Computational Study of Defects in Fusion Materials Containing Helium

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Atomic displacement cascades induce formation of point defects (i.e., vacancies, interstitial atoms, vacancy and interstitial clusters) and segregation of alloying elements, while nuclear transmutation reactions produce helium and hydrogen atoms. A standard parameter for the radiation damage in the material microstructure is the displacements per atom (dpa). The development of models for the accumulation of radiation defects and transmutation products, including helium and hydrogen, in complex microstructures is one of the priorities the EU Materials Modelling programme for the Horizon 2020. Computational studies of atom cascades due to the 14 MeV neutrons passage in α-Fe and W targets have been performed by transport Monte Carlo codes MCNP/MCNPX and FLUKA. The purpose was to determine the dpa and percentage of the formed helium atoms in α-Fe and W samples. The calculation of defects in fusion materials by positron lifetime could predict with high precision the defect structures.The second part of the study has covered the positron lifetime computer simulations by two component density functional theory (TCDFT) of defects in alpha-Fe and W samples, containing helium. We apply for calculations the dpa cross sections as a function of neutron energy. We performed calculations of displacements per atom (dpa) in W and α-Fe, due to 14 MeV neutron interactions. For 1MW/m^2 neutron fluence, damage in α-Fe is estimated to be 4.17 dpa for FPY. The calculation of positron wave function proceeds in exactly the same way as for electronic function. Once the positron wave function ψ^+ has been calculated, the positron annihilation rate λ, the inverse of the positron lifetime τ, can be calculated.

In summary: The results obtain by independent MCNP5 and FLUKA codes for neutron energy spectra are in agreement within a few %. The simulations of defects in fusion materials show that the morphology of the damage produced during the first few picoseconds in the collapse of a cascade influences significantly the nucleation and growth of defects during irradiation both in pure metals and in the presence of He. Large vacancy clusters are not directly formed in bcc metal displacement cascades. The presence of H and He stabilize the vacancy clusters into a three-dimensional defect configuration (voids or bubbles) in lattice volume. The positron lifetimes calculated by TCDFT correlate with the magnitude of electron density of the sample. The vacancy-clusters without gas atoms are active positron traps. The positron is bound to a mono-vacancy even it contains hydrogen or helium atoms. The lattice relaxation of atoms around vacancy reduces 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 nano-voids in tungsten and iron are clusters of many lattice vacancies, but nano-voids containing helium atoms are not equilibrium bubbles. The largest decrease in the positron lifetime is obtained for nano-voids with small size. Therefore the influence of the helium atoms is more significantly in small size nano-void containing helium. We assume that the pressure produced in small nano-voids will be higher than in the large size nano-voids.