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Simulating irradiation hardening in tungsten under fast neutron irradiation including Re production by transmutation

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Abstract

Simulations of neutron damage under fusion energy conditions must capture the effects of transmutation, both in terms of accurate chemical inventory buildup as well as the physics of the interactions between transmutation elements and irradiation defect clusters. In this work, we integrate neutronics, primary damage calculations, molecular dynamics results, Re transmutation calculations, and stochastic cluster dynamics simulations to study neutron damage in single-crystal tungsten to mimic divertor materials. To gauge the accuracy and validity of the simulations, we first study the material response under experimental conditions at the JOYO fast reactor in Japan and the High Flux Isotope Reactor at Oak Ridge National Laboratory, for which measurements of cluster densities and hardening levels up to 2 dpa exist. We then provide calculations under expected DEMO fusion conditions. Several key mechanisms involving Re atoms and defect clusters are found to govern the accumulation of irradiation damage in each case. We use established correlations to translate damage accumulation into hardening increases and compare our results to the experimental measurements. We find hardening increases in excess of 5000 MPa in all cases, which casts doubts about the integrity of W-based materials under long-term fusion exposure.

Keywords: fusion materials, transmutation, neutron damage, defect clusters, tungsten, rhenium

1. Introduction

Tungsten is being considered as a candidate structural material in magnetic fusion energy devices due to its high strength and excellent high temperature properties [1–4]. Upon fast neutron irradiation in the 600-1000°C temperature range, W transmutes into Re via either neutron multiplication (n,2n) or neutron capture (n,γ) reactions, followed by β-decay, at rates that depend on the shape and magnitude of the neutron flux spectrum [5], which varies with position in the reactor. For the DEMO (*DEMOnstration fusion power plant*) reactor concept, calculations show that the transmutation rate is 2000 and 7000 atomic parts per million (appm) per displacement per atom (dpa) in the divertor and the equatorial plane of the first wall, respectively (in each case, damage accumulates at rates of 3.4 and 4.4 dpa/year) [6, 7]. The irradiated microstructure initially evolves by accumulating a high density of prismatic dislocation loops and vacancy clusters, approximately up to 0.15 dpa [8–11]. Subsequently, a void lattice emerges and fully develops at fluences of around 1 dpa. After a critical dose that ranges between 5 dpa for fast (>1 MeV) neutron irradiation [10] and 2.2 dpa in modified target rabbits in the HFIR [11, 12], W and W-Re alloys develop a high density of nanometric precipitates with acicular shape at Re concentrations well below the solubility limit [10, 11]. The structure of these precipitates is consistent with σ (W_7Re_6) and χ (WRe_3) intermetallic phases, which under equilibrium conditions only occur at temperatures and Re concentrations substantially higher than those found in neutron irradiation studies [13]. A principal signature of the formation of these intermetallic structures in body-centered cubic (bcc) W is the