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A first-principles study of the avalanche pressure of alpha zirconium QING PENG, University of Michigan, WEI JI, JIE LIAN, Rensselaer Polytechnic Institute, FEI GAO, University of Michigan, SHUMING PENG, China Aademy of Engineering Physics, HANCHEN HUANG, Northeastern University, SUVRANU DE, Rensselaer Polytechnic Institute — We investigate the stability of a monovacancy in alpha zirconium under various strains and pressures by examining the vacancy formation energy through first-principles calculations. There is maximum formation energy of 2.35 eV under uniaxial strain corresponding to a c/a ratio of 1.75. Under volumetric strain, the formation energy increases as the strain increases. The formation energy as a function of the volumetric stress or pressure was also examined, with a minimum value of 2.00 eV at zero pressure. Using the equations of state method, we find that the formation volume of the vacancies decreases as the pressure increases, with a value of 0.6 unit-atom-volume at zero pressure. The formation enthalpy increases monotonically as the pressure increases. We predict that the avalanche pressure of alpha zirconium is -15 GPa, where vacancy formation is exothermic, causing avalanche swelling and the failure of the material.

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