacement energy by which a defect was created and survived beyond 5 ps was regarded as the threshold energy. 42 and 21 displacement directions were surveyed for Li and O, respectively, based on the symmetry of the Li2O crystal.

In both Li and O defect formations, [100] displacement shows significantly lower threshold energy than [111] displacement. Li defects were easily created than O defects almost in all directions. In fact, the average threshold energy except [111] displacement, which possesses extremely high threshold energy, was 21 eV for Li and 49 eV for O. In some cases, no defect could survive beyond 5 ps even by higher displacement energies than the threshold energy, due to the self-annealing effect. The self-annealing completed basically within 1 ps after introduction of displacement energy. At around this time, velocity distribution of all ions in the system became similar to the Maxwell-Boltzman distribution, indicating that the introduced energy can spread uniformly to the system within 1 ps, and that the relaxation time of the energy spread could relate to a time scale of the self-annealing. The relationship between the energy spread and the self-annealing will be discussed in detail.