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A MOLECULAR DYNAMICS SIMULATION STUDY OF DEFECT PRODUCTION IN VANADIUM

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ABSTRACT

We performed molecular dynamics simulations to investigate the process of defect production in pure vanadium. The interaction of atoms was described by the EAM interatomic potential modified at short range to merge smoothly with the universal potential for description of the high energy recoils in cascades. The melting point of this EAM model of vanadium was found to be consistent with the experimental melting temperature. The threshold energies of displacement events in the model system are also consistent with experimental minimum threshold in vanadium, and its average was found to be 44 eV. We evaluated the efficiencies of defect production in the displacement events initiated by recoils with kinetic energy up to 5 keV, and found that the probability of cluster formation is smaller than that of simulated events in fcc metals reported in the literature.

INTRODUCTION

Microstructural evolution during irradiation is a complicated, non-linear function of the initial defect production. The changes in mechanical properties due to irradiation are commonly supposed to result from irradiation-induced microstructural changes, such as the formation of point defects, dislocation loops, voids, surface craters and solute segregation. It is, therefore, critical that a clear understanding of these radiation damage processes be achieved, not only for prediction of a given material's response to irradiation but also for development of new, advanced materials. A physical description of the radiation damage process involves varying time- and length-scales from ballistic binary collisions to collective atomic motion in the thermal spike stage followed by the thermal activation process. The time scale of the radiation effects relevant to the field of nuclear materials ranges widely from 10^{-15} to 10^7 seconds, and the length scale ranges, also widely, from 10^{-9} to 10^{-3} meters.

The displacement cascade [1] is of fundamental importance to microstructural changes since it plays a role as a production source of defects in irradiated materials. Moreover, debris of point- and clustered-defects produced by the cascade has recently been a subject of increased interest since it has been suggested that this debris induces a diffusion bias [2] which acts during subsequent microstructural evolution. Molecular dynamics (MD) simulations can be used to study the space and time development of the cascade process [3-8]. With our MDCASK code [9], we can study systems with up to 10^6 atoms on massively parallel computers.

Vanadium-based alloys have significant advantages for use as structural materials in nuclear fusion devices because of their low activation and high radiation resistance. In the present study, in order to provide a first step towards the comprehensive model simulation of radiation effects in these alloys, we investigate cascade dynamics in pure vanadium at the atomic level by MD simulations with a many-body interatomic potential. First, we evaluated the displacement threshold energies and melting temperature of the model potential system. Second, we simulate the cascade process in vanadium for primary recoils with energy up to 5 keV. We discuss the production efficiencies of point- and clustered-defects produced by cascades in vanadium.

Table 1 Comparison of EAM-type many body potentials for vanadium. The activation energies of vacancy formation, E_v^f , vacancy migration, E_v^m and self diffusion, Q_v , and the fcc-bcc energy difference are listed in unit of electron volts.

	E_v^f	E_v^m	Q_v	$E_{fcc} - E_{bcc}$	Ref.
Adams & Foiles	2.22	0.98	3.20	0.035	[10]
Johnson & Oh	2.02	0.71	2.73	0.19	[11]
Finnis & Sinclair	1.83	0.72	2.55	0.14	[12]
		0.76	2.58		[13]
Ouyang & Zhang				0.046	[14]
Wang & Boercker	1.58			0.17	[15]
experiment	2.1	0.5	2.9		[16]
ab-initio LMTO				0.30	[17]

MOLECULAR DYNAMICS MODEL

All the simulations in the present study were performed with the molecular dynamics code, MDCASK [9] which runs efficiently on the Cray-2 supercomputer and T3D massively parallel computer at Lawrence Livermore National Laboratory. In order to evaluate existing interatomic potentials for vanadium, we compared the defect properties and fcc-bcc energy difference of several published potentials [10-15] to the experimental data [16] and ab-initio LMTO calculation results [17], respectively, as shown in Table 1. Based on the results, we use the Johnson and Oh EAM-potential [11] for our simulations. Since this EAM potential was, however, developed by fitting to just near equilibrium behavior of vanadium, we modified the high energy part of the potential for description of high energy recoils in cascades. The potential was splined to the universal potential of Biersack and Ziegler (ZBL) [18] by a similar scheme to that of Proennecke et al [19].

