Poster Session | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[PO-B2]Poster Session 2

Symposium B

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

[P2-16]Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] (1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine)

The microstructure evolution of cascade annealing in *α*-Zr crystals at *T*=300K, 400K, and 500 K for energy of 2, 6 and 10 keV with initially driving directions <0001> and <01-10> of primary knocked atoms (PKA) are investigated by using molecular dynamics simulations. The results show that the relaxation time (τ_r) of cascades can play a role of an effective parameter for describing radiation damages during molecular dynamics simulations. of cascade with the larger surface area but with the same volume is much smaller, which promotes faster recombination of defects during cascade annealing. Energy is a crucial factor in the formation of cascade displacements of atoms and appearing of defects compared with temperature and direction of movement for initially knocking atoms.

©The 9th International Conference on Multiscale Materials Modeling