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Atomistic simulation for strain effects on threshold displacement energies in refractory metals

Mosab Jaser Banisalman, Takuji Oda*

Department of Nuclear Engineering, Seoul National University, 1 Gwanak-or, Gwanak-gu, Seoul 151-742, South Korea

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ABSTRACT

To evaluate the extent of radiation damage for specific materials, defect formation energies and threshold displacement energies (TDEs) are important quantities. In this work, we study the influence of hydrostatic and uniaxial strains on the Frenkel pair formation energy (FP_E) and TDE for tungsten, molybdenum, and vanadium, which can be used in plasma devices and fusion reactors. With an applied tensile strain, the self-interstitial atom formation energy decreases significantly, while the vacancy formation energy slightly increases, which causes concurrent decreases in the FP_E and TDE. The opposite responses are observed with an applied compression strain. This result indicates that radiation defect formation is enhanced by a tensile strain and suppressed by a compressive strain. The strain effects on the TDE and FP_E are determined mainly by the volume change in the deformed crystal, regardless of the strain mode. Both the TDE and FP_E under strain conditions are described by linear functions of the volume change.

1. Introduction

In the materials used in nuclear reactors, the collision of an incident energetic particle with constituent atoms causes defect formation due to atomic displacement. Adverse effects on material properties, such as irradiation-induced hardening, shift of the ductile to a brittle transition temperature, and degradation of the thermal conductivity are often caused by the formed defects. Therefore, to understand and control adverse radiation effects, it is important to predict the types and number of radiation defects formed during reactor operation.

Refractory metals such as tungsten (W), molybdenum (Mo), and vanadium (V) are promising candidate materials for the components of fusion reactors. For example, W and Mo are considered for use as plasma-facing components for diverters in plasma devices. V-based materials have significant advantages as structural materials due to the high melting temperature and lower levels of long-term activation of V.

During reactor operation, materials suffer many sources of strain, such as irradiation-induced swelling, alloying/solute precipitates, void swelling, and solute segregation. Void-metal interactions sometimes become extremely high [1], and deuterium precipitates exhibit strain fields of up to 5% in one direction due to local volume expansion [2]. In addition, the diverters of fusion reactors will be subjected to combined thermal and mechanical stresses. Such stresses affect the stable defect type and the density and distribution of the formed defects, which changes the lifetime of the materials. Indeed, previous molecular dynamics (MD) studies of the collision cascades have shown that stress changes the number of defects generated by collision cascades in alpha-iron [3–5] and copper [6].

In determining the primary state of radiation damage in materials, the threshold displacement energy (TDE) is regarded as one of the most fundamental quantities. TDE is defined as the minimum kinetic energy needed for an atom to be displaced into a defect position in a material. In other words, TDE is the minimum energy required to form a stable Frenkel pair (FP). It is used in theoretical models, such as the Norgett-Robinson-Torrens (NRT) model [7], to evaluate the number of generated defects. In experiments, the TDEs for specific directions, such as ⟨1 0 0⟩ and ⟨1 1 1⟩, were obtained in W [8], Mo [9] and V [10]. In MD simulations, not only the TDEs of specific displacement directions but also the average values were calculated in W [11–13], Mo [11] and V [14,15]. However, all of these data were obtained for stress-free conditions.

Therefore, in the present work, we study the strain effects on TDE for W, Mo and V to predict how radiation damage is changed by stress. Specifically, the influence of applied uniaxial and hydrostatic deformation on TDE is evaluated through MD simulations. In addition, the formation energies of point defects are evaluated with the applied stresses. A model for roughly estimating the stress effects on TDE is derived from the results of the MD simulations.

* Corresponding author.
E-mail addresses: mosab123@snu.ac.kr (M.J. Banisalman), oda@snu.ac.kr (T. Oda).

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