MODELLING OF RADIATION EFFECTS: FROM IRON TO EUROFER97

Background

High chromium ferritic/martensitic steels are promising candidate structural materials for future fusion reactors. The safe application of these materials requires a careful assessment of their mechanical stability under high energy neutron irradiation. However, no experimental facility is currently capable of reproducing the expected hard neutron spectra and high neutron fluxes. Thus, the in-service behaviour of these steels must be *extrapolated* to the real conditions, from data obtained in existing irradiation facilities. In order to do so in a rational way, it is vital to reach a good level of understanding of the physical phenomena driving the material response to irradiation for different chemical compositions. For example, it has been observed that a yet unexplained minimum in radiation-induced ductile-brittle transition temperature shift appears at about 9 wt.% Cr. In addition, neutron irradiation experiments on Fe-Cr alloys show that adding Cr up to concentrations of 12-15 wt.% leads to a pronounced decrease in swelling compared to pure α-Fe, although for the highest concentrations embrittlement becomes an issue, due to α' phase formation.

Objectives

The present task aims at shedding light on the fundamental physical mechanisms producing the above-mentioned dependence on Cr concentration of important macroscopic parameters defining the mechanical stability under neutron irradiation of high-Cr steels, such as Eurofer97. For this purpose, a bottom-up multiscale modelling approach, using computer simulation techniques combined to state-of-the-art experimental examination of Fe-Cr model alloys, has been applied during the last few years at SCK•CEN in collaboration with other European labs.

Principal results

Computer simulation

Displacement cascades produced by recoiling atoms are the physical processes whereby damage, in terms of point-defects (vacancies and interstitials) and their clusters is produced in neutron-irradiated materials. It can be simulated using MD (molecular dynamics) computer techniques. About 300 displacement cascades in Fe and Fe-10%Cr with recoil energies up to 50 keV, have been simulated. We thereby found out that the main effect of the presence of Cr is to modify the chemical composition of interstitial defects. Namely, about 60% of the interstitial atoms are Cr atoms and interstitial clusters tend to contain more than 20% Cr atoms [1,2,3]. The discovery of this association of Cr atoms to interstitial clusters motivated a detailed MD study of the mobility of single interstitial and interstitial clusters in Fe-Cr alloys as a function of Cr concentration. The latter study has shown that interstitial clusters are indeed slowed down by Cr and that the largest reduction in mobility is obtained for small clusters at intermediate Cr concentrations (e.g. 7%), the slowing down being less pronounced for higher Cr content (e.g. 12%) [4]. This behaviour is similar to that observed in experimental data of swelling as a function of Cr concentration and indeed there exist a theoretical framework to establish a link between interstitial cluster mobility and swelling [4]. We rationalised these findings by an analytical model of a given cluster in Fe-Cr given the diffusion coefficient of that cluster in Fe, enabling us to extend the results to any concentration and any temperature [5]. The application of this analytical model for the mobility of clusters is compared to MD simulations and experimental data on swelling in the figures below, where the relationship between the two phenomena clearly appears.

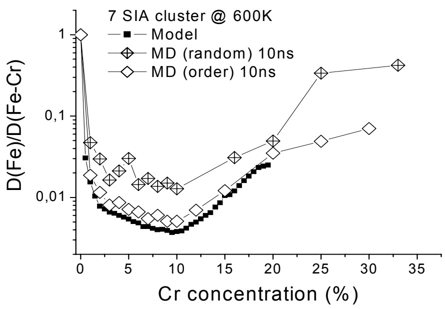

Fig. 1a – Reduction of the diffusion coefficient of a 7-interstitial clusters versus Cr concentration according to: MD simulations in random and ordered Fe-Cr alloys; analytical model.

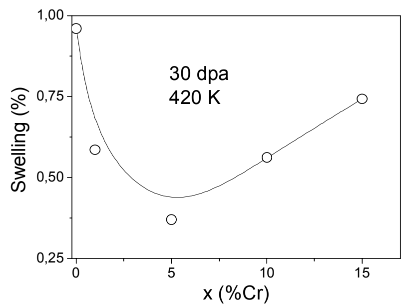

Fig. 1b – Experimental data on Fe-Cr swelling [from E.A. Little and D.A. Stow, J. Nucl. Mater. 87 (1979) 25].

