High-throughput screening of composition space for materials and process design

Ömer Büyükuslu* Moritz to Baben*

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Abstract

CALPHAD (CALculation of PHAse Diagrams) is a widely utilized method for modeling material systems at thermodynamic equilibrium. It enables the understanding and prediction of phase transformations in various inorganic materials. In this study, we demonstrate the effectiveness of performing numerous equilibrium calculations to efficiently screen composition space for materials design purposes. The composition space considered encompasses the elements Fe, Mo, V, Ni, Mn, Si, Cr, Ti, Al, Nb, B, and C, with a particular emphasis on high Fe contents. Following the calculations, a filtering process is applied to identify compositions that exhibit specific desired properties, including the formation of particular phases (e.g., austenite with subsequent martensite transformation), as well as melting and solidification temperatures. This high-throughput approach enables rapid analysis and interpretation of extensive thermodynamic data, facilitating the identification of promising alloy compositions for hardfacing applications in an efficient and dependable manner.

*GTT-Technologies