HYDROGEN ENHANCES CROSS-SLIP OF DISLOCATIONS IN THE VICINITY OF GRAIN BOUNDARIES

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Extensive experimental observations indicate the presence of nano-voids and the increase of free volume along the grain boundaries in hydrogen contaminated metals. This rate-dependent phenomenon motivates theoretical investigations of the underlying mechanisms. Here, a hydrogen enhanced cross-slip (HECS) mechanism in the close vicinity of the grain boundaries is demonstrated by direct molecular dynamics simulations. To this end, the interaction of the screw dislocations with a variety of symmetric tilt grain boundaries in H-charged and H-free bicrystalline nickel specimens is examined. The presence of segregated hydrogen atoms at the grain boundaries induces a stress field in their vicinity, and thus the barrier for cross-slip of screw dislocations considerably decreases. The enhanced cross-slip of dislocations facilitates the formation of jogs. These jogs can form vacancies during the glide process. This mechanism shows nano-scale evidence of enhanced vacancy formation and subsequent increase in the free volume along the grain boundaries in the presence of H. This increase of the free-volume along the grain boundary damages the material and induce further embrittlement in addition to the direct effect of hydrogen in decreasing the fracture energy.