8.6 Molecular Dynamics Modeling of Dislocation-Obstacle Interactions and Mechanisms of Hardening and Strengthening in Irradiated Metals — Y. N. Osetskiy and R. E. Stoller (Oak Ridge National Laboratory)

OBJECTIVE

The objective of this research is to investigate mechanisms of interaction between dislocations and obstacles (precipitates, voids, bubbles, etc.) induced at fusion irradiation conditions. These defects are usually very small, <10nm, and therefore atomic scale details are necessary to be understood.

SUMMARY

This extensive simulation program is design to investigate the basic mechanisms of strengthening and hardening during irradiation of fusion materials. Strength of spherical obstacles of different types and sizes is discussed for comparison. An interesting observation is that the relative strength of rigid particles (a model for oxide particles) depends on their size: small particles, 2 nm in diameter, are relatively weak compared to voids or equilibrium He-filled bubbles, while large particles are the strongest obstacle. The explanation is related to the atomic scale features of dislocation-obstacle interactions, particularly to cross-slip and climb mechanisms.

PROGRESS AND STATUS

Introduction

Structural materials subjected to fusion conditions are changing their microstructure and hence mechanical properties. Understanding the details of this process is necessary for predicting changes, estimation of structural components lifetime and design of new materials tolerant to fusion conditions. Experimental studies have demonstrated that depending on the structural material composition and particular conditions (temperature, neutron flux, He accumulation due to irradiation and/or transmutation, etc.) different microstructural features can form and affect dislocation motion and therefore mechanical properties. These obstacles can be voids, secondary phase precipitates, gas filled bubbles and other microstructure features relevant to fusion structural materials e.g. oxide nanoclusters. In many cases, for example voids and He-bubbles, modern radiation damage theory models based on rate theory, may predict evolution of their population however to bridge this to mechanical properties changes is not a trivial task. In general, simple phenomenological models used to account hardening/strengthening effects due to microstructural features are focused mainly on statistics of defects distribution having particular obstacle strength as an input parameter. It is therefore practically important to obtain information on the interaction mechanisms and strength for particular obstacle types. The corresponding extensive simulation program was designed and some preliminary results are presented here focused mainly on comparison spherical localized obstacles of different types.

Formalism

We used Molecular Dynamics (MD) modeling technique to investigate dislocation motion in the present of obstacles. The scale of modern models i.e. ~10^7 atoms, allows to cover the most important obstacles appeared under irradiation such as voids, bubbles, precipitates, oxide

nanoclusters and dislocation loops. A computer code developed at ORNL was used for these modelings is based on the atomic-scale dislocation model described in [1].

Voids and coherent Cu-precipitates in bcc iron matrix where considered earlier [2-4] and are used here for comparison. The current simulation program is focused mainly on He-filled bubbles and rigid inclusions simulating oxide-particles by introducing infinitely high shear modulus inside an inclusion. We have simulated equilibrium bubbles taking into account the earlier results on the equilibrium He-to-vacancy ratio [5]. At the first stage we have considered ½<111>{110} edge dislocation in bcc iron matrix. This choice was governed by two reasons:

1. Edge component in the dislocation network is increasing under irradiation due to formation and growth of dislocation loops;
2. Because of its inability to cross-slip an edge dislocation can be pinned by the rigid inclusions much stronger than a screw dislocation which can overcome rigid obstacles by cross-slip.

In the report we present data on spherical obstacles of three sizes 1, 2 and 4 nm in diameter all simulated at 300K and the applied strain rate 10^6 s^{-1}. More details on temperature and strain rate effects for voids and precipitates can be found in [2-4] and those for bubbles and rigid obstacles are under current study.

