Short-Range Order in High-Entropy Materials

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Abstract

Short-range order (SRO) in multicomponent alloys is complicated by the number of components, e.g., the number of Warren-Cowley SRO parameters for an M-component alloy is M(M-1)/2. Computational tools such as cluster expansion and machine-learned interatomic potential simulations, can be used to obtain SRO parameters, but these methods are too computationally expensive to survey a wide range of compositions in a high-throughput manner. In an effort to find high-throughput descriptors of SRO, we analyze the connection between SRO and LRO/phase diagrams for multicomponent alloys, and also investigate whether multicomponent SRO can be inferred from lower order (e.g., binary, ternary) information. We find that SRO cannot be determined from considerations of LRO alone, but the two can even qualitatively disagree. Based on energetics of ordered, disordered, and coherent phase separated states, we determine simple energetic descriptors of SRO, allowing us to classify SRO types in a variety of high-entropy alloy systems. We show illustrations of these ideas in high-entropy alloys with applications as structural materials, battery cathodes, and thermoelectrics.

Short Biography

Chris Wolverton is the Jerome B. Cohen Professor of Materials Science and Engineering at Northwestern University. Before joining the faculty, he worked at the Research and Innovation Center at Ford Motor Company, where he was group leader for the Hydrogen Storage and Nanoscale Modeling Group. He received his BS degree in Physics from the University of Texas at Austin, his PhD degree in Physics from the University of California at Berkeley, and performed postdoctoral work at the National Renewable Energy Laboratory (NREL). His research interests include computational studies of a variety of energy-efficient and environmentally friendly materials via first-principles atomistic calculations, high-throughput and machine learning tools to accelerate materials discovery, and multiscale methodologies for linking atomistic and microstructural scales. He is a Fellow of the American Physical Society and the American Society for Metals, and is an ISI Highly Cited Researcher. He has published more than 400 papers, with ~50,000 citations, and an h-index of 113.