Contribution ID: **22** Type: **not specified**

Interatomic potential development for H permeation in critical components

Tuesday, December 3, 2024 11:10 AM (20 minutes)

A long-term prediction of hydrogen permeation in fusion-relevant materials requires the use of atomistic calculations with necessary details on microstructures, the accuracy of which is predominantly determined by the performance of interatomic potentials. The purpose of this study is to understand the available forms of potential models and develop a new set of potentials based on the best functional form.

In the first phase of our study, we have reviewed the existing potential models for various material systems, selected a material system of interest, i.e. W-H binary system, for the further research and development. In the final two years, we have identified three key research areas to understand how the presence of hydrogen isotopes would change the microstructure-property relationship in W: (1) hydrogen permeation predictions from machine-learning potentials, (2) irradiation-damage changes, and (3) mechanics changes due to the presence of hydrogen.

In this talk, we present the progress in these three areas, and discuss the motion of hydrogen atoms. Since the studies have been done in parallel, the results have yet to be assimilated for a consistent understanding on the microstructure-property relationship. We also talk about the future direction of our research team.

This work was supported by IAEA-CRP, NRF grant (2020R1A2C201510913) and by Nano-Material Technology Development Program (RS-2024-00445448) through NRF funded by Ministry of Science and ICT.

Primary authors: LEE, Byeongchan (Kyung Hee University); Prof. KIM, Duho (Kyung Hee University); KANG, Keonwook (Yonsei University); Prof. ODA, Takuji (Seoul National University)

Presenter: LEE, Byeongchan (Kyung Hee University)

Session Classification: Atomistic Modelling II