

Analyzing the effect of pressure on the properties of point defects in γ UMo through atomistic simulations

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Abstract

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1. Introduction

2 Background on UMo fuel

Pressure state on UMo

4 Atomistic Calculations on UMo summary

What we will do

6 2. Computational Details

Molecular dynamics simulations are performed utilizing the LAMMPS [1] software package
8 and the U-Mo angular dependent potential (ADP) [2].

10 Relaxation is performed in an NPT-ensemble, relaxing each x, y, and z component individually, with a damping parameter of 0.1. A Nose-Hoover thermostat is utilized with the damping parameter set to 0.1 ps. Systems are investigated over a range of temperatures,

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12 from 600 K up to 1200 K. This temperature range was chosen due to the inherent prop-
erties of the potential, in that below 600 K γ U becomes mechanically unstable and above
14 1200 K the crystal structure is approaching the melting point.

Systems are relaxed for 100 ps, with energies averaged over the final 50 ps.

16 **3. Results**

Completed pressure-dependent defect formation energy calculations in UMo as a function
18 of composition and temperature. Results at 1200 K are below, and show that the pressure
does not dramatically affect trends in formation energy vs composition. The interstitial
20 formation energy is more sensitive to pressure with $\geq 50\%$ Mo, and the vacancy forma-
tion energy is more sensitive to pressure with $\leq 50\%$ Mo. The compositionally averaged
22 behaviors show that 1 GPa of pressure leads to approximately a 10% increase/decrease
in formation energy for interstitials and 1 GPa of pressure leads to approximately a 2%
24 increase/decrease in formation energy for vacancies. The results are almost identical at
800 K, but less pressure-sensitive. Data is being pursued at 600 K for formation energies.
26 Finally, diffusion coefficients for interstitials and vacancies as a function of pressure are
being determined

28 **4. Conclusions**

References

- 30 [1] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, J. Comp.
Phys. 117 (1995) 1–19.
- 32 [2] D. Smirnova, A. Kuksin, S. Starikov, V. Stegailov, Atomistic modeling of the self-
diffusion in gamma u and gamma u-mo, Phys. Met. and Metall. 116 (2015) 445.