RESULTS AND DISCUSSION

VALIDATION OF INTERATOMIC POTENTIAL

To validate our model potential (EAM-ZBL potential) for cascade dynamics simulation, the displacement threshold energies and melting temperature were investigated. First, we evaluated displacement threshold energies for the various directions of recoil atom. The initial lattice temperature was 0K. The threshold energies of our model potential are shown in Fig. 1. The threshold energy for displacing an atom is highly dependent on the direction of recoil atoms, as many previous theoretical and experimental studies have shown [20-22]. The stable configuration of the produced interstitial is found to be the split configuration whose axis lies along $\langle 110 \rangle$, which is generally the most stable configuration of interstitials in bcc metals. Our result shows a minimum threshold of ~ 25 eV, which is consistent with the experimental minimum threshold [23]. An average value over all directions is found to be 44 eV, in excellent agreement with the suggested ASTM standard [24].

Second, we evaluated the melting temperature of our model potential system. An MD crystal containing a stacking fault in the center was annealed at several temperatures ranging from 2100 to 2400 K during several psec. No melting was observed at 2100 K. However, melting was observed to nucleate at the defect layer during 4 psec simulation at more than 2200 K. To estimate crystalline order upon melting quantitatively, we investigated the squared magnitude of the planar

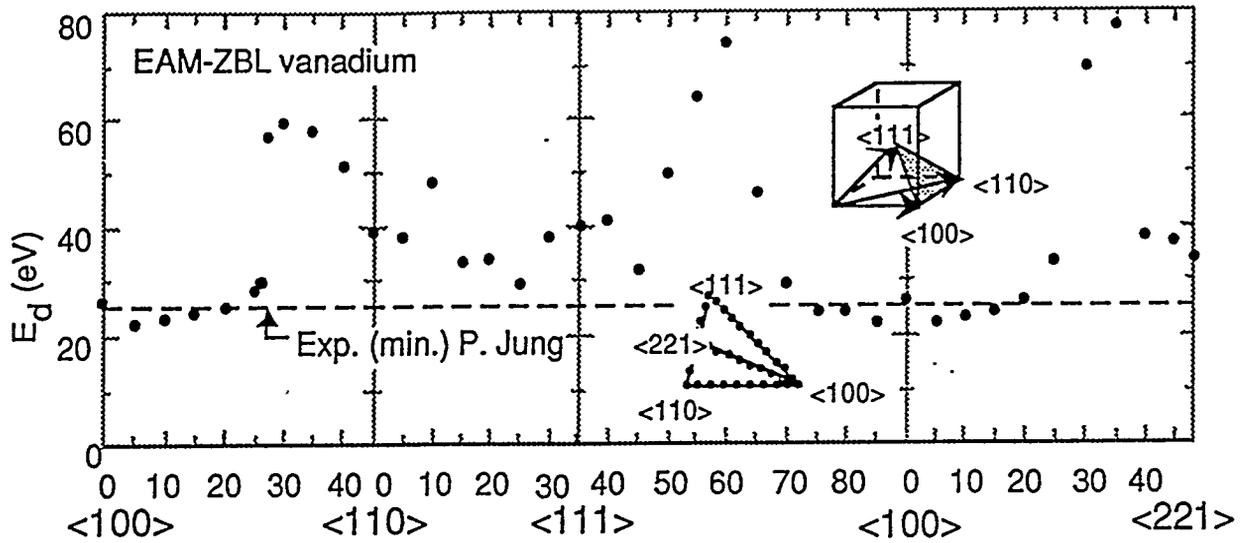


Fig. 1 Displacement threshold energies for point defect production in vanadium. Final configuration of displaced atoms is observed to be $\langle 110 \rangle$ split, the most stable configuration of an interstitial in bcc metals.

