MECHANISMS OF HYDROGEN TRAPPING AND CLUSTERING AT NANOVOIDS AND DISLOCATIONS IN BCC METALS

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Interactions between hydrogen and nanovoids and dislocations are central to understanding hydrogen induced damages in structural metals. Focusing on the BCC metal group, we systematically investigated these interactions using computational simulations. For nanovoids, we elucidated the complete process of hydrogen trapping therein, explicitly demonstrating sequential adsorption of hydrogen adatoms on dedicated geometric interstitial sites of nanovoids with distinct energy levels, with interaction between hydrogen adatoms dominated by pairwise power law repulsion. Based on the results, a predictive model has been established for quantitative determination of configurations and energetics of hydrogen adatoms in nanovoids. This model was then further combined with equation of states of hydrogen gas to predict the conditions of hydrogen bubble formation in nanovoids. Furthermore, multiscale simulations based on our predictive model were then performed, yielding good agreement with recent thermal desorption experiments. Meanwhile, for hydrogen at dislocations, we showed that hydrogen clustering can be strongly facilitated by anisotropic stress field along particular crystalline directions, and demonstrated that platelet-shaped hydrogen cluster formation can be thermodynamically enabled around certain dislocations. Such hydrogen clustering can further promote the formation of dislocation junctions which are otherwise unstable in absence of hydrogen. These hydrogen-enabled dislocation junctions can stay stable under loading, subsequently promote vacancy loop formation and growth. The above findings provide critical mechanistic pieces to advance our understanding of hydrogen induced damages in metals.