

**ON THE CHARACTER OF SELF-INTERSTITIAL LOOPS IN VANADIUM**--L. A. Zepeda-Ruiz (Lawrence Livermore National Laboratory), J. Marian (Lawrence Livermore National Laboratory), B. D. Wirth (University of California Berkeley), and D. J. Srolovitz (Princeton University)

## ABSTRACT

Isolated self-interstitial atoms (SIA) and SIA clusters produced during collision cascades are key components of the microstructure observed when metals are irradiated with high-energy particles. The evolution of these defects may cause undesirable changes in the mechanical properties of the material under irradiation. Therefore, knowledge of the properties, formation and diffusion mechanisms of SIA is essential for understanding and predicting the effects of radiation damage.

In this study, we used molecular statics and molecular dynamics (MD) simulations based on a new Finnis-Sinclair potential, fit to first-principles calculations of point defect properties, to investigate the energy and structure of SIA dislocation loops in vanadium. We found that SIA dislocation loops with  $a/2\langle 111 \rangle$  Burger's vector were the lowest energy configuration in vanadium, and migrated rapidly along their  $\langle 111 \rangle$ -glide cylinder. Initial dislocation loop configurations with Burger's vector of  $a/2\langle 110 \rangle$  or  $a\langle 100 \rangle$  rotated into  $a/2\langle 111 \rangle$  orientations at very low temperatures during the computational relaxation scheme used in this work and indicate that the formation energy of  $a/2\langle 110 \rangle$  and  $a\langle 100 \rangle$  loops is much higher than  $a/2\langle 111 \rangle$  loops. Our results were compared to experimental observations and recent results in ferritic alloys which detail the formation mechanism responsible for the nucleation and growth mechanism of  $a\langle 100 \rangle$  dislocation loops. Unlike in Fe, where a metastable  $a\langle 100 \rangle$  loop is very close in energy to the ground-state  $a/2\langle 111 \rangle$  orientation, constrained  $a\langle 100 \rangle$  loops in V have considerably higher formation energies than  $a/2\langle 111 \rangle$  loops, and the energy difference increases with size.

Finally, our MD simulations of the interaction between two mobile  $a/2\langle 111 \rangle$  clusters, according to the reaction proposed for  $a\langle 100 \rangle$ -loop formation in Fe, revealed the formation of a single resulting  $a/2\langle 111 \rangle$  loop. The simulations indicated that while a junction reaction occurs (a  $\langle 100 \rangle$ -junction does form), the junction has a low thermal stability and rotates into a  $a/2\langle 111 \rangle$  orientation at temperatures of 600-800K. The simulations performed to date provide no indication that the smaller  $a\langle 100 \rangle$  junctions will propagate across the loop, but instead will dissolve with low thermal stability.

## Reference

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