
[PO-B2]Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-06]Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

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Tungsten (W) is considered as a promising candidate for the plasma facing wall material at divertor in nuclear fusion reactors. In order to assess the lifetime of the divertor for safe operation of the nuclear fusion reactors, mechanical response to the irradiation of high energy neutrons and helium atoms should be precisely understood from atomistic scale. Under the irradiation of high energy neutrons, not only defects are formed but also transmutation occurs, which will produce a few percent of rhenium (Re) concentration within several-year operation of nuclear fusion reactor. Thus the effect of solute Re atoms on the mechanical behavior of host material, W, should be taken into account, such as recovering rate after cascading damage, H/D/T retention, He bubble formation, or dislocation mobility. In this study, we create a neural-network (NN) potential for quaternary system, W-Re-H-He, combined to an EAM potential for W-Re binary system. It is known that machine-learning (ML) potentials such as NN can well reproduce DFT energies of wide variety of atomic configurations, but it requires big data to learn a lot of free parameters and it is usually much slower than the classical potentials such as EAM. By combining the NN with EAM potentials, we can construct a potential with smaller number of reference data and make it much faster than fully NN potential. The properties of the potential and the effect of Re on the recovering rate after cascading damage, He bubble formation/growth rate, and dislocation punching will be discussed.