RESULTS

The results on Critical Resolved Shear Stress (CRSS), which is the measure of the strength of the individual obstacle, obtained for coherent Cu-precipitates, voids, He-filled bubbles and rigid inclusions are presented in the Fig. 1 together with the data obtained in simulation of the Orowan mechanism for the corresponding obstacle size. One can see that in the size range studied, from 1 to 4 nm, coherent Cu-precipitates are the weakest obstacles. The interaction mechanism in this case is a simple shear without any additional changes in precipitate or dislocation structures. Voids are stronger obstacles and cause some climb due to absorption vacancies by an edge dislocation line. The comparative strength of He-bubbles depends on their size. Thus small bubbles (1nm) are stronger than voids however larger ones (4nm) are compatible. We expect that larger bubbles (>4nm) might be weaker obstacles than voids however more studies are necessary to reveal this. The mechanism of this size dependence is not understood yet but it might be related to the pressure of He inside bubbles which for equilibrium bubbles decreases when size increases. The size dependence of the rigid inclusion strength is even stronger as can be seen in

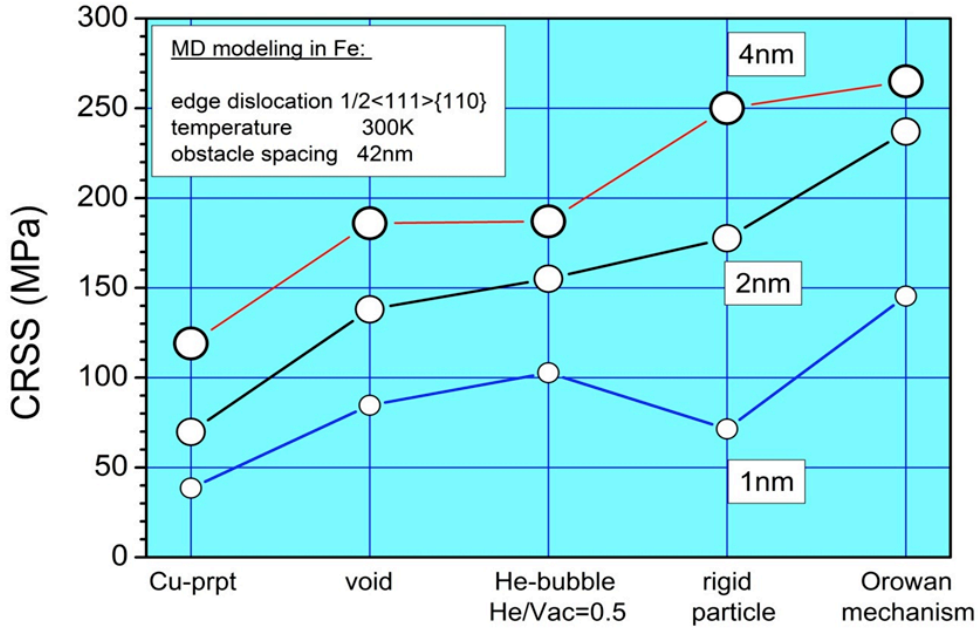

Figure 1. Critical resolved shear stress for different obstacles obtained in MD modeling.

Fig.1. Thus 1 nm inclusion is very weak, compatible with the corresponding Cu-precipitate. The 2nm inclusion is stronger than precipitate, void and bubble but still significantly weaker than the Orowan obstacle. And, finally, 4nm inclusion is compatible with the maximum possible strength given by the Orowan mechanism. Atomic-scale modeling allows to rationalize mechanisms responsible for such behavior. Thus, small 1nm inclusion is so weak because edge dislocation can easily emit few vacancies to climb around the rigid obstacle and to drag the corresponding interstitial atoms out as a superjog. At 2nm inclusion dislocation achieves shape of two parallel screw segments with spacing just below 2nm. Strong interaction between dipole leads to their cross-slip and unzipping from the obstacle when one of the screw dislocation segments reaches the edge of the obstacle. In this case a large superjog created on the dislocation line and the mechanism is similar to that discussed in [4] for voids. However, at large inclusion, 4nm, although the dislocation achieves the screw dipole configuration the driving force for cross slip is smaller because the separation is large. Moreover, the successful cross-slip that would release the dislocation from the inclusion must be more significant because of the large obstacle. Therefore, in this case the dislocation dipole is elongating until attraction force exceeds the Peierls stress for these screw segments, dislocation segments annihilate and the Orowan loop is left around the inclusion. The maximum possible stress is realized for this mechanism. We expect that larger obstacles will reproduce exactly the Orowan stress.

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