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Modelling radiation effects using the ab-initio based tungsten and vanadium potentials

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ABSTRACT

The Embedded Atom Model (EAM) Derlet–Nguyen–Manh–Dudarev tungsten and vanadium potentials were modified to correctly reproduce the experimentally obtained defect threshold energies. This was done by letting the interactions at short distances be dictated by the universal screened Coulomb potential. Both the repulsive part and the electron density function of the potentials were modified. The potentials were then used in collision cascade simulations and the resulting defects were compared with the corresponding defects in iron. Based on this comparison, factors affecting the outcome of a cascade were identified.

1. Introduction

Structural materials in a fusion power plant will be subjected to neutron irradiation, which affects the lifetime of components because of radiation damage that neutrons generate in the materials. Understanding, assessing and, desirably, predicting the type of the damage is one of the significant directions of fusion materials research, and molecular dynamic (MD) simulations is one of the effective and powerful tools capable of addressing the problem. Simulations of irradiation phenomena in tungsten and vanadium is of particular interest. This is because, owing to its low tritium retention and low sputtering yield [1], W has been chosen as divertor material in the fusion reactor ITER [2], and V alloys are among promising candidate materials for the first-wall and blanket applications, due to their excellent thermal and activation properties [3].

Interatomic potentials provide crucially important input to MD simulations, and correct description of not only equilibrium but also of defect properties are required before a potential can be used to model more complex collective events and processes. The short-range part of a potential is of particular significance when dealing with high-energy interactions. In this work we have modified the repulsive part of two recently parametrized potentials for V and W [4]. The potentials reproduce the correct point defect structures and, after suitable modification, they also describe well the observed experimental threshold energies.

We also performed simulations of recoil cascades in V and W. The resulting primary damage was compared to that in Fe where a similar potential and same simulation and analyzing methods were used [5,6]. This gives insight into the effect of the geometric structure of radiation defects, since V and Fe are similar in atomic mass and threshold energies, but differ when it comes to the structure of the most stable interstitial configuration. In V the ⟨111⟩ crowdion is the ground structure [4,7], while the ⟨110⟩ dumbbell is the most stable in body-centred cubic Fe [5,6,8]. The ground state interstitial in W is also the ⟨111⟩ crowdion, and in addition W differs strongly from V and Fe in terms of the atomic mass, threshold energies and defect formation energies.

In addition to the identification of similarities and differences between radiation damage created in the three bcc metals noted above, we note a significant pragmatic aspect of systematic MD investigation of radiation damage in these three materials. Predicting microstructural changes in materials under neutron irradiation

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requires relating the incident flux of neutrons bombarding the material with the concentration of radiation defects produced by neutron impacts. In engineering applications semi-empirical rules are often used, for example, the Norgett–Robinson–Torrens (NRT) model [9] where the number of defects generated by fast neutrons is assumed to be proportional to the energy of neutrons initiating collision cascades, and inversely proportional to the threshold Frenkel pair formation energy. Finding the pre-factor in the NRT equation determining the rates of formation of Frenkel pairs in materials under irradiation requires carrying out atomistic simulations similar to those described below.

2. Method

2.1. Modification of the repulsive part

A merging interpolation function $V_{int}(r)$ was used to spline the universal potential of Ziegler, Biersack and Littmark $V_{ZBL}(r)$ [10] with the original W and V pair potentials $V^{W,V}_{orig}(r)$. This approach was also used for Fe in [6] and for W, although with a different interpolation function, in Ref. [11]. The modified repulsive potentials thus take the form

$$V^{W,V}_{BN}(r) = V^{W,V}_{ZBL}(r), \quad r \leqslant r^{W,V}_1 = V^{W,V}_{int}(r), \quad r^{W,V}_1 < r < r^{W,V}_2 \\ = V^{W,V}_{orig}(r), \quad r \geqslant r^{W,V}_2, \tag{1}$$

where r_1 and r_2 are the cutoffs for the interpolation functions. These cutoffs were fitted in order to get the threshold energies correct without affecting the interstitial energies. The interpolation function is a fifth order polynomial,

$$V_{int}(r) = a_0 + a_1 r + a_2 r^2 + a_3 r^3 + a_4 r^4 + a_5 r^5, \tag{2}$$

which was constructed to give a continuous potential and first and second derivatives at r_1 and r_2.

