

Structure, Energy and Mobility of Self-Interstitial Dislocation Loops in Vanadium



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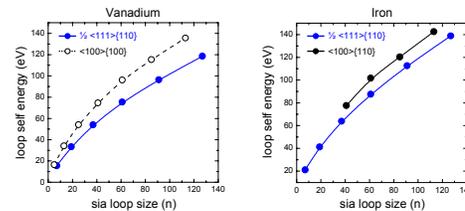
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Introduction

- In Fe, dislocation loops with Burger's vector $\langle 100 \rangle$, along with a population of $\frac{1}{2}\langle 111 \rangle$, form during irradiation
- In V, dislocation loops are observed with Burger's vector of both $\frac{1}{2}\langle 110 \rangle$ and $\frac{1}{2}\langle 111 \rangle$, but not $\langle 100 \rangle$
- Recently, a model has been proposed to explain the formation of $\langle 100 \rangle$ loops in Fe based on the interaction of mobile $\frac{1}{2}\langle 111 \rangle$ loops*
- In this work, we apply MD simulations to discover the properties of self-interstitial dislocation loops in V and explain the different observed behavior between Fe and V

*J. Marian, B.D. Wirth, and J. M. Perlado, *Phys. Rev. Lett.* **88**, 255507 (2002).

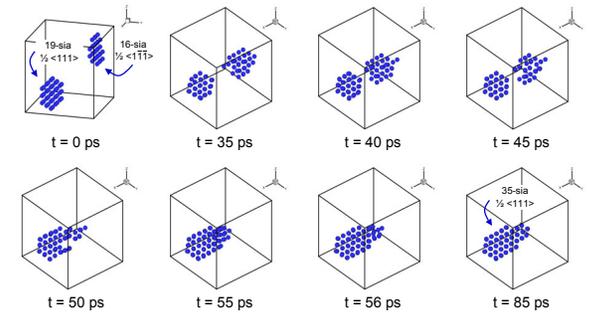
Dislocation Loops Formation Energies



- In both V and Fe, the stable loop morphology is $\langle 111 \rangle$
- However in Fe, unlike V, a metastable $\langle 100 \rangle$ is very close in energy*
- $\langle 111 \rangle$ clusters in both Fe and V rapidly migrate along their $\langle 111 \rangle$ glide cylinder

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MD Simulation of Loop Intersection in V



Simulation Method

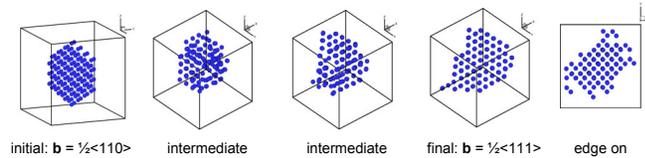
- Molecular Statics and Molecular Dynamics simulations to:
 - Study the mobility and thermal stability of dislocation loops in V with a variety of sizes and shapes
 - Understand the different observed dislocation loop morphology in Fe and V
- MD simulations:
 - Parallel version of MDCASK
 - Computational cell: $40a_0 \times 40a_0 \times 40a_0$ (128,000 + sia atoms)
- Requires a reliable interatomic potential – use a new Finnis-Sinclair potential for V parameterized by *ab-initio* calculations

Dislocation Loop Evolution

- Comprehensive MD-MS relaxation scheme reveal that the final loop configuration is highly kinked, with $\frac{1}{2}\langle 111 \rangle$ Burger's vector, irrespective of initial condition*

*L.A. Zepeda-Ruiz, J. Marian, and B.D. Wirth, *Phil. Mag.*, in press.

Dislocation Loop Evolution: $\frac{1}{2}\langle 110 \rangle \rightarrow \frac{1}{2}\langle 111 \rangle$



Energetics of Point Defects in Vanadium

- Existing EAM type potentials give very different predictions for Vanadium
- None of the EAM potentials correctly predict the stable form of the defect

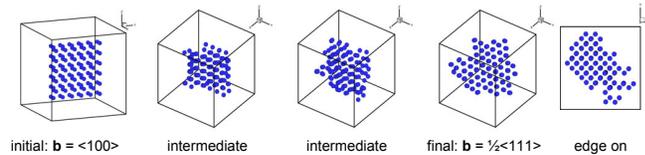
	vacancy	$\langle 100 \rangle$ split	$\langle 110 \rangle$ split	$\langle 111 \rangle$ split	$\langle 111 \rangle$ crowdion
First Principles	2.60	3.57	3.48	3.14	3.15
Finnis-Sinclair	2.63	3.60	3.66	3.27	3.27

units: eV

- Present work* is in excellent agreement with first principles calculations

* S. Han, L. A. Zepeda-Ruiz, G. J. Ackland, R. Car, and D. J. Srolovitz, *Phys. Rev. B* **66**, 220101 (2003); *J. Appl. Phys.* **93**, 3328 (2003).

Dislocation Loop Evolution: $\langle 100 \rangle \rightarrow \frac{1}{2}\langle 111 \rangle$



Conclusions

- We have used an improved Finnis-Sinclair potential for Vanadium, fit to an *ab-initio* database of point defect properties, to investigate the characteristics of self-interstitial clusters
- Self-interstitial clusters (dislocation loops) with $\frac{1}{2}\langle 111 \rangle$ Burger's vector are the lowest energy configuration in Vanadium, and migrate rapidly along their $\langle 111 \rangle$ glide cylinder
- Initial cluster configurations with Burger's vector of $\frac{1}{2}\langle 110 \rangle$ or $\langle 100 \rangle$ rotated into $\frac{1}{2}\langle 111 \rangle$ orientations at very low Temperatures during the computational relaxation scheme and indicate that the formation energy of $\frac{1}{2}\langle 110 \rangle$ and $\langle 100 \rangle$ loops is much higher than $\frac{1}{2}\langle 111 \rangle$ loops
- Unlike Iron, a metastable (e.g. nearly equivalent formation energy) $\langle 100 \rangle$ loop configuration does not exist
- MD simulations of the interaction between two mobile $\frac{1}{2}\langle 111 \rangle$ clusters, according to the reaction proposed for $\langle 100 \rangle$ loop formation in Fe*, reveal the formation of a single resulting $\frac{1}{2}\langle 111 \rangle$ loop. The simulations suggest that while the reaction occurs (a $\langle 100 \rangle$ -junction does form), the junction has a very low thermal stability and rotates into a $\langle 111 \rangle$ orientation at Temperatures of 400-700K

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