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Investigation of Possible Phase Separation in Rapidly Quenched $Fe_{1-x}Co_x$ Alloys with Cluster Expansion Model XIN ZHAO, MANH CUONG NGUYEN, MIN JI, IVER E. ANDERSON, M.J. KRAMER, R. WILLIAM MCCALLUM, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University — Recently, experiments observed phase separation in rapidly quenched $Fe_{1-x}Co_x$ alloy in the ordered α' phase [J. Alloys Compd. 424, 145 (2006)]. It is also believed that this is not an equilibrium result because of phase rule violation in the published phase diagram. To clarify this situation, we calculate the phase diagram of the system using cluster expansion in combination with a genetic algorithm. We calculated free energy of the system using super-cells up to 32 atoms with compositions ranging from 35 to 100 at. % Fe. Possible explanations for the experimental observations will be discussed.

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