**Advanced high-entropy alloys design and fundamental understanding aided by neutron scattering(1,2)**

Peter K. Liaw (pliaw@utk.edu)

Department of Materials Science and Engineering, The University of Tennessee, Knoxville, USA

**Abstract**

Recently, exceptional properties that are continuously found in an intriguing new class of metallic structural materials, high-entropy alloys (HEAs), demonstrate their great potential for engineering applications particularly in extreme environments where conventional alloys reach their limits. The concept of HEAs has revolutionized traditional alloy design, in particular in terms of their endless composition space, which meanwhile brings a new challenge of how to effectively design HEAs with targeted properties. In this presentation, we will give an introduction on HEAs first. Following that, we will focus on the design of advanced precipitate-strengthened lightweight as well as fatigue-resistant HEAs by integrating computational methods and advanced experimental techniques, such as neutron scattering. We will discuss how to design high-strength, low-cost, and lightweight and fatigue-resistant HEAs by the Calculation of Phase Diagrams (CALPHAD)-based high-throughput computational method (HTCM). A fundamental understanding of the precipitation-strengthening, order-disorder-transition, and fatigue behavior in these newly designed HEAs is revealed by *in-situ* neutron scattering, advanced microscopies, Monte-Carlo (MC) simulations, and *ab initio* molecular dynamics (AIMD). This study provides in-depth insights into the discovery of advanced structural materials by the HEA concept. Moreover, the potential applications of HEAs are discussed.

1. *R. Feng, C. Zhang, M.C. Gao, Z. Pei, F. Zhang, Y. Chen, D. Ma, K. An, J.D. Poplawsky, L. Ouyang, Y. Ren, J.A. Hawk, M. Widom, P.K. Liaw, High-throughput design of high-performance lightweight high-entropy alloys, Nature Communications 12(1) (2021) p. 4329.*
2. *R. Feng, R., Rao, Y., Liu, C., X. Xie, D. Yu, Y. Chen, M. Ghazisaeidi, T. Ungar, H. Wang, K. An, and P.K. Liaw, Enhancing Fatigue Life by Ductile-transformable Multicomponent B2 Precipitates in a High-entropy Alloy, Nature Communications, 12(1) (2021) p. 3588.*