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Resistivity of Frenkel Pair in BCC W from First Principles

Tungsten is a key material for both nuclear fusion and as a spallation target for neutron sources. In nuclear fusion, W is being considered for heat divertors thanks to its good thermal conductivity, resistance to irradiation damage, and high melting temperature. Furthermore, due to its high density and atomic mass, W is an excellent material as a target for neutron sources. In both settings, W is exposed to high amount of damage measured as displacement per atoms (DPA), which results in the creation of Frenkel pairs, voids, dislocations, and transmutation reactions. Tungsten will see irradiation damage of 10-35 DPA in its working lifetime. This amount of damage will negatively affect the properties of the material. In this work, we propose a method to calculate from First Principles using Density Functional Theory the changes in resistivity due to a Frenkel Pair. Specifically, a vacancy and a self-interstitial (crowdion in the [111]). The calculated resistivity from a vacancy is 8.07 μΩm, while the experimental value is 7 μΩm. For the Frenkel pair, the resistivity is 31.5 μΩm, while the experimental value is 27 μΩm. This method can be expanded in multiple ways. First, to consider the changes in resistivity due to presence of transmutation elements like rhenium, osmium, and tantalum under neutron irradiation in W. Second, with hexagonal closed-packed materials like titanium, which are being considered as containment and window material for the graphite target for the Long Baseline Neutrino Facility. Finally, this method can be further developed to calculate changes in electronic contribution to thermal conductivity. Knowing how the properties of the material change due to irradiation can help in maximizing its service life, finding ways of improving the properties of the material, and enables to test novel materials before manufacturing.

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