Accepted Manuscript

Design of high-entropy alloys with a single solid-solution phase: Average properties vs. their variances

Yiming Tan, Jinshan Li, Shaowu Tang, Jun Wang, Hongchao Kou

PII: S0925-8388(18)30259-7

DOI: 10.1016/j.jallcom.2018.01.252

Reference: JALCOM 44716

To appear in: *Journal of Alloys and Compounds*

Received Date: 30 November 2017

Accepted Date: 17 January 2018

Please cite this article as: Y. Tan, J. Li, S. Tang, J. Wang, H. Kou, Design of high-entropy alloys with a single solid-solution phase: Average properties vs. their variances, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.01.252.

Design of high-entropy alloys with a single solid-solution phase: Average properties vs. their variances

Yiming Tan, Jinshan Li*, Shaowu Tang, Jun Wang, Hongchao Kou

State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, P.R. China

Abstract

The empirical thermo-physical parameters for designing of high-entropy alloys (HEAs) with a single solid-solution phase (SSP) are based on the average properties of constituent elements, significant derivation from which might make them out of work. In the current work, both the important roles of average properties and their variances were studied. After an introduction of the variance of dimensionless enthalpy of mixing to characterize the chemical bond mismatch and a comparative study between two typical collections of HEAs to show the validity of previous designing rules, it was found that all the previous parameters to some extent fail to predict the formation of HEAs with a single SSP whereas the variance of dimensionless enthalpy of mixing is able to separate the regions of HEAs with a single SSP, with multi-phases and with an amorphous phase. Application to three typical HEA systems proved further that the lower value of the variance of dimensionless enthalpy of mixing corresponds to the higher possibility to form HEAs with a single SSP. The current work provides some necessary conditions for designing of HEAs, based on which preparation of potential HEAs with a single SSP could be accelerated.

Keywords: High-entropy alloys; Atom size difference; Chemical bond mismatch; Thermodynamics; Designing rules.

* Corresponding author
E-mail address: lish@nwpu.edu.cn (Jinshan Li)