Mobility of dislocations in thermal aged and irradiated Fe-Cr alloys

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The choice of the Cr concentration in reduced-activation ferritic/martensitic steels for fusion applications is largely based on the observed minimum radiation-induced embrittlement, in terms of ductile-to-brittle transition temperature shift (ΔDBTT), found around 9%Cr [1]. To date, no physical explanation for the existence of this minimum has been provided. It is known that in high-Cr ferritic alloys the precipitation of the Cr-rich, coherent α’ phase occurs for concentrations above 9% Cr, both due to irradiation or thermal ageing at high enough temperature [2]. The formation of a fine dispersion of precipitates can therefore explain the increased embrittlement above this concentration, but it is unclear why the ΔDBTT should increase also for lower Cr concentrations. In addition, it is suspected that under irradiation α’ precipitation may be induced also for Cr contents below 9% [3]. At the same time, it is known that below 9% Cr ferritic alloys exhibit a tendency to ordering, i.e. Cr atoms are not distributed as in a random solid solution and try to be as far apart as possible from each other, thereby tending to create a superlattice [4].

In order to cast some light on the effect that these phase changes may have on dislocation motion in the presence of radiation damage, we study at the atomic level the mobility of dislocations in FeCr alloys of different concentrations where Cr is distributed in different fashions (i.e. ordered, clustered or in a random solid solution) and in the presence of radiation damage (e.g. point-defect clusters created by cascades). The microstructure will be obtained by making the system evolve according to the acting thermodynamic driving forces (also in the presence of defects) using Metropolis Monte Carlo techniques. Subsequently, the simulation of the dislocation motion will be performed using large scale molecular dynamics, whereby the corresponding stress-strain curve can be obtained. The simulations will be performed using an existing interatomic potential for FeCr which has been proven to provide a satisfactory description of both phase stability and point defects in pure Fe and in FeCr alloys, in agreement with density functional theory calculations [5]. The information obtained in this study is expected to be of use to parameterise dislocation dynamics models for the prediction of the mechanical behaviour at the mesoscopic level of the corresponding alloys.


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