8.7 STRENGTHENING DUE TO HARD OBSTACLES IN FERRITIC ALLOYS- Y. N. Osetskiy and R. E. Stoller (Oak Ridge National Laboratory)

OBJECTIVE

The purpose of this research is to understand atomic level hardening mechanisms in materials with rigid precipitates such as ODS alloys. Because of the lack of interatomic potentials, direct modeling of such systems is not yet possible. We therefore have developed a model of rigid uncompressible precipitates embedded in a metallic matrix interacting via an empirical EAM potential.

SUMMARY

We have developed a molecular dynamics (MD) based model to simulated dislocation dynamics in the presence of rigid, impenetrable inclusions. These inclusions simulate rigid oxide particles as obstacles to dislocation motion. Interactions between a moving edge dislocation ½<111> {110} and rigid inclusions was modeled over a wide range of parameters such as inclusion size, temperature, strain rate and interaction geometry. It was found that the interaction mechanism depends strongly on the inclusion size and interaction geometry. Some new mechanisms were observed and are now under detailed investigation.

PROGRESS AND STATUS

Introduction

ODS materials have a number of properties making them very attractive for nuclear energy applications [1, 2]. Some of these such as interactions between oxide-particles and other solute elements are strongly related to chemical properties. For example it is expected that existence of small oxide-particles may suppress He-bubble formation and growth. However due to significant complications in describing interatomic interactions such studies are mainly limited by low-scale firs-principle DFT calculations of elementary interactions between constituting elements but not modeling real oxide particles [3, 4]. However, in application to mechanical properties of ODS materials the problem can be resolved in a relatively simple and accurate way. The main issue here is the dislocation interaction with oxide particles and the fact that these particles are much harder than the metallic, e.g. Fe, matrix material. Oxide particles are “strong” obstacles that interact with moving dislocations by the Orowan-like mechanism and the important is not the behavior of dislocations inside the particle or on its interface but the self-interaction of dislocation segments heavily-curved around the obstacle. Therefore, omitting the details of particle-matrix interface does not affect the dislocation particle interactions.

Simulation method

We have developed a molecular dynamics (MD) based model to simulated dislocation dynamics in the presence of rigid, impenetrable inclusions. These inclusions simulate rigid oxide particles as obstacles for dislocation motion. At the MD scale such an inclusion is considered as a super-atom of the corresponding size whose motion follows the usual Newtonian equations. Modeling of atomic-scale dislocation dynamics is a very resource-demanding process for a) the simulated crystal should be large to accommodate long enough dislocation which can be strongly curved around the large obstacle and b) large number of time steps should be integrated to model a relatively slow dislocation. In practice, the largest obstacle we simulate at the moment, 7 nm in diameter, needs ~6.3 million mobile atoms integrated over a few million steps to model dislocation moving at about 1 m/s. Using this model we are studying dislocation – rigid inclusion interactions over a wide range of parameters such as inclusion size, interaction geometry, dislocation velocity and applied deformation strain rate, ambient temperature etc.

Current progress

For the last six months we have continued modeling of the largest at that time obstacles, 6 nm in diameter and have started a larger, 7 nm, inclusion. The necessity of this came from the observation that the mechanism of interaction between a moving dislocation and rigid inclusion depends very much on the obstacle size. More precisely it depends on the inclusion curvature and therefore on the cross-section of the inclusion in the dislocation glide plane. We therefore investigate this particular effect and have found that it is more important for large inclusions. The results were treated and we have found that the obstacle critical resolved shear stress (CRSS) follows the dependence versus the actual obstacle size where it is intersected by the dislocation slip plane. A certain asymmetry was found for the obstacle above the slip plane, which is stronger than the equivalent obstacle below the slip plane. An example of CRSS dependence as a function of the interaction geometry is presented in Figure1. We explain this by the fact that interatomic potentials are asymmetric as well and the absolute value of forces generated during compression is higher than that for tension. This therefore affects to the obstacle strength through the compression and tension regions around edge dislocations. We do not expect a similar effect for screw dislocations. It is interesting that not only CRSS depends on the interaction geometry but also the interaction mechanism itself. This is illustrated in Figures 2 and 3. Thus in Figure 2 shows the edge dislocation ½<111>(110) and 6 nm inclusion with its equator in the dislocation slip plane before (a) and after (b) interaction. The Orowan sheared loop shown in Figure 2b is formed due to this interaction. This mechanism provides the maximum strengthening as shown in Figure 1.

Figure 3 show the same obstacle but in the configuration when its equator is half of the radius below the dislocation slip plane and the corresponding CRSS in Figure 1 is for R=0.5. The position of slip plane can

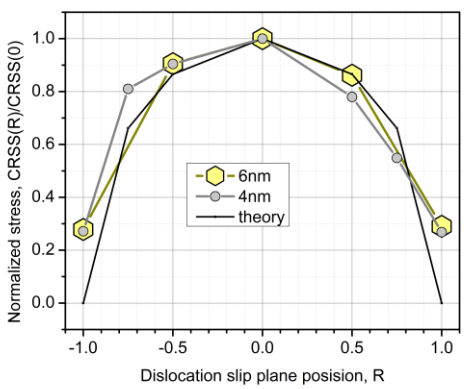

Figure 1. Dependence of the CRSS vs distance between the inclusion equator and dislocation slip plane. Black solid line shows the estimation based on the area of the corresponding cross-section through the inclusion.

be clearly seen on Figure 3a as a red line and it moves from left to right.

