Constructing Compositional Gradients in Many-Element Systems

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Abstract

Dissimilar joining of shape memory alloys has gained attention in recent years due to their use in aerospace and biomedical industries. At present, joints are made mechanically (e.g., bolting or crimping) because metallurgical bonds produce deleterious phases and poor joint efficiencies. To be considered successful, a joint must have a final composition gradient that results in favorable (strong, ductile) phases, while avoiding unfavorable (weak, brittle) ones. This requires: a target final gradient that is known or predicted to be favorable; and a technique for guiding the joining process to such a targeted final gradient.

Previous work has used path planning algorithms from the field of robotics to quickly create paths in composition spaces – while also minimizing a particular cost function – that were predicted by CALculation of PHAse Diagrams (CALPHAD) software. However, these approaches require surrogate models of the unfavorable phase regions prior to path planning, necessitating extensive sampling of CALPHAD before path construction can even begin. This becomes impossible to scale when working considering industrial structural alloys, which can easily have 8 elements. Here, we introduce the concept of frontier algorithms that can sample CALPHAD on-the-fly and decrease computational time by orders of magnitude.

Short Biography

McCue is a tenure-track Assistant Professor and the Morris E. Fine Junior Professor in Materials and Manufacturing at Northwestern University in the Department of Materials Science and Engineering. His research group focuses on designing materials for extreme applications – e.g., aerodynamic, radiation, and corrosion – and understanding how their microstructures evolve in these environments. He received his PhD degree in Materials Science and Engineering from Johns Hopkins University in 2015, and received a Materials Research Society Silver Graduate Student Award in 2014 for his dissertation work. He then held a postdoctoral appointment at Texas A&M University studying the fabrication and mechanical testing of metal nanocomposites. Prior to joining Northwestern University, he was a Senior Scientist at the Johns Hopkins University Applied Physics Laboratory, where he developed and studied new high temperature alloys for extreme environments. He has been an invited speaker at two Gordon Research Conferences: the 2019 Physical Metallurgy, and 2022 Structural Nanomaterials. He received a NASA Early Career Faculty Award in 2021 to develop solutions to bonding nitinol to dissimilar alloys, and a DARPA Young Faculty Award in 2023 to develop a new high-strain rate mechanical test method.