Abstract Submitted
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Structure Defect Property Relationships in Binary Intermetallics[1] BHARAT MEDASANI, Lawrence Berkeley National Lab, HONG DING, University of California Berkeley, WEI CHEN, KRISTIN PERSSON, ANDREW CANNING, MACIEJ HARANCZYK, Lawrence Berkeley National Lab, MARK ASTA, University of California Berkeley — Ordered intermetallics are light weight materials with technologically useful high temperature properties such as creep resistance. Knowledge of constitutional and thermal defects is required to understand these properties. Vacancies and antisites are the dominant defects in the intermetallics and their concentrations and formation enthalpies could be computed by using first principles density functional theory and thermodynamic formalisms such as dilute solution method. Previously many properties of the intermetallics such as melting temperatures and formation enthalpies were statistically analyzed for large number of intermetallics using structure maps and data mining approaches. We undertook a similar exercise to establish the dependence of the defect properties in binary intermetallics on the underlying structural and chemical composition. For more than 200 binary intermetallics comprising of AB, AB2 and AB3 structures, we computed the concentrations and formation enthalpies of vacancies and antisites in a small range of stoichiometries deviating from ideal stoichiometry. The calculated defect properties were datamined to gain predictive capabilities of defect properties as well as to classify the intermetallics for their suitability in high-T applications.

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