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Invited Paper

The effect of the atomic hydrogen on the behavior of a single dislocation in bcc tungsten: atomistic study

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ABSTRACT

Tungsten (W) has been widely studied and spotlighted as a plasma-facing material (PFM) in the extreme environment of nuclear fusion due to its excellent physical properties. It is important to investigate the effect of hydrogen on the material behavior of tungsten as it was used in the hydrogen-rich fusion environment Solute hardening is a typical phenomenon, and it is traditionally understood by dragging or pinning effect when hydrogen atoms act like solute atoms that impede dislocation motion. On the other hand, there were several experimental studies reporting softening associated with enhanced dislocation activity, either by easy nucleation or increased mobility, or both. In order to shed light on these controversial observations, the authors focused on the hydrogen effect on dislocation mobility in W using molecular dynamics simulations with different dislocation types, hydrogen concentrations, stress, and temperature. At a high concentration of 1 at.%, H atoms are often strongly clustered around a dislocation core and produce a super-pinning effect in that both edge and screw started to move at a stress far beyond Peierls stress. This critical stress reduces with temperature increase, and thermally assisted kink or jog formation helps a dislocation escape from the H-cloud trapping. At a low concentration of 0.01-0.1 at.% or a high concentration of 1 at.% without super-pinning, hydrogen dragging barely appeared with a screw dislocation, and the intrinsic lattice resistance dominated the motion of a screw. For an edge dislocation under the same condition, an appreciable reduction in mobility was observed with the increase of H concentration at a low temperature of 300 K, and this change in mobility becomes inconspicuous for higher temperatures. In conclusion, this study predicts the hardening of W at a high H concentration of 1 at.% due to dislocation trapping at the H cluster.

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