SAND2014-0663C

Nanomechanics of Helium-3 Bubble Growth in Aging Palladium Tritides

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Palladium is an attractive material for hydrogen and hydrogen-isotope storage applications due to its properties of large storage density and high diffusion of lattice hydrogen. For the storage of tritium, the material's structural and mechanical integrity is threatened by both the embrittlement effect of hydrogen, and the creation and evolution of additional crystal defects (e.g. dislocations, stacking faults) caused by the formation and growth of nanometer-sized helium-3 bubbles. Gaining a fundamental understanding of the mechanics of this phenomenon is accomplished using atomic-scale simulation, which requires inter-atomic potentials that accurately capture the structural, mechanical and physical properties of the system, including the miscibility gap between dilute and concentrated phases of hydrogen in palladium. Here, we present embedded-atom potentials for the palladium-silver-hydrogen system. This ternary model is used to examine the effects alloying has on the structure of the hydride, such as decreasing the miscibility gap and increasing the likelihood of hydrogen occupying tetrahedral interstitial sites over octahedral sites. Using these potentials, we perform atomistic simulations of helium bubble growth. Our simulations show the evolution of a distribution of material defects (e.g. dislocations, stacking faults), and observations are made on how alloying affects the aging process.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.