Korringa-Kohn-Rostoker Electronic Structure Theory 50 Years On
Understanding the Physical Properties of Concentrated Solid Solution and High Entropy Alloys"

G. Malcolm Stocks[1], Sai Mu[1], German Samolyuk[1], Sebastian Wimmer[2], Sergiy Mankovsky[2], Markus Eisenbach[1], Junqi Yin[1] and Markus Daene[3]

[1] *Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*
[2] *Ludwig-Maximilians-Universität München, 81377 München, Germany*
[3] *Lawrence Livermore National Laboratory,*

At Oak Ridge, the history of the development and application of Korringa-Kohn-Rostocker (KKR) multiple scatter theory (MST) electronic structure methods dates back 50 years and the reporting, by Sam Faulkner, Harold Davis and Hugh Joy, of a KKR-band theory code able to perform a highly precise calculation the Fermi surface of Cu in under 10 minutes using a IBM 360-75 computer – the laboratories 'supercomputer' of the time. This work marked the beginning of KRR derived research effort, including development of KKR-CPA method for calculating the electronic states of disordered alloys and the linear scaling Locally Self-consistent Multiple Scattering (LSMS) large system electronic structure code, that continues today. In addition to solving the band structure problem for periodic solids, MST Green's function methods provide an ideal framework for implementing the coherent potential approximation (CPA) for calculating the configurationally averaged electronic properties of disordered systems. Implemented within MST and DFT, the resulting KKR-CPA method provides a first principles theory of the electronic, magnetic, transport and other properties of solid solutions and non-stoichiometric compounds. The recent discovery of a new class of, so called, "High Entropy Alloys" (HEA) that contain 4, 5, or more elements, at or near equiatomic composition, yet form as single phase solid solutions, has led to renewed interest in understanding the physical properties of disordered alloys; in particular, to provide insights into the underlying electronic mechanisms responsible for their extraordinary physical and mechanical properties and enhanced radiation tolerance. Here, we present experimental measurements, as well as corresponding theoretical calculations, of the electrical and magnetic properties of an expanded class of equiatomic, fcc, concentrated solid solution alloys (CSA) that is based on the *3d*- and *4d*-transition metal elements Cr, Mn, Fe, Co, Ni, Pd; a set of alloys that ranges from simple binary alloys, such as $Ni_{0.5}Co_{0.5}$ and $Ni_{0.5}Fe_{0.5}$, to the quinary $Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}$ an $Cr_{0.2}Pd_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}$ HEA themselves. Theoretically, we present the results of first principles KKR-CPA calculations that show how the complex electronic and magnetic structures and resulting transport properties evolve as a function of the number and type of alloy constituents and discuss the role that increasing chemical complexity has on the underlying electronic structure and scattering mechanism that determine the electrical transport properties.

Work supported by US-DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division and the *Energy Dissipation to Defect Evolution (EDDE)*, Energy Frontier Research Center.