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ATOMISTIC MODELING OF HIGH TEMPERATURE URANIUM-ZIRCONIUM ALLOY STRUCTURE AND THERMODYNAMICS

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Abstract

A semi-empirical Modified Embedded Atom Method (MEAM) potential is developed for application to the high temperature body-centered-cubic uranium-zirconium alloy (γ-U-Zr) phase and employed with molecular dynamics (MD) simulations to investigate the high temperature thermo-physical properties of U-Zr alloys. Uranium-rich U-Zr alloys (e.g. U-10Zr) have been tested and qualified for use as metallic nuclear fuel in U.S. fast reactors such as the Integral Fast Reactor and the Experimental Breeder Reactors, and are a common sub-system of ternary metallic alloys like U-Pu-Zr and U-Zr-Nb. The potential was constructed to ensure that basic properties (e.g., elastic constants, bulk modulus, and formation energies) were in agreement with first principles calculations and experimental results. After which, slight adjustments were made to the potential to fit the known thermal properties and thermodynamics of the system. The potentials successfully reproduce the experimental melting point, enthalpy of fusion, volume change upon melting, thermal expansion, and the heat capacity of pure U and Zr. Simulations of the U-Zr system are found to be in good agreement with experimental thermal expansion values, Vegard's law for the lattice constants, and the experimental enthalpy of mixing. This is the first simulation to reproduce the experimental thermodynamics of the high temperature γ-U-Zr metallic alloy system. The MEAM potential is then used to explore thermodynamics properties of the high temperature U-Zr system including the constant volume heat capacity, isothermal compressibility, adiabatic index, and the Grüneisen parameters.

1. Introduction

In this work, an interatomic potential for uranium zirconium alloys is developed. Since the Clementine reactor in 1949, the first nuclear fast reactor, metallic alloy fuels have been of interest to the nuclear community, and a number of experimental fast reactors have employed nuclear metallic fuel, including the Experimental Breeder Reactor (EBR) series, Los Alamos Molten Plutonium Reactor Experiment (LAMPRE) series, Dounreay Fast Reactor (DFR) and the Fermi reactors [1]. Metallic alloys have advantages over the conventional ceramic nuclear fuels in the areas of thermal conductivity, burnup, ease of fabrication, favorable plutonium (Pu) breeding efficiency, fuel-recycling and other thermo-physical and neutronic properties [2, 3]. However, metallic fuels undergo various physical phenomena whose fundamental processes are