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

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**Abstract** this is the abstract

# Introduction

Background on UMo fuel

Pressure state on UMo

Atomistic Calculations on UMo summary

What we will do

# Computational Details

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

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

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

# Results

Completed pressure-dependent defect formation energy calculations in UMo as a function of composition and temperature. Results at 1200 K are below, and show that the ressure does not dramatically affect trends in formation energy vs composition. The interstitial formation energy is more sensitive to pressure with ¿50% Mo, and the vacancy formation energy is more sensitive to pressure with ¡ 50% Mo. The compositionally averaged 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% 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. Finally, diffusion coefficients for interstitials and vacancies as a function of pressure are being determined

**4. Conclusions**

# References

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

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