Deviation from High-Entropy Configurations in the $Al_{1.3}CoCrCuFeNi$ Alloy

Louis J. Santodonato[1,2], Yang Zhang[3], Mikhail Feygenson[2], Chad M. Parish[2], Michael C. Gao[4,5], Richard J.K. Weber[6,7], Joerg C. Neuefeind[2], Zhi Tang[8], and Peter K. Liaw[1]

1. *Dept. of Materials Sci. & Eng., The University of Tennessee, Knoxville, Tennessee, USA*
2. *Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.*
3. *Dept. of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA*
4. *National Energy Technology Laboratory, Albany, OR*
5. *URS Corporation, Albany, Oregon, USA*
6. *Materials Development Inc., Evanston, Illinois, USA*
7. *Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, USA*
8. *Dept. of Materials Sci. & Eng., Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, Virginia, USA*

Presenter and corresponding author: Prof. Peter K. Liaw, pliaw@utk.edu

The alloy-design strategy of combining multiple elements in near-equimolar ratios has shown great potential for producing exceptional engineering materials, often known as "high-entropy alloys". Understanding the elemental distributions, and thus the evolution of the configurational entropy during solidification, is the goal of the present research. The case of the $Al_{1.3}CoCrCuFeNi$ model alloy is examined, using integrated theoretical and experimental techniques, such as *ab initio* molecular dynamics simulations, neutron scattering, synchrotron X-ray diffraction, high-resolution electron microscopy, and atom-probe tomography. It is shown that even when the material undergoes elemental segregation, precipitation, chemical ordering, and spinodal decomposition, a significant amount of disorder remains, due to the distributions of multiple elements in the major phases. The results suggest that the high-entropy-alloy-design strategy may be used to develop a wide range of complex materials, which are not limited to single-phase solid solutions. The integrated experimental and theoretical techniques, discussed here, are particularly well-suited to studying partially-ordered materials, produced using the high-entropy-alloy design strategy.

Acknowledgements:

The U.S. Department of Energy (DOE) Office of Basic energy Sciences sponsors the national user facilities where the present neutron scattering, synchrotron X-ray diffraction, and high-resolution electron microscopy were conducted. The *ab initio* molecular dynamics simulations were conducted in support of the DOE Innovative Processing and Technologies Program of the National Energy Technology Laboratory (NETL). Prof. P.K. Liaw further acknowledges the support from the U.S. Army Office Project (W911NF-13-1-0438) with the program manager, Dr. S.N. Mathaudhu. The National Science Foundation (NSF) (DMR-0909037, CMMI-0900291, and CMMI-1100080), the DOE Office of Nuclear Energy's Nuclear Energy University Programs (NEUP, grant #00119262), and the DOE Office of Fossil Energy, NETL (DE-FE0008855 and DE-FE-0011194), with Drs. C.V. Cooper, A. Ardell, Z.M. Taleff, R.O. Jenseng, Jr., L. Tian, V. Cedro, S. Lesica, and S. Markovich as program managers, provided additional funding, particularly for Prof. Liaw (NSF) and the students (DOE) at The University of Tennessee.