Molecular Dynamics simulation of cascades in Fe-0.1%He steel with various empirical interatomic potentials

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Helium in the ferritic/martensitic steels foreseen for the future fusion reactor is an important issue to address as it degrades their mechanical properties. Because of the extremely low solubility of helium in materials, helium atoms tend to cluster with vacancies in bubbles or to be trapped at defects such as interstitials, dislocations and grain boundaries, and may promote the formation of voids.

The effect of He on subsequent damage produced by the 14 MeV fusion neutron in pure Fe is investigated by molecular dynamics simulation, as a model for ferritic/martensitic steels, with various empirical interatomic potentials. Cascade energies range from 1 to 20 keV and temperatures from 10 to 523 K. The resulting number of point defects, clusters of those and their size, and the ratio of helium to self point defects in the clusters are assessed. In a previous study \cite{1} we have used the Ackland ‘97 potential, the Wilson-Johnson \cite{2} potentials and the Beck ‘68 potential to describe Fe-Fe, Fe-He and He-He interactions, respectively. The morphology of the clusters is further analysed within the standard stereographic triangle to identify interstitial types. The magnitude of the difference in formation energy between He substitutional (He\textsubscript{s}) and He interstitial (He\textsubscript{i}) by the empirical potentials is overestimated (2.09 versus 0.17 eV from \textit{ab initio} \cite{3}). In the present study a recent Fe-He potential \cite{4} is used, which gives in particular the appropriate difference in formation energy. In addition, various potentials for Fe-Fe will be deployed, consisting in the one of Mendelev ‘03 and Dudarev-Derlet ‘05, in combination with the new Fe-He potential. The implications of the choice of the potentials on the resulting microstructure will be discussed.

\cite{1} J. Yu, Z. Yao, G. Yu and R. Schaeublin to be published in \textit{Journal of Nuclear Materials}, 2007
\cite{2} W.D. Wilson and R.D. Johnson, Rare gases in metals, in \textit{Interatomic Potentials and Simulation of Lattice Defects}, P.C. Gehlen, J.R. Beeler Jr., R.I. Jaffee (Eds.), Plenum (1972) 375.

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