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Computational Study of Defects in Fusion Materials Containing Helium

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The interaction of the intensive neutron fluxes with the first wall components of the fusion reactors result on serious structure damages in fusion materials. 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. The measure for the radiation damage in the material microstructure is dpa. The development of models for the accumulation of radiation defects and transmutation products, including helium and hydrogen, in complex microstructures will be one of the priorities for the EU Materials Modelling programme for the Horizon 2020. Computational studies of atom cascades due to the 14 MeV neutrons passage in 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 Fe and W samples. We plan also to compare the computational data from FLUKA and MCNPX.
The second part of the study has coved the positron lifetime computer simulations by TCDFT for 14 MeV neutrons in alpha-Fe and W samples, containing helium. The positron lifetimes calculated by TCDFT correlate with the magnitude of electron density of the sample.

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