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A multiscale approach to study the effect of chromium and nickel concentration in the hardening of iron alloys

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ABSTRACT

A multiscale approach is presented to study the effect of chromium and nickel concentration on the deformation behavior of iron systems. A combination of molecular dynamics (MD) and dislocation dynamics (DD) simulations are employed. In this framework, the critical information is passed from the atomistic (MD) to the microscopic scale (DD) in order to study the degradation of the material under examination. In particular, information pertaining to the dislocation mobility is obtained from MD simulations. Since accurate measurements of dislocation velocity are difficult to obtain through experiment, atomistic simulations constitute an adequate alternative tool. Then this information is used by DD to simulate large systems with high dislocation and defect densities. In particular, we study the effect of nickel and chromium concentration on the strength, as well as the effect of dislocation loops concentration on the yield stress of the aforementioned systems. The results reveal, among other, defect free zones, in accordance to experimental observations, and an evolution law for the defect density.

1. Introduction

The development of new-generation nuclear reactors depends on the availability of materials that can operate safely in severe environments for an extended service lifetime [1,2]. Materials operating in such a harsh environment are subjected to high doses of irradiation which cause changes in microstructure. These changes are responsible for dimensional instabilities, such as swelling and irradiation creep, and mechanical property evolution and degradation, such as irradiation hardening and post-yield deformation behavior including plastic flow and subsequent localization, which impact component performance and reliability.

The evolution of microstructural features with irradiation dose and temperature involves coalescence of vacancies and interstitials into voids and dislocation loops that cause swelling. In steels, void swelling can occur at temperatures up to about 800 K [3,4]. Modern steels used in nuclear reactors include high strength, ferritic, martensitic and oxide dispersion strengthened steels. These steels reduce the occurrence of void swelling and are more stable in the presence of defects that arise due to their severe functional environment. These steels are used in conditions subjected to creep and stress corrosion in the reactor environment that adversely affect their useful service life. Although ferritic–martensitic steels are quite resistant to swelling and maintain good fracture toughness at irradiation above 673 K [5,6], they are prone to loss of ductility at lower irradiation temperatures [7,8].

Over the past two decades, significant advances have been made in understanding the effects of irradiation on materials microstructure and mechanical properties by focusing theory, experiments and modeling on the basic underlying physical mechanisms [9]. For example, it is well established that the effect of irradiation on ferritic/martensitic alloys at low to intermediate temperatures is to increase yield stress, reduce strain hardening capacity and initiate flow localization at lower strains [10]. Furthermore, the predominant microstructural features include dislocation loops, voids, regions of solute segregation and second phase precipitates. The initial density and evolution of these features depends on some key variables, such as irradiation temperature, dose and dose rate, helium production rate and alloy composition. The mechanical properties on their part depend on the interaction of dislocations with the defects as well as the interaction between dislocations.

Due to the cost of the development and testing of such new materials, the use of computational techniques has been proven to be highly preferable and cost-effective. These techniques include, among others, first-principle, molecular and dislocation dynamics and were used by a number of authors [11–14], to model the behavior of prospective materials in future nuclear energy systems. Previous empirical models are being replaced by more

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physical ones taking advantage of new results at the microscopic level, of the tremendous improvements of computing technology and science, and of the breakthrough in physical metallurgy at the atomic scale. However, the prediction of the material behavior based on this knowledge is still an open problem, mainly due to its multiscale nature that involves processes spanning a wide range of length and time scales. Current models that address the issue of defect production and interaction are limited to one scale only without any interaction between the different scales. At the smallest scales (nanometer and picoseconds), irradiation dose and temperature cause the coalescence of vacancies and interstitials into voids and dislocation loops. These defects and clusters diffuse over macroscopic length and time scales, altering significantly the chemistry and microstructure of the material. In order to effectively predict the mechanical behavior of the materials under irradiation at the continuum scale, critical information should be determined and progressively passed from one scale to another.

In the heart of any macroscopic model is the collective behavior of dislocations inside the material under study. Among the available computational techniques, dislocation dynamics is the most commonly used to study the materials behavior at the mesoscale. However, in order for this method to work, a detailed knowledge of the dislocation mobility in an analytical form inside the materials is required. In the literature various studies can be found to deal with the mobilities of dislocation using molecular dynamics simulations [15–17]. This work comes to add to the already published research in dislocation mobility in alloy systems [18–25] by computing the effect of the solute concentration on the mobility of two different alloys, e.g. Fe–Cr and Fe–Ni. Recently work has been done in calculating the mobility of screw dislocations in α-iron and to derive analytical expressions for the use within the dislocation dynamics [26]. Although the motion of screw dislocations is dominant in the deformation of bcc structures, the role of edge dislocations is not insignificant. Furthermore, in the dislocation dynamics framework, the mobility of a screw dislocation is considered to be a constant fraction of the mobility of the edge dislocation therefore, if the mobility of either an edge or a screw dislocation is known, the mobility of the other type can be calculated in terms of this mobility [27,28].

