Impurity effects on He diffusion in $\alpha$-Fe

C.J. Ortiz$^a$, M.-J. Caturla$^b$, C.C. Fu$^c$ and F. Willaime$^c$

$^a$Dept. Fisica Aplicada, Universidad de Alicante, E-03690 Alicante, Spain
$^b$Universidad de Alicante, Dep. Fisica Aplicada, Alicante, Spain
$^c$SRMP - Service de Recherches de Métallurgie Physique, CEA/SACLAY, 91191 Gif sur Yvette, France
mj.caturla@ua.es

The diffusion of He in $\alpha$-Fe in the presence of defects produced by irradiation (vacancies and self-interstitials) is studied using both rate theory and kinetic Monte Carlo models with input from \textit{ab initio} calculations. Comparison between the model based on He in pure Fe and experimental data of He desorption from Fe under different conditions shows discrepancies. Increasing the vacancy migration energy and decreasing the binding energy of a vacancy to a He substitutional and a vacancy to a He interstitial provides good agreement with experimental measurements at all temperatures and conditions studied. This difference in energies from the original \textit{ab initio} data for pure Fe is attributed to the presence of impurities in the experimental samples, with carbon being the most likely candidate. In order to check the validity of this assumption, \textit{ab initio} calculations were performed to study the energetics of He-V-C complexes in $\alpha$-Fe. These data have been included in a full model of He migration in $\alpha$-Fe in the presence of carbon. Calculations are presented on the effect of carbon on He migration for different conditions, in particular different He-to-vacancy ratios, temperatures and carbon concentrations. Finally the effect of carbon on He desorption in $\alpha$-Fe is evaluated.

This work was performed in the framework of the European Fusion Materials Modelling programme.