
Laser powder bed fusion of Fe–Co–Ni–Cu high-entropy alloys guided by computational simulation

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Abstract

High-entropy alloys have tantalized both academia and industry in recent years due to their impressive mechanical and physical properties. However, efficient approaches to screen the immense compositional space for promising candidate alloys are limited. Herein, thermodynamic and molecular dynamics simulations are employed to design novel Fe–Co–Ni–Cu high-entropy alloys for laser powder bed fusion. The thermodynamic simulations reveal that the content of Ni and Cu significantly affects the solidification temperature range and, in turn, the printability of the alloy. Molecular dynamics simulations unveil that increasing the content of Ni and Co increases the stacking fault energy, while increasing the content of Fe decreases it. High-throughput in-situ alloying via laser powder bed fusion of mixed elemental powder is performed to fabricate compositionally graded samples and screen the Fe–Co–Ni–Cu compositional space. The tensile properties and dislocation evolution of Ni_{50–x}Fe₂₅Co₂₅Cu_x alloys are explored using experimental characterization and atomistic simulations. This work provides a framework for developing novel high-entropy alloys by laser powder bed fusion.

Keywords: High entropy alloys, Laser powder bed fusion, Additive manufacturing, Molecular dynamics simulations, Calculation of phase diagrams

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