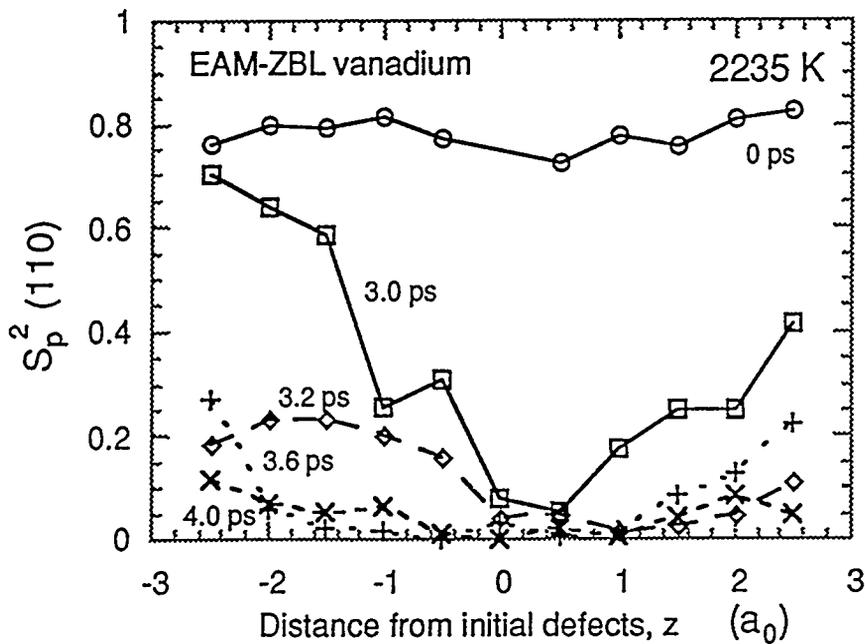


Fig. 2 Propagation of defect-nucleated melting in vanadium at 2235 K. Initial defects are located at $z=0$ at the beginning. The melting is characterized by planar structure factor of $k=(110)$.

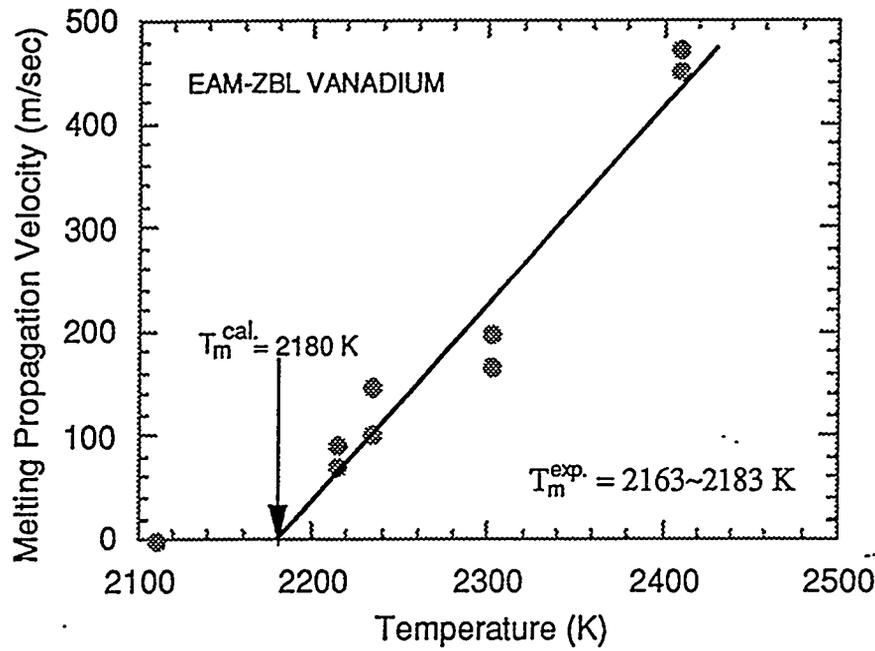


Fig. 3 The propagation velocity of defect nucleated melting as a function of lattice temperature. The calculated melting temperature, 2180 K, is consistent with experimental value.

structure factor, $S_p^2(k)$, as defined by

$$S_p^2(k) = \left[\frac{1}{N} \sum_{i=1}^N \cos(k \cdot q_i) \right]^2 + \left[\frac{1}{N} \sum_{i=1}^N \sin(k \cdot q_i) \right]^2, \quad (1)$$

where k is a reciprocal lattice vector and q_i is the position vector of i -th atom in a given plane. For an ideal crystal lattice at zero temperature, $S_p^2(k)$ equals unity for any wave vector k , and in the liquid state it fluctuates near zero. Fig. 2 shows the values of the planar structure factor for (001) planes in the MD crystal heated at 2235 K. As shown in the figure, atomic disordering due to melting is observed to take place from the central (001) plane, $z=0.0$ where the defects were initially introduced. The propagation velocity of the melting front depends on the lattice temperature, and goes to zero at the melting point. Fig. 3 shows the melt propagation velocity as a function of temperature. An extrapolation to zero velocity yields a melting temperature of 2180 K, which is in agreement with experimental melting point (2163-2183 K) [25].

DEFECT PRODUCTION

MD simulations of displacement cascade in vanadium were performed using the EAM-ZBL potential at initial lattice temperature of 10 K. In the present study, primary recoil atoms with kinetic energy up to 5 keV were simulated. The initial directions of motion of recoils were chosen randomly. We present results for 2 events at each energy.

