Accepted Manuscript

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PII: S0925-8388(18)31033-8

DOI: 10.1016/j.jallcom.2018.03.165

Reference: JALCOM 45395

To appear in: *Journal of Alloys and Compounds*

Received Date: 7 December 2017

Revised Date: 5 March 2018

Accepted Date: 12 March 2018

Please cite this article as: M. Jafary-Zadeh, Z.H. Aitken, R. Tavakoli, Y.-W. Zhang, On the controllability of phase formation in rapid solidification of high entropy alloys, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.03.165.

On the controllability of phase formation in rapid solidification of high entropy alloys

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Abstract

The demonstration of high entropy alloys (HEAs), or more generally multi-principal-element alloys (MPEAs), which display a greater resistance to softening at elevated temperatures and embrittlement at cryogenic temperatures, has offered an accessible alternative alloying process for materials scientists and engineers. Although solidification is a fundamental process in synthesis of alloys which strongly affects their microstructure and properties, a firm understanding of this process in HEAs is scarce. Here, using molecular dynamics (MD) simulations, we study the rapid solidification of the multi-principal-element CoFeNiPd alloy as a prototypical single-phase HEA. Our simulations reveal an intense competition between fcc and bcc structures during homogenous nucleation in this alloy. According to our numerical analyses, the crystalline fcc phase is thermodynamically the most stable structure in this alloy, which is in agreement with the experimental observations. We show that formation of the fcc structure can be facilitated through heterogeneous nucleation by including a pre-existing fcc seed in the liquid phase. Interestingly, we illustrate that altering the phase of the seed from fcc to bcc leads to obtaining a single phase bcc alloy. Our detailed analyses confirm that the tendency of HEA systems to undergo crystallization (rather than amorphisation) at fast cooling rates is owing to the neutral chemical affinity and similar atomic size of their constitutive elements. Our findings suggest that rapid solidification accompanied with heterogeneous (*e.g.* seed-assisted) nucleation could be a promising processing route to control the microstructure and properties of the HEAs.

Keywords: high entropy alloys; solidification; crystallization; homogeneous; heterogeneous; molecular dynamics.