A systematic method to construct potential models: for tungsten materials in fusion reactors

Takuji Oda[1]

[1]*Department of Nuclear Engineering, Seoul National University*

Molecular dynamics (MD) calculation is an important computational method for materials science and engineering. For nuclear materials, the importance of MD is further emphasized because a large scale simulation of defect dynamics is needed to study radiation damage processes and effects. To obtain meaningful results from MD simulations, one has to prepare a quality potential model, which must work appropriately not only in around equilibrium states but also in non-equilibrium states caused by high-energy particles.

In this presentation, I will introduce a systematic method to construct empirical potential models, specifically (i) two-body model (distance function) [1], and (ii) embedded-atom method (EAM) model (a kind of function of distance function) [2]. In this method, potential functions are expanded with cosine/sine series in reference to energies, forces and stresses calculated by first-principles calculations. By adding first-principles calculation results of, for example, atomic collision events into the reference data, a constructed potential model is expected to reasonably work even for recoil simulations. As test cases, I will present a comparison result of the performance of several constructed potential models for nuclear materials, including tungsten (plasma-facing components; d-electron metal), tungsten-hydrogen systems, and sodium (coolant for fast reactors; s-electron liquid metal).

[1] T. Oda, W.J. Weber, H. Tanigawa, Comp. Mater. Sci. **111**, 53 (2016).
[2] T. Oda, submitted.