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On the prediction of low-cost high entropy alloys using new thermodynamic multi-objective criteria

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Abstract

In an attempt to identify new low-cost metallic materials with interesting thermophysical properties from the Fe-Cr-Mn-Ni-V-Ti-Al- (Co,Mo) system, we present here an original tool for the design of first-generation High Entropy Alloys (HEAs). The composition of potential HEAs is calculated under a set of nonsmooth and non-linear constraints and multi-objective functions linked to the single phase start temperature, the room-temperature driving force for phase assemblage evolution and the solidification range. These are all new thermodynamic criteria for the design of HEAs. This tool links a constrained Gibbs energy minimization algorithm that uses accurate thermodynamic databases to a optimization algorithm implemented for solving "blackbox" objective functions and constraints. As a result of this work, we have identified entire sets of new FCC and BCC first-generation HEAs potentially suitable for future industrial applications.

1. Introduction

The design of the optimal material for a given application is a challenging task: the optimized chemistry is often obtained as a result of a complex trial and error process of the simultaneous tuning of the corrosion properties, specific mechanical properties and cost. In most cases, the ideal alloying element

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