



An approach for screening single phase high-entropy alloys using an in-house thermodynamic database

Antonio João Seco Ferreira Tapia, Dami Yim, Hyoung Seop Kim, Byeong-Joo Lee*

Department of Material Science and Engineering & Center for High-Entropy Alloys, Pohang University of Science and Technology (POSTECH), Pohang, 37673, Republic of Korea

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ABSTRACT

A new screening methodology is proposed to aid in the development of high-entropy alloys (HEAs). This approach takes into account three commonly used criteria and methods to guide the design of HEAs: empirical parameters, binary phase diagram inspection and the Calculation of Phase Diagrams (CALPHAD) method. In addition, two novel concepts are introduced: a criterion to evaluate the likeliness of single phase solid solution in an alloy system's non-equiatomical compositional space, and a binary priority list, which allows us to make the employed in-house thermodynamic database a more reliable tool for solid solution screening in a time-effective manner.

1. Introduction

Research on high-entropy alloys (HEAs) has become increasingly complex since their recent advent [1,2]. Early studies focused on single phase HEAs and were motivated mainly by the desire to understand the basic properties of these newly discovered materials, elaborate phase formation rules and prediction mechanisms to aid the screening of candidate alloys for solid solution and investigate viable fabrication routes and applications [3–13]. Although current studies also deal with these issues at much deeper levels [14–21], the progress of emerging research fronts such as the study of the metallic strengthening mechanisms, influences on the fatigue behavior and design of light-weight alloys (well-established in steels and other widespread materials) has elevated HEAs research, resulting in more complex structures with a wider range of properties and potential applications [22–31]. However, the ability to screen the essentially infinite compositional space of the HEAs in a methodical and efficient way, being able to identify new single phase solid solution alloy systems, is still relevant, if not key, to the further development of HEAs research [32].

This relevance can be easily seen in the ongoing interest to develop new screening methodologies and improve traditional ones by the review and modification of their assumptions and procedures. The diversity of the empirical parameters designed throughout the years for the parametric approach provides clear evidence of this effort. The quantification of the atomic misfit in a multicomponent alloy, for example, can be entrusted to several empirical parameters, each having

their own set of underlying assumptions about the atomic packing instability, lattice distortion origins or intrinsic strain energy formulations [33–36]. The prominent role of thermodynamics, particularly in the absence of kinetic factors, has also directed attention to parameters that could accurately reproduce the effects of the competition between the enthalpy of mixing ΔH_{mix} and entropy of mixing ΔS_{mix} over phase selection [15,37–39].

Newly developed thermodynamic parameters are able to overcome previous limitations, such as with the usage of the semi-empirical Miedema model [40] for evaluating ΔH_{mix} and the overlapping of calculated values between single phase HEAs and multiphase alloys. Nevertheless, the complexity (associated with elevated costs and computational time) and sometimes lack of rigorosity in their formulation has limited their usage [32,37,41]. The formulae for the original and most widely used empirical parameters for the atomic misfit δ and the enthalpy of mixing ΔH_{mix} are given by

$$\delta = 100 \sqrt{\sum_{i=1}^N x_i \left(1 - \frac{d_i}{\sum_{j=1}^N x_j d_j} \right)^2} \quad (1)$$

and

$$\Delta H_{mix} = \sum_{i=1, i \neq j}^N 4\Delta H_{AB}^{mix} x_i x_j \quad (2)$$

where N is the total number of elements, x_i and x_j are the atomic percentages of the i th and j th element, d_i and d_j are the diameter of the

* Corresponding author.

E-mail address: calphad@postech.ac.kr (B.-J. Lee).

