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Hydrogen Segregation in Crystalline Palladium and Effects on Mechanical Properties HIEU PHAM, AMINE BENZERGA, TAHIR CAGIN, Texas A&M University — Calculations of tensile strength and tensile modulus were carried out to investigate the effects of hydrogen interactions, diffusion and segregations in palladium single crystal, high-vacancy crystal and bicrystal, by using the embedded atom method. Elevated temperature, hydrogen absorption and defects such as vacancy and grain boundary (GB) individually induce a loss in mechanical strength of palladium in a monotonous manner. The hydrogen-induced mechanical degradation was noticed at the grain boundary, as well as in bulk. The failure induced by hydrogen in palladium up to x_H=0.1 is plastic rather than brittle, even around grain boundary region, by formation of dislocations. At high H absorption, the global hydrogen concentration is a dominant factor over crystal defects. However, a high-angle grain boundary such as $\sum$5 (2 1 0) provides a great driving force for diffusion and tendency for physical trapping of hydrogen. Therefore, the existence of grain boundary makes materials more susceptible and easily exposed to high hydrogen absorption and segregation. Also, our simulation shows that hydrogen maintains the highest localization at GB in the vicinity of ambient temperatures; and this finding coordinates with experimental observation that hydrogen embrittlement are generally observed at room temperatures.

Hieu Pham
Texas A&M University

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