The configuration obtained after the dislocation bypassed the inclusion is shown in Figure 3b. One should take into account that in this figure dislocation is seen again on the left side of the obstacle where it appeared due to periodic boundary conditions in the slip plane. A small interstitial loop is left behind the inclusion and the corresponding negative superjog was created on the dislocation line. This can be seen more clearly in Figure 3c where the view along the dislocation Burgers vector is shown. The loops size and shape is approximately equivalent to the upper part of the inclusion above the dislocation slip plane.

These examples demonstrate clearly how the interaction mechanism depends on the interaction geometry. The mechanism on Figs.3 is observed for the first time and was not described yet in the literature. The usual deformation mechanisms result in formation vacancy-type defects because this is energetically more favorable. Formation of interstitial-type defects occurred on these inclusions is because they are very strong obstacles. In fact, they are obstacles of maximum possible strength. We are going to investigate these mechanisms in more details because we think they should have important

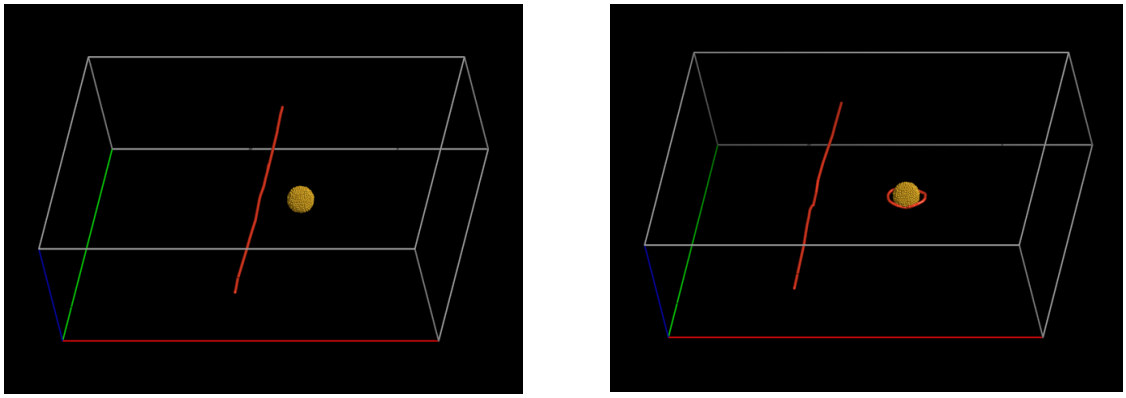

Figure2. Edge dislocation ½<111>(110) and 6nm inclusion with its equator in the dislocation slip plane before at) and after (b) interaction. The Orowan sheared loops shown on the right is formed due to this interaction. This mechanism provides the maximum strengthening.

influence to the creep behavior of ODS alloys.

We have also concluded that 6 nm obstacle might be too small for the treatment within the continuum approach to find out the general description of the effect. So we have launched a new series of deformations for 7 nm rigid particle. The full set of parameters to be studied includes temperature: 100, 300, 450 and 600 K, different levels of the dislocation slip plane relatively to the particle equator: 0, +-0.5R, +-0.75R and +-R, where R=7 nm is the particle radius and applied strain rates: 1, 2 and 5 in units of 10^6 s^{-1}. This work is in progress now.

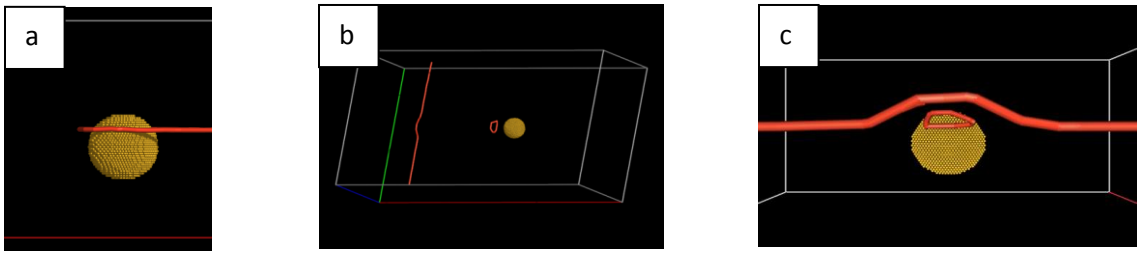

Figure 3. Edge dislocation ½<111>(110) and 6nm inclusion with its equator half of the inclusion radius below the dislocation slip plane. a – view to the inclusion along the dislocation slip plane where red line is the bowing around. Dislocation glides from left to right. Centre – total view to the crystal after the interaction. Dislocation has a negative created due to an interstitial dislocation loop left behind the inclusion. Right – view along the dislocation Burgers vector.

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