

Local chemical environment effects on the energetics of stacking faults and vacancy platelets in α -zirconium

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Zirconium alloys are subject to irradiation growth, a volume conservative deformation in the absence of stress, due to the inherent anisotropy of the α -zirconium hexagonal close-packed crystal structure. The resulting growth strains are small at low-to-moderate fluences, but accelerate once a threshold, or incubation, dose has been reached. This accelerated growth behavior has been termed “breakaway” irradiation growth and its onset is correlated with the nucleation and growth of faulted vacancy c -loops on basal planes. One theory for the stabilization of c -loops at high fluences is the reduction in their stacking fault energy by impurity or solute segregation. Here, we report the density functional theory calculations of the binding energies for iron, tin, niobium, chromium, and nickel to basal extrinsic, basal intrinsic, and prismatic stacking faults in α -zirconium. These *ab initio* binding energies have been correlated to segregation profiles that contribute to the modification of stacking fault energies. Our results demonstrate that iron and tin are both tightly bound to basal stacking faults with weakly attractive or repulsive binding to prismatic stacking faults. Thus, these elements are expected to preferentially segregate to faulted basal c -loops. As a result of the corresponding reduction in their formation energy, the vacancy-type basal c -loop becomes thermodynamically preferred to perfect prismatic a -loops. An impurity-assisted nucleation mechanism by iron and tin segregation can then be supported for the nucleation and growth of c -loops at high fluences. Based on our DFT calculations, niobium, chromium, and nickel do not have a significant effect on c -loop formation energies. Additionally, the binding energies of iron, tin, niobium, chromium, nickel, and hydrogen to a nineteen-vacancy platelet were calculated to confirm the extrapolation from the behaviour of the stacking fault interactions. The vacancy platelet introduces a high-energy contact of similar atomic rows in α -zirconium and may act as a nucleation barrier for faulted c -loop formation. Iron and chromium in particular show strong binding to the periphery of this structure and may reduce this nucleation barrier.

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