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

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Abstract

this is the abstract

1. Introduction

Background on UMo fuel

Pressure state on UMo

Atomistic Calculations on UMo summary

What we will do

2. 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 γU 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.

3. 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 self-diffusion in gamma u and gamma u-mo, Phys. Met. and Metall. 116 (2015) 445.