Effects of Neutron Damage on Hydrogen Near Grain Boundaries in Tungsten

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Nuclear fusion, the reaction that powers the Sun, plays an important role in the search for alternative energy sources. A fusion test reactor known as ITER is currently under construction in France that will provide a facility in which to study magnetic-confinement fusion. The reaction that will occur inside, the deuterium–tritium fusion reaction, involves two hydrogen

isotopes (^{2}H and ^{3}H) fusing to produce helium (^{4}He) and a high-energy neutron. A magnetic field will sweep the hydrogen and helium atoms towards a component known as the divertor, which is responsible for extracting the hydrogen and helium plasma and the associated energy from the bottom of the reaction vessel. The divertor of ITER will be made of tungsten; understanding the effects that the hydrogen, helium, and energetic neutrons produced by the fusion reaction can have on its structure is critical to the effective use of ITER and future magnetic fusion reactors. This project investigates hydrogen transport near grain boundaries caused by collisions with nearby neutrons. By running molecular dynamics simulations, we observe the behavior of deuterium that is trapped on a grain boundary after it interacts with an energetic tungsten atom representative of a neutron-induced cascade. Simulations are run for energy values of 10, 20, and 30 keV imparted on the primary knock-on atom, which are representative of secondary neutron collisions (neutrons that have interacted with metal or hydrogen atoms deeper in the material, losing some of their kinetic energy). We find surprisingly little displacement of hydrogen from the grain boundary and similarly low levels of defect formation in the nearby regions, meaning that grain boundaries may reduce the amount of damage caused by neutrons near tungsten surfaces. We also find it unlikely that neutron damage, at least at these energies, will significantly alter hydrogen transport in polycrystalline tungsten.