Modeling of Li diffusivity in Li$_2$O by molecular dynamics simulation

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Radiation effects are one of the important issues for materials used in fusion reactors. Since diffusion process plays a main role in defect annihilation and aggregation, its modeling is essential to predict long-term effects of radiation. In Li-containing oxides of candidate tritium breeders, diffusion behavior of Li is complicated compared with that of other constituents, because (i) Li vacancies are abundantly formed by tritium breeding reaction and facilitate Li diffusion, and (ii) some Li-containing materials have superionics of Li as reported in Li$_2$O and Li-Si-O system. In the present paper, we aimed to model Li diffusion in Li$_2$O as a function of Li burn-up (Li defect concentration) to imitate reactor conditions, by means of molecular dynamics simulation (MD).

DL_POLY code was used for MD. NPT ensemble was utilized for Li$_{1000}$O$_{500}$ supercell under periodic boundary conditions. In order to reduce potential model dependences of calculation results, we employed a few different potential models having various features, and compared simulation results. In simulation, two types of defective systems were studied together with the perfect system (Li$_{1000}$O$_{500}$): a system containing Li vacancy (e.g. Li$_{998}$O$_{500}$) or Schottky type defect (e.g. Li$_{999}$O$_{499}$). For Li$_{999}$O$_{500}$, the effective charges of Li and O ions were slightly changed to keep charge neutrality.

In defective systems, three characteristic Li diffusion behaviors were distinguished in a solid phase: (i) diffusion assisted by introduced defects ($< 0.5 \times [\text{melting point}]$), (ii) diffusion below the critical temperature of the superionics, and (iii) diffusion above the critical temperature. Calculated critical temperatures were about $0.7 \times [\text{melting point}]$, which is in the general tendency of PbF$_2$-type superionics. These behaviors were observed under any potential models used in the present study, although absolute values of diffusion coefficient were dependent on potential models.

In comparison between Li$_{999}$O$_{500}$ and Li$_{999}$O$_{499}$, Li diffusion coefficients were different each other despite the same concentration of Li vacancies. In Li$_{999}$O$_{499}$, Li and O vacancies formed a defect cluster, and thus diffusion coefficients became lower than those in Li$_{999}$O$_{500}$. In the presentation, diffusion coefficients will be shown as a function of Li defect concentration, and details of diffusion mechanisms will be discussed.

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