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ABSTRACT:

Lattice Distortions and Non-Sluggish Diffusion in BCC Refractory High Entropy Alloys

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Refractory high-entropy alloys (RHEAs) are promising candidates for extreme high-temperature applications. In our recent studies, we investigated self- (Zr) and impurity (Co, Mn, and Zn) diffusion in single phase (BCC solid solution) HfTiZrNbTa and HfTiZrNbV RHEAs. The results of the radiotracer diffusion measurements are analysed accounting for ab initio-based calculations of substitutional and interstitial solution energies, local lattice distortions, and short-range order effects. A ‘non-sluggish’ diffusion behavior for Zr is clearly observed, highlighted by an enhancement of the measured diffusion rates with respect to the geometric mean of the diffusivities in the corresponding pure elements. Co diffusion is found to be dominated by an interstitial mechanism, exhibiting fast diffusion, while impurity diffusion of Mn and Zn is vacancy-mediated. The findings for impurity elements reveal important structure–property relationships between the local atomic environments and diffusion kinetics in BCC RHEAs.