8.2 STRENGTHENING DUE TO RADIATION INDUCED OBSTACLES IN FE AND FERRITIC ALLOYS.

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OBJECTIVE

The purpose of this research is to understand atomic level strengthening mechanisms in materials with radiation induced localized microstructures such as voids, gas-filled bubbles, secondary phase precipitates and oxide particles. These microstructures work as obstacles to dislocation motion and cause radiation induced hardening and embrittlement. Currently, we are investigating the map of mechanisms depending on the obstacle type and size.

SUMMARY

Irradiation of structural alloys by neutrons and ions lead to formation of a high density of nanoscale objects such as secondary phase precipitates, voids and gas-filled bubbles. These objects are obstacles for dislocation motion and cause wanted or unwanted changes in mechanical properties. In order to predict materials behavior these obstacles must be characterized as well as their individual strength to be estimated. The only technique that allows this at the scale of nanometers is classical molecular dynamics (MD). In this work we modeled vacancy voids, He-filled bubbles, Cu precipitates and rigid inclusions in bcc-Fe matrix. At the current stage of the research we investigated ½<111>{110} edge dislocation. During its motion this dislocation cannot change its glide plane (cross-slip) to avoid interaction with obstacles and therefore produces maximum strengthening effect. The results obtained in this research will be used to improve theoretical prediction of mechanical properties changes.

PROGRESS AND STATUS

We now have finished modeling obstacles of up to 7 nm in diameter and continue with 8 nm obstacles. This demands larger modeling crystals, $>8x10^6$ atoms. Unlike small obstacles, <4 nm, which show individual mechanisms with different hardness, large obstacles are strong and according to the dislocation line shape that adopts a long dipole of screw dislocations the mechanism is assumed to be the Orowan-type. However, as our modeling has demonstrated, the classical Orowan mechanism [1] i.e. with formation of a sheared dislocation loops around the obstacle is applicable only to rigid obstacles. Other obstacles demonstrate the shear mechanism with a similar strength. This can be seen in Figure1 where a comparison of critical resolved shear stress (CRSS) is presented for different obstacles of different size. Rigid obstacles are found to be the strongest. The dependence of their strength is also exceptionally strong within the range studied as can be seen in Figure2 where the comparison of atomistic modeling of rigid obstacles from 1 to 7 nm in diameter at 300K (circles) with theoretical estimation from [2,3] (lines) is presented.

Our data demonstrate that obstacles of a few nanometers in diameter have individual dependence of their strength versus their size. This is especially important for the irradiation conditions for the majority of obstacles is typically small, within a few nanometers. Our calculations provide parameters for the prediction of mechanical properties change due to irradiation. This work was already started within the corresponding task. Within the current task we now are finalizing investigation of the interaction geometry effect for large obstacles. The main issue is if a simple usage of mean defect size is appropriate for strengthening estimation. We have already some evidences that interaction between an obstacle and a dislocation gliding above and below its equator can be strongly asymmetric for some obstacles. In this case a simple usage of dispersed barrier hardening model [4] with a mean obstacle size can be inaccurate especially for small obstacles.

