Intricacies of helium effects on displacement cascades in tungsten

WAHYU SETYAWAN, GIRIDHAR NANDIPATI, HOWARD HEINISCH, KENNETH ROCHE, RICHARD KURTZ, Pacific Northwest Lab, BRIAN WIRTH, University of Tennessee — MD simulations were performed to study the effect of He on displacement cascades in W. The ability of He clusters to displace W atoms (kick-out mechanism) was studied with thermalization of interstitial He for 200 ps. The minimum cluster size to initiate kick-out decreases from 7 (1025 K) to 5 (2050 K). No kick-out was found at 300 K even at 4600 appm. Effects on damage were studied with 75 keV PKA for 55 ps with no initial He clustering. At 1025 K, data with 100% interstitial He shows the number of surviving SIAs remains unchanged: 81 (pure), 82 (2300 appm), while vacancy count drops to <50 at 2300 appm due to He filling the vacancies. Further study was done for 460 appm at several T. For 100% interstitial, the number of He-filled vacancies is 7 (300 K), 8 (1025 K) and 15 (2050 K) due to increased mobility. For 50% substitutional, the number of vacancies is minimum at 1025 K (65) compared to 87 (300 K) and 73 (2050 K) indicating there is an interplay between increased He mobility to find a vacancy vs decreased He+vacancy stability. The 100% substitutional data confirms the observation. The seemingly decreased stability of He+vacancy cluster may be due to increased mobility of SIAs and overtake vacancies from those clusters. More studies are planned to elucidate the competition.

Wahyu Setyawan
Pacific Northwest Lab