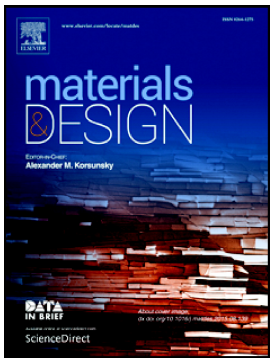

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Designing high entropy alloys employing thermodynamics and Gaussian process statistical analysis

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Abstract

High entropy alloys (HEAs), a category of highly concentrated multicomponent alloys, have become a subject of interest in the past years due to their combination of properties. The development of these single phase solid solution alloys, containing between 5% and 35% of at least five different elements, has mainly relied on trial-and-error experiments, and more recently on modelling. The latter has notably focused on criteria to guide the formation of a single solid solution: (1) Hume-Rothery rules or their modification based on elemental variations in atomic radius, electronegativity, valence or number of itinerant electrons; (2) the use of thermodynamic concepts relying on estimates of enthalpy or entropy of mixing, and/or on melting or spinodal decomposition temperatures; (3) criteria based on lattice distortion; and (4) computational thermodynamics using the CALculation of PHAse Diagrams (CALPHAD) method. However, none of these criteria or methods, taken alone, can reliably predict the formation of a single solid solution. Instead, based on a critical assessment and a Gaussian process statistical analysis, a robust strategy to predict the formation of a single solid solution is proposed, taking into account most of the previously proposed criteria simultaneously. The method can be used as a guide to design new HEAs.

Keywords:
HEA; Neural network; Thermo-Calc; data mining