Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic properties and electron-phonon interaction in complex, multicomponent alloys in application to high-entropy alloys GERMAN SAMOLYUK, Oak Ridge National Laboratory, MARKUS DAENE, Lawrence Livermore National Laboratory, GEORGE MALCOLM STOCKS, Oak Ridge National Laboratory, JOSE ALFREDO CARO, Los Alamos National Laboratory, ROGER STOLLER, Oak Ridge National Laboratory — High-entropy alloys (HEAs) have recently been developed as nontraditional alloy systems. They are composed of multiple elements at or near equiatomic ratios that form random solid solutions on simple underlying fcc or bcc lattices. In recent years HEAs have attracted significant attention due to their high strength, ductility and possible high radiation resistance. The complexity of the alloys results in very interesting electronic system behavior. Even in thermal equilibrium, disorder, especially extreme disorder, has important impacts on all electronic, atomic, and magnetic properties. In the current work we present results of first principle investigation of the electronic and magnetic properties of Ni-based multicomponent concentrated alloys using the coherent potential approximation (CPA). The influence of electronic structure modifications on the electron mean free path and values of electron-phonon coupling are calculated, together with preliminary results on similar quantities obtained by Time Dependent DFT. We discuss possible effects of tuning the mean free path and energy dissipation mechanisms to defect production and recombination in HEAs under irradiation.

German Samolyuk
Oak Ridge National Lab

Date submitted: 14 Nov 2014 Electronic form version 1.4