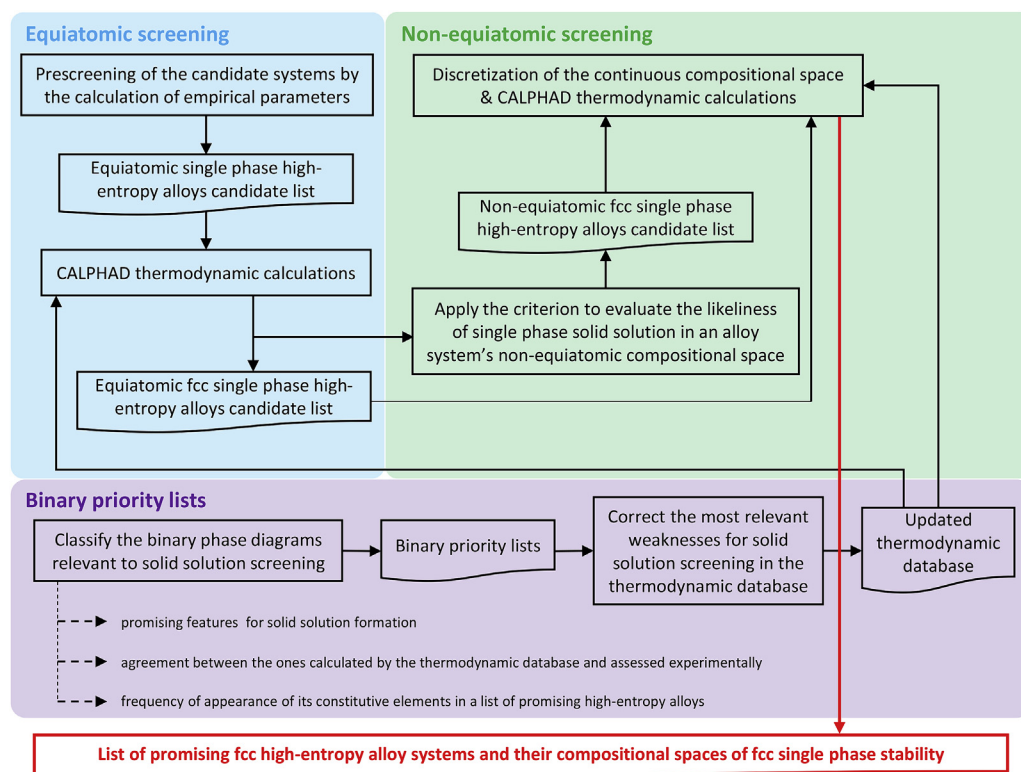


Fig. 1. Main steps of the fcc single phase screening methodology developed. The steps related directly with the equiatomic screening, non-equiatomic screening and binary priority lists are located in the blue, green and purple regions, respectively. For simplification purposes, supporting files such as the codes used during the thermodynamic calculations are left out of the flowchart and commented in details in ref. [50]. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

i th and j th element and ΔH_{AB}^{mix} is the enthalpy of mixing for the equiatomic binary liquid AB alloys [5].

In this research, two novel concepts (a criterion to evaluate the likelihood of single phase solid solution in an alloy system's non-equiatomic compositional space and binary priority lists) are employed with commonly used techniques in the design of HEAs (empirical parameters, binary phase diagram inspection and the Calculation of Phase Diagrams [CALPHAD] method) in a convenient manner in order to efficiently screen for potential face-centered cubic (fcc) single phase HEAs as well as provide a means of improving the reliability of the thermodynamic database used for solid solution screening in a time-effective manner.

2. Methods

2.1. Solid solution screening

A flowchart of the complete methodology developed in this study is shown in Fig. 1. An upgraded version of the TCFE2000 thermodynamic database [42,43] is used with the Thermo-Calc software [44] for the thermodynamic calculations. The screening process developed in this study evaluates both equiatomic and non-equiatomic compositions. An atomic misfit of $\delta = 7$ (Eq. (1)) is used to limit the equiatomic alloys that had their phase fractions calculated over a temperature range, similar to Fig. 2a. Not only is this value slightly higher than what is accepted in literature ($\delta = 6.6$) as the threshold for solid solution formation in multicomponent alloys [38], it also roughly marks the point from which, for the alloy systems available in our in-house thermodynamic database, higher atomic misfits translate into considerably higher computational costs and a longer time needed to calculate the equilibrium state as the latter becomes more complex; the stability of multiple intermetallic phases is observed in nearly all alloy systems. Unlike previous studies in which both the thermodynamic and topological parameters are used to make prediction maps of HEA systems, the enthalpy of mixing ΔH_{mix} (Eq. (2)) and the Ω parameter are not used as additional criteria for these calculations. The increase of the

computational cost associated with this decision is found to be negligible since only a relatively small amount of alloy systems are added to the overall calculation procedure.

The equiatomic alloys that fall within the atomic misfit criterion are then investigated using the thermodynamic calculation technique. Unlike typical approaches, we do not focus only on alloy systems in which a fcc single phase solid solution is stable within an appropriate temperature range; all alloy systems that show any solid solution regions (regardless of the size or the location of the temperature range) are selected for further investigation. Since our final goal is to identify new fcc single phase HEAs, the only feature required for these solid solutions is the presence of at least one fcc structured phase in their constitution. This approach enables not only to identify equiatomic alloys that are good candidates for single phase HEAs, but also alloy systems inclined to show similar features at non-equiatomic compositions. The possibility to evaluate the presence of single phase solid solution regions in an alloy system's non-equiatomic compositional space through the calculation of its equiatomic phase fraction plot can be seen more clearly in the analysis of the CoCrFeMnNiV equiatomic alloy, Fig. 2. This alloy is illustrative because it shows in its phase fraction plot a double phase solid solution region that qualifies it for further screening of its non-equiatomic compositions, Fig. 2a. Furthermore, the criterion of using any solid solution region that contains at least one fcc structured phase becomes clear when observing that in the two pseudo-binaries the fcc phase field region is undetectable at equiatomic compositions, Fig. 2b and c.

The alloy systems selected during the first analysis are subsequently submitted to a second screening, focused in their non-equiatomic compositions. This requires the continuous compositional space of HEAs to be turned into a set of discrete values that is representative and also allows the calculation of its phase fraction plots with a minimum sampling effort. The concentration values chosen for the individual elements in the quaternary, quinary and senary alloys are shown in Table 1. In the quinary alloy systems, for example, the five values selected yield a total of 241 compositions that need to be evaluated for each specific alloy system. It is important to notice that the quantity of

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