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FTP/P7-18: Simulation of Defects in Fusion Materials Containing Hydrogen and Helium

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Simulations of damages in beryllium, alpha-iron and tungsten, irradiated by fusion neutrons have been performed using molecular dynamics (MD). We applied three codes MCNP5, GEANT4 and FLUKA for simulation of 14 MeV neutron interactions in beryllium, iron and tungsten lattices. The displacement cascades induced by the Primary Knocked-on Atoms (PKA), produced by the bombardment of fast neutrons destroys locally the crystalline structure. The displacement cascades efficiency has been calculated using the Norgett-Robinson-Torrens (NRT) formula, the pair potential of Ziegler-Biersack-Littmark (ZBL) and the more realistic EAM interatomic potential.
The second part of the study has coved the positron lifetime computer simulations for 14 MeV neutron irradiated Be, alpha-Fe and W samples, containing hydrogen and helium. The positron lifetimes calculated by TCDFT correlate with the magnitude of electron density of targets. The positron is bound to a mono-vacancy even it contains hydrogen or helium atoms. The vacancy-clusters without helium are active positron traps, if once they are bound with helium or hydrogen, they become less effective in the trapping of positrons. The lattice relaxation of atoms around vacancy, reduce the effective vacancy volume, which decreases the positron lifetime at a vacancy location. Positron lifetime is proportional to the increasing of the nano-void size while an increase the number of helium atoms into nano-void decrease the lifetime. The model calculated positron lifetimes of nano-void containing gases atoms are shorter than in the empty nano-void of the same size.

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