# Atomistic Modeling of the Effect of He on Vacancy Clustering Energetics in Ni

E.K. Stirrup[1] and B.D. Wirth[1]

[1]The University of Tennessee, Knoxville, TN, USA

The behavior of structural materials in nuclear environments is ultimately controlled by defect physics. In nickel-based alloys, helium will be produced at varying rates depending on the energy-dependence of the neutron flux. In this work, we report on the results of atomistic and molecular statics simulations to investigate the role of nickel in modifying the structures and energetics of vacancy-type defect clusters. These simulations use the EAM potential calculated by Mendelev et al. in 2012 for Ni-Ni type interatomic interactions, a simple ZBL potential for He-Ni interactions, and the potential calculated by Beck in 1968 for He-He type interactions. Alternative simulations using a variety of potentials for Ni-He interactions are used to demonstrate the effect of varying interatomic potentials on the interactions between the nickel matrix, helium interstitials, and defect structures. In particular, these simulations evaluate the relative stability of vacancy-Frank loop, stacking fault tetrahedron, and cavities as a function of the quantity of nearby helium. These simulation results provide important insight on the role of helium in mediating defect cluster evolution and high energy particle irradiated nickel-based alloys, needed to both interpret both experimental results and inform multi-scale simulations.