Crystal Nucleation and Growth in High-Entropy Alloys Revealed by Atomic Electron Tomography

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Crystal Nucleation and Growth in High-Entropy Alloys Revealed by Atomic Electron Tomography

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High-entropy alloys (HEAs) have emerged as a pinnacle of materials design, spanning both structural and functional fields. For example, they offer an exceptional balance between strength and ductility in metallurgy, while exhibiting near-continuum adsorbate binding energies in catalysis. However, despite significant advancements in synthesizing HEAs, characterizing their structural and chemical order, and pursuing their broad applications, fundamental insights into the crystal nucleation and growth of HEAs at the atomic scale—essential for understanding their synthesis-structure-property relationships—remain elusive. Here, we advance atomic electron tomography to determine the three-dimensional atomic structure and chemical composition of 8,094 HEA nuclei, captured at different stages of nucleation. We observe that early-stage nuclei exhibit a structural order that gradually decreases from the cores to the boundaries and is correlated with local chemical order. As the nuclei grow, their cores become more crystalline, and the structural order extends further along the radial direction. In the late stage of nucleation, most nuclei coalesce without misorientation, while a small fraction forms twin boundaries. Since these results differ from classical nucleation theory and the two-step nucleation model, we develop an equation called gradient nucleation pathways to better explain our experimental observations. These findings provide a fundamental understanding of crystal nucleation and growth in HEAs. Moreover, we expect that gradient nucleation pathways can be broadly applied to elucidate a wide range of nucleation processes [8].

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