2.2. Modification of the electron density function

The electron density function $f(r)$ in both potentials was also modified. This was done to better correctly reproduce the contribution of the attractive electron d-states. The electron density in the EAM formalism is of the expression

$$\rho_i = \Sigma_{j,j\neq i} f(r_{ij}) \tag{3}$$

and it contributes to the embedding energy through $F(\rho) = -A\sqrt{\rho}$, where A is a fitted constant found in Ref. [4]. The modified density function $f^{W,V}_{BN}(r)$ looks like

$$f^{W,V}_{BN}(r) = \rho^{W,V}_0, \quad r \leqslant r^{W,V}_3 = \rho^{W,V}_{int}(r), \\ r^{W,V}_3 < r < r^{W,V}_4 = \rho^{W,V}_{orig}(r), \quad r \geqslant r^{W,V}_4. \tag{4}$$

ρ_{orig} is Eq. (2) in Ref. [4] and ρ_{int} (r) is a third order polynomial

$$\rho_{int}(r) = b_0 + b_1 r + b_2 r^2 + b_3 r^3, \tag{5}$$

which was constructed assuming that the bonding part of the potential approaches a constant value for interatomic distances smaller than r_3, and that it smoothly joins the original density function at r_4. The cutoff radii r_3 and r_4 for the interpolation procedure were determined by requiring that the bonding part of the potential does not diverge in the limit of small separation between atoms, and instead it saturates in this limit. The characteristic interatomic distance at which this saturation occurs is related to the spatial extent of overlapping d-orbitals (the 3d orbitals in the case of V atoms and 5d orbitals in the case of W atoms), which provide the dominant contribution to the cohesive energy in these transition metals. Figs. 2 and 3 show normalized radial distributions of electron density in the atomic orbitals of V or W atoms, calculated by solving the relativistic Dirac equation in the local spin density approximation. These distributions were used for assessing the values of the cutoff radii r_3 and r_4.

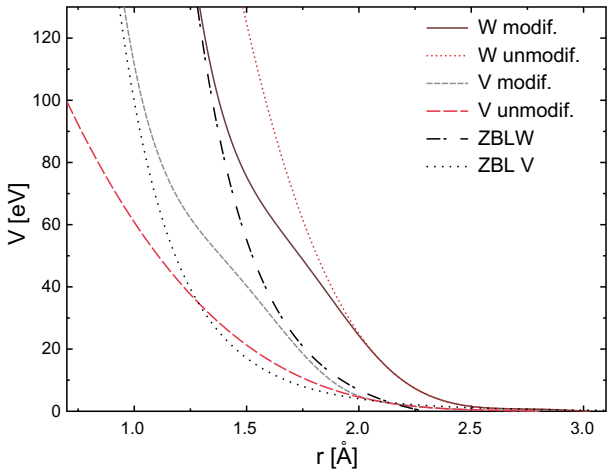

Fig. 1. The original and modified repulsive potentials for vanadium and tungsten. The universal ZBL potentials are also included.

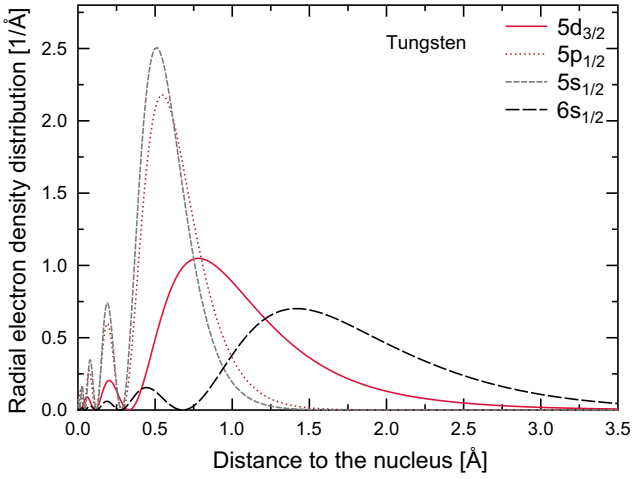

Fig. 2. The radial electron density distribution of tungsten.

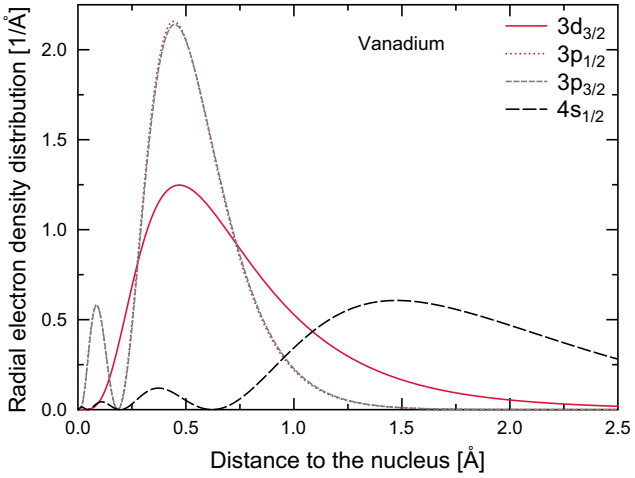

Fig. 3. The radial electron density distribution of vanadium.