Efficient first-principles methods of calculating stacking fault energies in high entropy alloys: comparison of FCC and BCC lattices

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Due to their unusual structure and composition, high entropy alloys (HEAs) have favorable properties such as high service temperatures, strength, and ductility, making them potential candidates for high performance engineering material applications. In the present work, first-principles based calculations using density functional theory (DFT) were used to analyze stacking fault energies (SFE) in candidate BCC and FCC single-phase quinary HEA systems. Special quasi-random structures (SQS) and the GGA-PBE exchange correlation functional were used. Intrinsic stacking faults on the {111} planes in FCC are investigated on the CoCrFeNiMn system. "Twinning-sense" and "non-twinning-sense" stacking faults (SF) on the (112) plane, with ABCDEFA stacking, are explored. Two methods for making the calculations more efficient are employed: a lower ordering averaging method on a quinary's constituent ternary systems, and the use of inferential statistics to apply predictive error bars on a subset of the global population. Results are compared to known literature where available, and the implications for using both methods for HEA database development are discussed.

Bio: Dr. Chelsey Hargather is an Assistant Professor of Materials & Metallurgical Engineering and runs the Advanced Computational Metallurgy Lab (ACML) at New Mexico Tech. She teaches undergraduate courses in engineering design, materials engineering, thermodynamics and physical metallurgy, as well as graduate courses in metallurgical phase transformations, phase equilibria, and materials applications to density function theory. Dr. Hargather's research group focuses on uses computational and experimental techniques to understand the behavior of specific alloying elements in or improve the performance of metallic engineering alloys. Dr. Hargather's research group has evolved over the past few years to include research on energetic materials and additive manufacturing of solid composite rocket propellant. Her current projects are funded by National Science Foundation, Army Research Lab, Sandia National Laboratories, and DOE NNSA. Dr. Hargather advises PhD, Masters, and undergraduate students on her research projects.

Chelsey received a PhD in Materials Science and Engineering from The Pennsylvania State University in 2012. Her research developed an improved understanding of Ni-base superalloys through computational techniques, including the calculation of phase diagrams, and first-principles calculations of diffusion coefficients. Chelsey received a BS in Materials Science and Engineering with a minor in French from Virginia Polytechnic Institute and State University in 2008.