

MOLECULAR DYNAMICS STUDY OF THE THRESHOLD DISPLACEMENT ENERGY IN VANADIUM--

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ABSTRACT

One of the most important physical parameters for describing radiation damage is the threshold displacement energy (TDE). The TDE is the minimum kinetic energy transferred to an atom in the lattice from an impinging particle necessary to permanently displace an atom from its lattice site, thus generating stable defect, such as a Frenkel pair. In the case of high kinetic energy particle impingement (such as 14 MeV neutrons in a fusion reactor environment), the initial cascade gives rise to a series of subcascades which stop when the highest energy particle has kinetic energy smaller than the TDE. Hence, threshold displacement energies are critical parameters for both low and high energy irradiation conditions. The TDE provides a lower limit on particle kinetic energies that must be considered in molecular dynamics (MD) simulations of radiation damage and, hence, is a key parameter for enabling MD simulations of displacement cascades.

Threshold displacement energies in V were calculated as a function of temperature ($100 < T < 900$ K) and orientation of the incident particle momentum by molecular dynamics simulation using a new parameterization of an embedded atom method/Finnis-Sinclair-type potential for V. A primary knock-on atom (PKA) was chosen near the center of the simulation cell and assigned a velocity along a particular direction, consistent with a chosen knock-on energy. The trajectories of all of the atoms in the system were traced for 10 ps following the knock-on event. The TDE was defined as the minimum kinetic energy transferred by the PKA to a lattice atom that resulted in the formation of a stable Frenkel pair.

It was found that the minimum TDE in V is approximately 13 eV. This corresponds to a displacement along the $\langle 100 \rangle$ -direction. The maximum TDE observed in the simulations was 51 eV, in a direction close to $\langle 101 \rangle$. Since the simulations did not span all possible angles, it is likely that the true maximum TDE is even larger, especially when allowing for longer time recombination processes. A comparison of the TDE for V with experimental values for other body centered cubic metals (Fe and Mo) showed that the directional anisotropy is comparable in Mo but the TDE ordering in $\langle 110 \rangle$ and $\langle 111 \rangle$ orientations is different in Fe. In addition, it was found that the TDE in V is almost independent of temperature since the magnitude of the TDE is very much greater than thermal energies, even at temperatures approaching the melting point.

REFERENCE

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