Ab initio modeling of radiation effects in NiFeMnCr high entropy alloy

Congyi Li[1], Khorgolkhuu Odbadrakh[2], Sai Mu[3], Phil Sterne[4], Brian Wirth[1]

[1]*University of Tennessee, Knoxville, TN 37996*
[2]*Oak Ridge National Laboratory, TN 38831*
[3]*University of California, Santa Barbara, CA 93106*
[4]*Lawrence Livermore National Laboratory, CA 94550*

High entropy alloys (HEAs) are potential candidates for high-temperature fission structural applications due to their attractive mechanical properties. Recently, a novel, near-equimolar 28%Ni-27%Fe-27%Mn-18%Cr (in wt%) high entropy alloy has been synthesized and exhibited improved resistance to void swelling and elemental segregation than austenitic stainless steel at similar ion irradiation conditions. Preliminary neutron irradiation test revealed unique changes in electrical resistivity and positron lifetime spectroscopy. However, little theoretical modeling has been conducted to understand the physics behind these ion and neutron irradiation effects.

In this study, *ab-initio* methods are utilized to understand radiation effects in NiFeMnCr HEA. Atomic level stress calculation provides a qualitative interpretation of elemental segregation trend at grain boundary after ion irradiation. Positron lifetime calculation for vacancy-type of defects is compared with the experiment, revealing the evolution of vacancy cluster size at different annealing temperatures. Finally, electrical resistivity calculation investigates the effects of atomic displacement scattering, chemical disorder scattering, magnetic disorder scattering and point defect concentration on HEA's electrical resistivity. These results provide insights on the feasible cause of significant electrical resistivity enhancement due to the neutron-irradiation.