A- Experimental validation

In order to provide experimental support to the models and to produce well documented results to be modelled, a campaign of neutron irradiation was launches in SCK•CEN's BR2 reactor of pure Fe, ultra-pure Fe-9%Cr, Fe-12%Cr and Fe-15%Cr single crystals, and Fe-(2 to12%)Cr-C model alloys, together with Eurofer97 and T91 steels. The as received materials have been characterised in detail using advanced experimental techniques for the observation of the microstructure and the determination of the macroscopic properties, especially the mechanical ones [6]. The irradiation campaign at 300°C is underway to achieve three different irradiation doses, from few tens of dpa to more than 1 dpa, to study the evolution of the microstructure under cascade damage conditions. The post-irradiation examination will consist of the identification of the type of defects produced under irradiation, their size and density, as functions of neutron-dose, in each material. The ultimate goal is to link the microstructural evolution under irradiation with changes in both the flow properties of the material and its mechanical resistance. Fig. 2a shows results of tensile tests after irradiation to 0.06 and 0.6 dpa for the binarys alloy containing ~100 ppm C, as compared to the two technological steels, T91 and EUROFER 97. As it can be seen, already at very low dose all materials harden by about 100 MPa, with a tendency to decrease when the Cr content becomes higher than 5%. The increase of the irradiation dose by one order of magnitude makes all materials much harder, by about a factor 2.5. The material containing 12%Cr is the hardest, indicating different mechanisms of damage accumulation in these alloys depending on Cr concentration. Fig 2b, illustrates the ductility properties of the same alloys and doses: by increasing irradiation dose, all materials lose to some extent their uniform and total elongations, but EUROFER 97 seems to have lost almost all its ability to deform plastically. This unexpected behaviour of this steel compared to the others shows the need for a quantitative characterisation of the defects created by irradiation and also the mechanisms of interactions between dislocations and these defects.

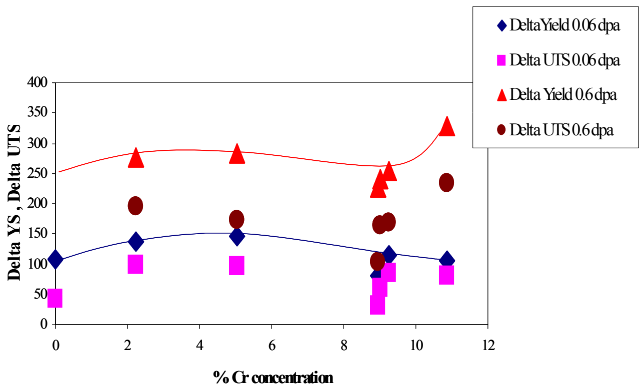

Fig. 2a – Change of tensile properties in Fe-Cr-C model-alloys and in T91 and Eurofer97 versus Cr concentration, for two neutron irradiation doses.

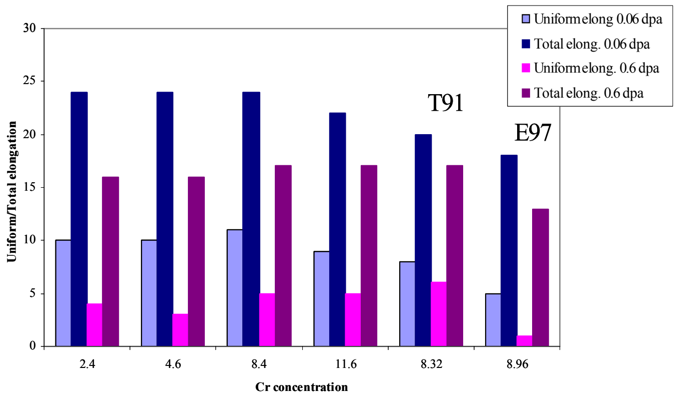

Fig. 2b – Uniform and total elongation for the same materials and radiation doses as in Fig. 2a.

Future work

Further studies of interstitial cluster mobility in Fe-Cr alloys as a function of different variables, including phase transformation (formation of Cr-rich α' phase) using improved interatomic potentials are ongoing. These results are expected to allow the longer term simulation of radiation damage accumulation using kinetic Monte Carlo tools, capable of providing direct comparison with experimental data, including those produced in the BR2 irradiation campaign at SCK•CEN. The materials extracted from the reactor will be characterised in terms of microstructure as a function of their composition and irradiation dose. In a later stage their deformation mechanisms will also be studied.

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