8.4 Radiation-Induced Obstacles in Iron and Ferritic Alloys: An Atomic-Scale View —

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EXTENDED ABSTRACT - paper submitted to J. Nucl. Mater. after ICFRM-16, with new results on the largest modeled 6nm obstacles added.

Radiation produces nanoscale defects which strongly affect mechanical properties. An extended study using atomic-scale modeling investigated strengthening mechanisms in irradiated iron and ferritic alloys, considering ***inclusion-like*** obstacles (precipitates, voids, bubbles). Both types have unique features, different strengthening mechanisms and demand different models for predicting hardening. The strengthening mechanism for dislocation loops depends on their size, interaction geometry and on impurity segregation to the loops and may vary from practically zero resistance to the maximum strength of an Orowan mechanism. Conditions which lead to the maximum strengthening resulting from different types of individual obstacles and a combination of multiple obstacles were investigated and the results are discussed in terms of existing experimental data.

Model To study dislocation dynamics at atomic scale we used a standard MD based model described earlier (Osetsky&Bacon, MSMSE, 2000) and schematically depicted in the Figure 1. Within this model we studied screw and edge dislocations moving through a periodic array of obstacles under applied stress or stain and temperature. Typical system consists of 2-10 million mobile atoms interacting by EAM-type interatomic potentials and with a simulated dislocation density of ~10^{13}-10^{14}m^{-2}. Applied strain rates of 10^6-10^8s^{-1} provide dislocation velocity from 10 to 1000 m/s simulated over physical times 100 to 2000 ps. Typical output information include stress-strain dependence, crystal energy and visualization of a dislocation and obstacles.

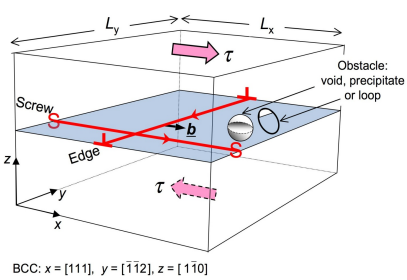

Figure 1. Atomic scale model for dislocation-obstacle interaction study.

Voids, precipitates and bubbles. Static modeling, i.e. 0K relaxation to the minimum energy state at a certain strain, allows a direct comparison with continuum models and dislocation dynamics modeling. The result is a set of equilibrium crystal states, which yields stress-strain and energy-strain dependences, Critical Resolved Shear Stress (CRSS) and dislocation-obstacle interaction mechanisms. Results for voids and Cu-precipitates are compared with continuum models in Figure 2. Here ***D*** is obstacle diameter and ***L*** is period along the dislocation line, all are in units of the edge dislocation Burgers vector ***b*** = ½<111>. Large enough obstacles are strong "Orowan-like" and their

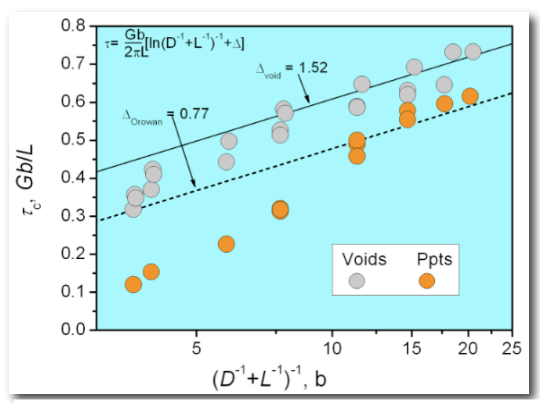

Figure 2. Comparison of atomistic and continuum results for void and precipitate hardening.

strengthening is well described by the continuum approach. However, small obstacles involve local atomic scale effects, which cannot be accounted for by continuum methods.

Temperature effects in Cu-precipitate strengthening.

The Fe-Cu system is relevant to the experimentally observed radiation-induced precipitate hardening in pressure vessel steels. Small precipitates are coherent with bcc-Fe matrix while large precipitates, >4-7nm, transform to fcc structure. Transformation and hardening depend on temperature and geometry of dislocation-precipitate interactions. An extensive study provided understand the basic mechanisms of Cu-precipitate hardening, phase transformation and their temperature dependence. The results are presented in Figure 3: weak temperature dependence of CRSS for small precipitates is consistent with numerous data for neutron irradiated ferritic alloys where precipitates do not grow above 2nm while the stronger temperature dependence for large precipitates consistent with experiments in overaged alloys.

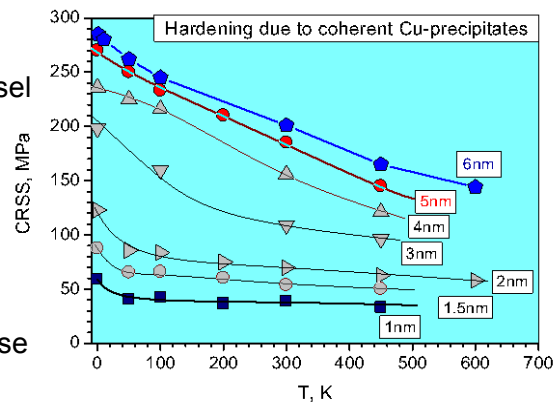

Figure 3. Temperature dependence of hardening due to Cu-precipitates of different size.

Comparison of different inclusion-like obstacles.

Other inclusion-like obstacles important in irradiated ferritic alloys include He bubbles and oxide nanoclusters as in ODS-alloys. The equilibrium state of He-bubbles and the effect of He-bubbles on moving dislocations have been studied. The bubble-dislocation interaction mechanisms are generally similar to that with voids. Near the equilibrium He-to-vacancy ratio (He/Vac) bubbles are stronger obstacles than voids, with their strength decreasing at higher He/Vac. Oxide particles we "simulated" as rigid inclusions coherent with bcc-Fe matrix. The inclusion had infinitely high elastic modulii while the whole inclusion interacted with the matrix atoms by the same Fe potential and can move inside matrix. Dislocation interaction with such an inclusion depends strongly on its size: small inclusions are weak obstacles and even an edge dislocation can overcome it whereas large ones, ≥4nm, are classical Orowan obstacles and Orowan loops are formed after the dislocation breaks away. A comparison of strength of all studied inclusion-like obstacles is presented in Figure 4.

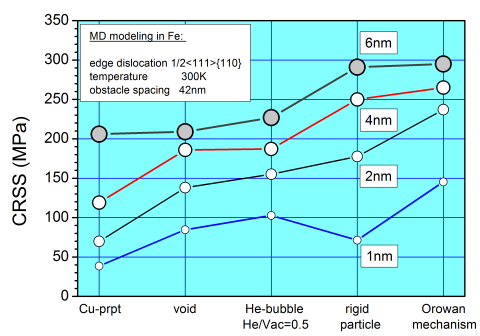

Figure 4. Comparison of strength of different types of obstacles of different size.