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ABSTRACT:

Grain Boundary Diffusion in Compositionally Complex Alloys

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Grain boundary (GB) diffusion plays a critical role in controlling microstructural stability, phase evolution, and high-temperature performance of compositionally complex alloys (CCAs). In this work, we present a comprehensive radiotracer-based investigation of GB diffusion in prototypical FCC CCAs, including CoCrFeNi and CoCrFeMnNi, with diffusion data obtained for multiple constituent and impurity elements.

The results reveal that GB diffusivities in CCAs do not follow a universally sluggish trend when compared to simpler, lower-component systems such as pure metals and binary alloys. Instead, a nuanced picture emerges while certain elements exhibit reduced mobility, others display comparable or even enhanced diffusivities. This demonstrates that the widely invoked concept of “sluggish diffusion” cannot be treated as a blanket characteristic of CCAs.

A key outcome of this study is the clear identification of element-specific GB diffusion behavior. The variation in diffusivities across different tracers highlights the role of local chemical environments and atomic interactions in governing GB transport. Such behavior underscores the importance of considering individual atomic mobilities rather than relying on averaged or simplified descriptions.

Further insight into GB kinetics is obtained from deformation-processed CoFeNi, where GB diffusion of Co tracers reveals a pronounced retardation in the relaxation of non-equilibrium GB states. These findings indicate that deformation-induced excess energy and structural disorder persist over extended timescales in medium-entropy alloys, contributing to enhanced and time-dependent GB diffusivity.

The talk also highlights the inherent challenges in accurately characterizing GB diffusion in multi-principal element alloys, given their broad compositional variability and complex microstructures. A00192C