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ABSTRACT:

Co-segregation Phenomena and Stability Issues in High-Entropy Alloys using Density-Based Phase-Field Modelling

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Several recent studies have revealed that the phase decomposition in medium- and high-entropy alloys is triggered by solute segregation at grain boundaries. The chemically complex nature of these alloys already clues that such segregation in materials should be something more than the interaction between solutes and grain boundary, but also affected by the solute-solute interactions during the segregation. In fact, experiments indicate the significance of such solute-solute interaction. Yet, the mechanisms of co-segregation in multi-component alloys are rather challenging to explore and rarely studied quantitatively. Recently, a CALPHAD-integrated density-based phase-field model has been proposed for studying grain boundary phenomena [1]. Several applications of this model have shown its expansive capacity for investigating grain boundary segregation and phase behavior [2-8]. In this talk, the applications of this model to studying co-segregation phenomena and grain boundary phase diagrams in multi-component alloys are presented —the term 'co-segregation' here refers to co-evolution and any mutual interplay among the solutes and grain boundary during the segregation. In particular, the iron-based ternary and quaternary alloys are discussed. I show how a grain boundary may have its own miscibility gap and how this immiscibility can influence the co-segregation behavior. As an alternative to grain boundary phase diagrams, rather suited for binary and ternary alloys, a new concept of co-segregation maps for screening and segregation design in multi-component alloys is presented. Applying the co-segregation maps, the nonlinear Mn and Cr co-segregation in Fe-Co-Mn-Cr is discussed.

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