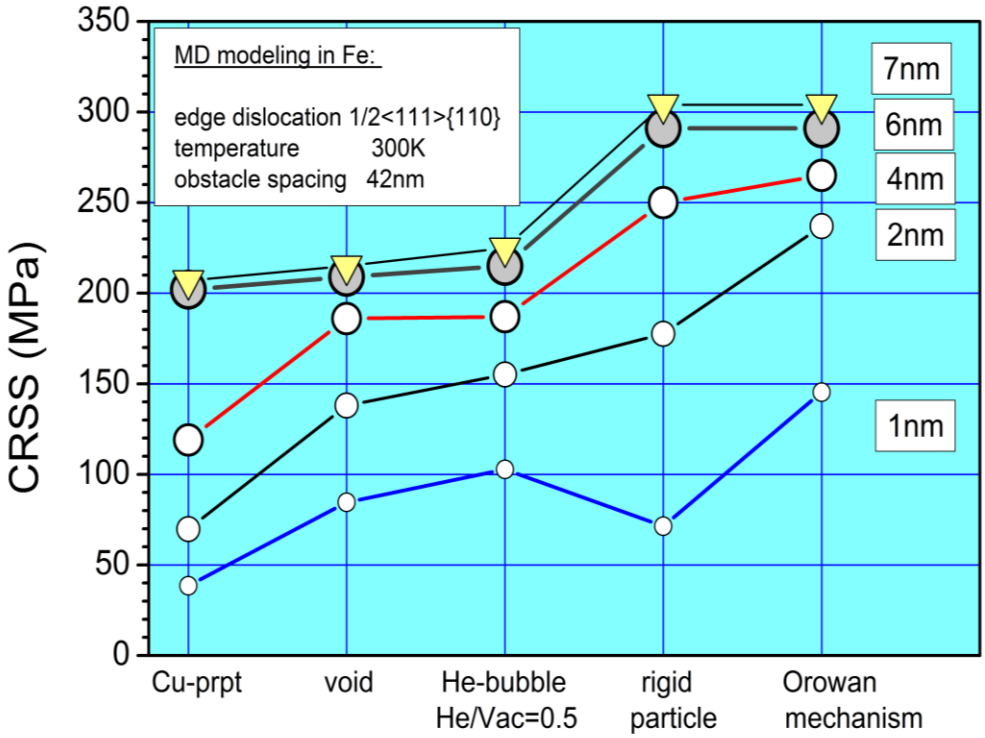

Figure 1. Critical resolved shear stress for different obstacles of different size obtained by molecular dynamics modeling at 300K.

Future Studies

1.Development of the enhanced dispersed barrier hardening model able to include dislocation obstacles interaction mechanisms revealed in atomic-scale modeling.

2. Extension of modeling program to screw dislocation to cover all possible interactions.

3. Extension of modeling program to dislocation-type obstacles such as dislocation loops. So far dislocation loops are threated in the same way as inclusions however their interaction with dislocations is quite different and this must be taken into account.

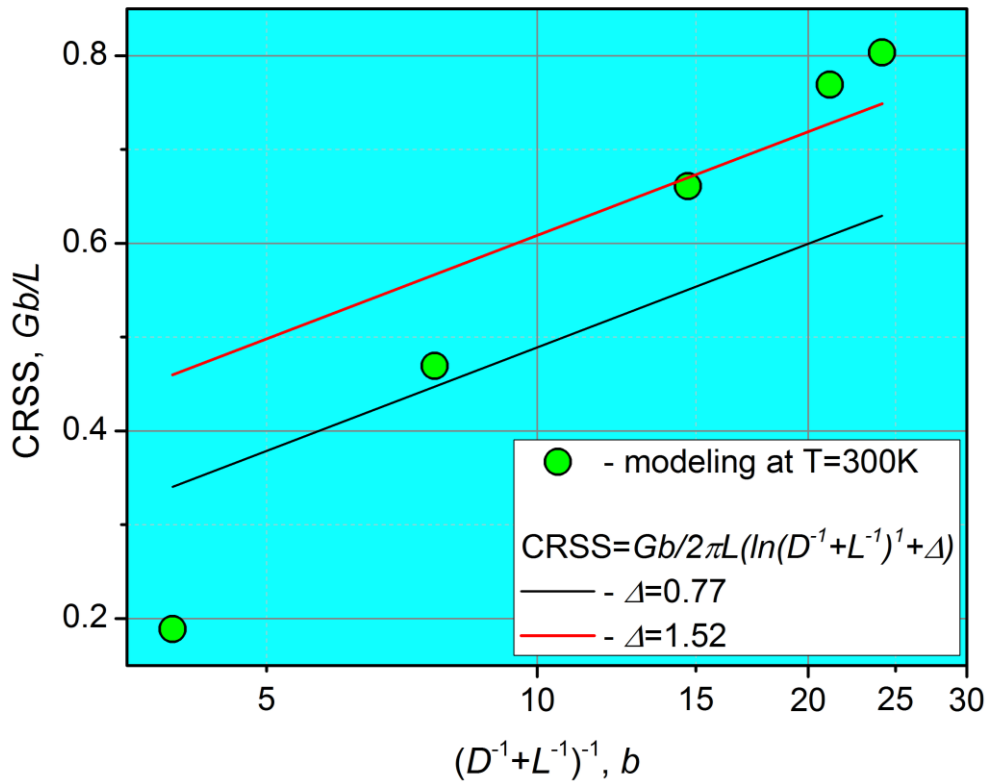

Figure 2. Critical resolved shear stress in reduced units as a function of harmonic mean of an obstacle diameter, *D*, and spacing between them along the dislocation line. Circle - rigid inclusions simulated in current work, lines are dependences obtained in dislocation dynamic modeling for Orowan mechanism (black line) and void (red line) in [1,2].

References

[1] Orowan E., A type of plastic deformation new in metals, *Nature,* 1942, vol.149, p.643.
[2] Bacon, D. J., Kocks, U. F., and Scattergood, R. O., 1973*, Phil. Mag.,* 28, 1241.
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[4] Seeger A., Proc. 2nd UN Int. Conf. on Peaceful Uses of Atomic Energy (Geneva, Switzerland, September 1958), 1058, vol.6, p.250.