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Effects of biaxial strain on diffusivity of low index tungsten surfaces ZHENGZHENG CHEN, NASR GHONIEM, Mechanical & Aerospace Engineering Department, University of California Los Angeles — Detailed knowledge of diffusion behaviors is necessary toward fully understanding of damage of tungsten serving as reactor pressure vessels. Using first-principles calculations, we observed different diffusion scenarios on W(001) and W(110) surfaces with external biaxial strains. Hopping is the major diffusion mechanism on the W(110) surface under all kinds of loadings in the present work. On the other hand, the main mechanism on the W(001) surface transfers between the adatom hopping and the formation and movement of surface crowdions depending on biaxial strains. Our results also indicate high mobile and strong anisotropy of surface crowdions on both surfaces. The microscopic explanation is presented by analyzing the charge density. We have built up the diagram of diffusion on the W(001) surface. This diagram presents that not only the diffusion mechanism, but also the diffusion direction can be modulated by patterns of biaxial strains. These results are important to the future dynamical modeling and simulations. We have further performed kinetic Monte Carlo simulations and observed (1) the modulation of diffusion of single adatom on W(001) surface by strains and (2) the aggregation of multiple adatoms on W(110) surface.

Zhengzheng Chen
Mechanical & Aerospace Engineering Department,
University of California Los Angeles

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