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| <b>Subject</b>        | Study of radiation effects in FeCr alloys for fusion applications using computer simulation |
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| <b>Faculty</b>        | Solid State Physics   |
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### Abstract

Radiation effects in FeCr alloys, as model materials for ferritic/martensitic steels, using computer simulation tools, were studied in order to provide interpretation of the experimentally observed effect of Cr on the radiation response of these alloys, as compared to Fe. In particular, after assessing the effect of Cr on the primary damage state (displacement cascades), the migration properties and mutual interactions of thereby produced defects and their clusters, are investigated using Molecular Dynamics simulations. Phase separation processes under thermal ageing are treated with the help of Monte Carlo techniques. Rate theory equations are finally applied to reproduce the defect annealing stages in Fe and Fe-Cr alloys, using the results obtained in this work.

The results obtained show that the thermodynamic properties of the Fe-Cr system can be reproduced, using semi-empirical interatomic potentials, in good agreement with experimental and *ab initio* data. The primary damage state distributions (such as number of produced defects, volume and density of created atomic cascades) are not affected by the presence of Cr. Whereas the effective migration energy and the diffusion coefficient of the interstitial defects are lower in FeCr alloys (of studied concentrations) than in pure Fe, the migration energies of small 3D migrating SIA clusters being much higher than those in pure Fe. With the increase of the Cr concentration, therefore, the diffusivity of 1D migrating interstitial clusters drops, reaches a minimum and then rises again. The depth of the minimum and the critical concentration at which the minimum is reached depend on the size of the interstitial cluster. This effect was explained by the existence of a strong interaction between crowdion and Cr atoms. The main impact of this effect was seen on small SIA clusters, with sizes up to one hundred interstitials.

An explanation for the origin of the experimental measured swelling vs Cr concentration is proposed, relying on the observations of the non-monotonic dependence of SIA cluster mobility on Cr content and the results on the interaction between Cr-rich precipitates and SIA clusters. A description of the defect annealing stages in Fe and FeCr has been given by applying rate equation (RE) methods, using the results on mobility of defects for the parameterization. The obtained results show that the application of the RE method for the description of the defect annealing provides very close results to those obtained by other researchers using the a kinetic Monte Carlo method, and in agreement with experimental results. The parameterization of defect migration properties obtained in the present work also predicts the positions of the recovery peaks in Fe, in good agreement with experimental data, but corresponds to an alternative interpretation of the recovery stages, based on the ideas of the existence of sessile configurations for small SIA clusters. Finally, the calculation of the defect recovery in Fe-Cr alloys (with  $C_{Cr} = 5, 10$  and  $15\%$ ) has shown that reasonable agreement for stage I, II and III is obtained, assuming the presence of traps (of one type only) for single SIAs. The concentration of traps and their trapping energies depend on the Cr content in the alloy. An approximate estimation of their values is given in this work.