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BCA-KMC Hybrid Simulation with Meta-Modeling for Hydrogen Dynamic Retention in Tungsten Material

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To achieve the fuel balance and recycling in ITER and DEMO reactors, it is necessary to understand hydrogen behaviour in plasma facing materials. Because the plasma-wall interaction is determined by particle balance between the flux of plasma particles and the diffusivity in materials, the reproduction of realistic flux and fluence corresponding to experiments is a key issue in simulation. In the previous conference, the formation of the fuzzy nano-structure induced by helium plasma irradiation had been successfully represented by Molecular Dynamics and Monte-Carlo (MD-MC) hybrid simulation which can treat the realistic flux, 10^{22} m^{-2}s^{-1}, and fluence, 0.5×10^{22} m^{-2}, corresponding to experimental conditions. In this paper, we further develop the hybrid simulation and propose Multi-Scale Meta-Modelling (MSMM) as follows.

To estimate retained hydrogen amount in tungsten materials under the realistic flux and fluence condition, Binary Collision Approximation and Kinetic Monte-Carlo (BCA-KMC) hybrid simulation has been developed. In the BCA-KMC hybrid simulation, the BCA part treats the collision cascade process of incident plasma particles and the KMC part treats the diffusion processes of hydrogen isotope atoms and vacancies in a tungsten material. The elapsed time can reach 10^{-2} s beyond 10^{10} times the gap of their time scales. By the the BCA-KMC hybrid simulation, hydrogen retention amount at laboratory experiment flux, 10^{20} m^{-2}s^{-1}, to ITER divertor environment flux, 10^{24} m^{-2}s^{-1} have been estimated. As a result, the retained hydrogen amount in the case of 10^{24} m^{-2}s^{-1} is at least 10 times higher than that of 10^{22} m^{-2}s^{-1}.

Furthermore, we enhance the reproducibility of the KMC in terms of grain boundaries. In general, the KMC model is created by using the Density Functional Theory (DFT) calculation. However, the calculation speed of the DFT is too slow to find many migration paths in grain boundaries. In the MSMM, the KMC model for the migration paths is automatically constructed by using the MD. The reliability of this automatic KMC modelling depends on the accuracy of the potential model of MD. The potential model of MD is improved by comparison with the DFT in terms of many sample structures. Thus, in the MSMM, the almost all parameters are determined from the MD with the DFL level accuracy.

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