In view of this, molecular dynamics simulations were performed in iron alloys with various concentrations of nickel and chromium [29]. These systems were chosen because of the availability of the interatomic potentials and their similarity to the systems considered for the next generation nuclear reactors. Due to the generality of the technique, other materials and alloys can be studied as well. Then the calculated mobilities has been used to formulate rules of the mobility as function of temperature and concentration in a suitable form for the dislocation dynamics framework. This information can be used to study the degradation of the material at the microscale. This paper is organized as follows. First, the multiscale methodology is presented. Then, the geometry of the simulation box, the methodology of creating and moving an edge dislocation and the boundary conditions are reviewed. Then, the mobility of an edge dislocation in α-Fe is calculated and compared with similar results in the literature to validate our simulations. Later, the mobility of an edge dislocation in Fe–Ni and Fe–Cr structures with various Ni and Cr concentrations is calculated and the results are used to develop rules of the mobility as function of temperature and concentration in a suitable form for the dislocation dynamics framework. Following that, DD simulations are performed and the results gathered are presented along their analysis that leads to the evaluation of the critical resolved shear stress in Fe–Ni–Cu alloys as a function of concentration, as well as irradiation damage. Finally, semi-empirical expressions are developed for future use in a dislocation-based crystal plasticity framework, followed by discussion and the conclusions of this work.

2. Methodology

The modeling methodology involves a hierarchical approach integrating molecular dynamics (MD) simulations and dislocation dynamics (DD) simulations, over the relevant length and time scales to model the fates of defects and solutes and thus, predict microstructural evolution in irradiated ferritic/martensitic steels. The evolution of the microstructure under irradiation will be linked to a quantitative prediction of irradiation hardening and post-yield deformation behavior through the use of dislocation dynamics (DD) simulations, crystal plasticity and continuum internal variable models. The following procedure is a summary of the multiscale approach that we have adopted.

(a) MD simulations: Dislocation mobility and defect properties in Fe-alloys (Fe–Cr, and Fe–Ni) are obtained from atomistic simulations based on semi-empirical EAM and/or MEAM potentials. Specifically, defect cluster energetics, physical insight into kinetic processes and interactions are obtained from large-scale atomistic simulations, including the fate of moving defect–solute clusters with dislocations and grain boundaries, the mechanisms of moving dislocation interactions with dislocation loops, defect clusters and second phase particles.
(b) DD–MD linkage to mechanical property changes: The dislocation mobility and microstructure predicted by the atomistic simulations serves as input to three-dimensional DD simulation to quantitatively predict radiation-induced mechanical property changes. Specifically, MD lead information about the dislocation mobility and its dependence on solute concentration.
(c) MD-informed dislocation dynamics simulations: The collective behavior of an ensemble of dislocations in a crystal is modeled by calculating the forces on each dislocation and taking into account all possible reactions among dislocations, as well as between network of dislocations, and the radiation-induced defect microstructure.

2.1. Molecular dynamics

The MD simulations consists of a box with orientations $x = \langle 111 \rangle$, $y = \langle \bar{1}01 \rangle$ and $z = \langle 1\bar{2}1 \rangle$. Periodic boundary conditions were used along x and z directions, while the y direction was kept free so that a shear stress to be applied. The box was divided into two regions, an upper and a lower with the lower region having one atomic plane fewer in the x direction than the upper region. Then, the upper region was elongated and the lower compressed so that both regions to have the same length. By minimizing the energy of the resulted structure using the conjugate gradient method, an edge dislocation with line parallel to z and moving on the x–z plane was formed at the center of the simulation box. The final configuration is shown in Fig. 1. This configuration is designed to simulate a dislocation of infinite length inside an infinite size box. This technique was first adopted in [30] and allows the dislocation to traverse the simulation box multiple times without leaving the simulation cell and at the same time eliminating any undesirable end effects and inducing very low to negligible stresses to the crystal. The dimensions of the simulation box at 0 K were approximately $120b \times 80b \times 114b$, in accordance with other similar works [31,26].

All the molecular dynamic simulations presented in this paper were performed using the code LAMMPS [33]. The Embedded Atom Method (EAM) [34] potentials developed by Mendelev et al. [35], Stukowski et al. [36] and Bonny et al. [37] for the pure iron, Fe–Cr and Fe–Ni respectively were used. All three potentials were