The average number of Frenkel pairs produced per cascade is 5.5, 11 and 27 for 1, 2 and 5 keV events, respectively. They correspond to a defect production efficiency of 55, 55 and 54 % of the prediction of binary collision models [26] where defect production is described as $N_{NRT} = 0.8 E_p / 2 \bar{E}_d$. Here, \bar{E}_d is the effective average threshold energy for Frenkel pair production. The value of \bar{E}_d employed in the present study is 40 eV which is suggested in the

ASTM standard [24]. The defect production efficiencies obtained here for bcc vanadium are somewhat higher than those of other fcc metals in this energy range. Although these results are for limited statistics, the trend is in agreement with the previous work of Bacon et al. [6-8], which shows that the efficiency of bcc iron is higher than those of other close-packed metals. Furthermore, the defect clustering efficiencies obtained here for vanadium are similar to those of bcc iron [6,7], as shown in Fig. 4; a higher fraction of produced defects is single- and di-defects and smaller fraction is taken up in clusters for bcc vanadium than those in other fcc metals [3-6]. This suggests that direct cluster formation in cascades is greatly influenced by lattice type, and seems to be consistent with experimental observation of lower probability of cascade collapse in bcc metals than that in fcc [27].

SUMMARY

We modified the EAM interatomic potential for vanadium of Johnson and Oh to describe high energy part of atom interaction by connecting it with the universal ZBL-potential, and investigated the displacement threshold energies and melting temperature of the system. We further used this potential to investigate defect production during irradiation in vanadium. Our cascade simulation results show a higher production efficiency of defects and lower defect clustering in bcc vanadium compared to other fcc metals. This is similar to results in bcc iron, suggesting that defect production in cascades, including clustering features, are strongly dependent on lattice type.

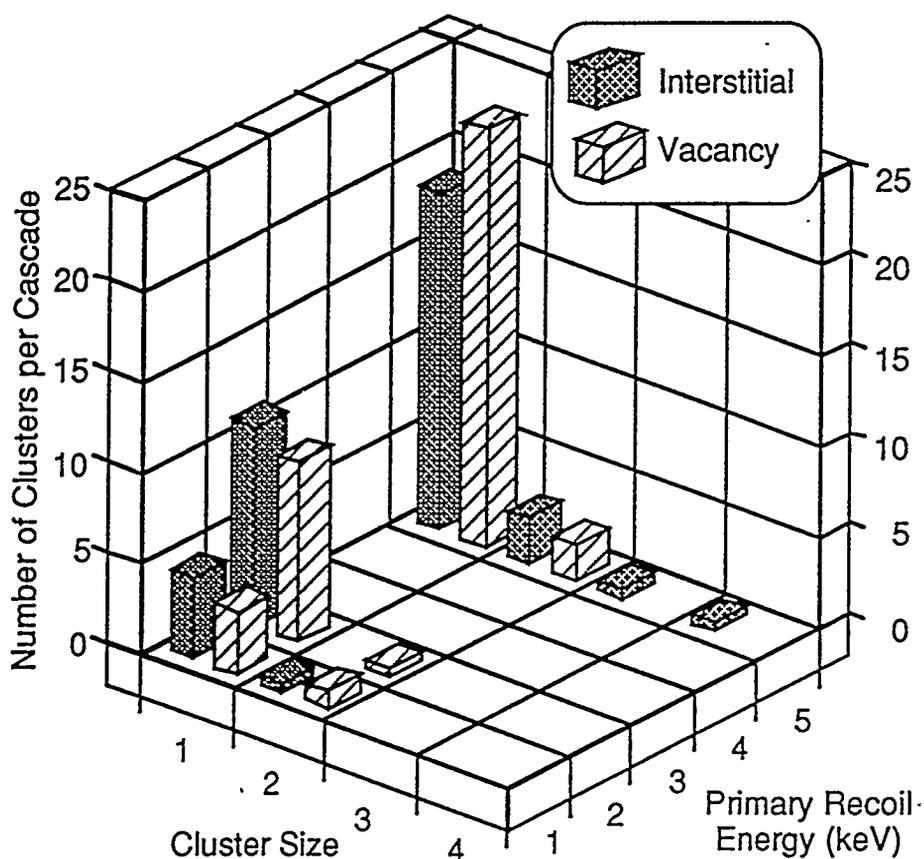


Fig. 4 Size distribution of cascade defects in vanadium at 10 K as a function of recoil energy.

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