FLAIR Colloquium

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Metastable Defect Phase Diagrams as a Road Map for Defect Design

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Recent experimental studies show the formation of secondary phases that cannot be explained by bulk phase diagrams. For example, for various alloys excess solutes well above the solubility limit have been observed to form planar defects rather than the secondary bulk phases predicted by the phase diagram. This discovery opens up exciting possibilities to engineer material defect structures using chemical, rather than mechanical, driving forces. However, to realize such applications, it is essential to have computational tools that can predict whether defect formation is exothermic at a given chemical composition and temperature, as well as the type of defect phase that will form. In this talk, we will present a novel approach, called the metastable defect phase diagram (MDPD), that goes beyond conventional defect phase diagrams by incorporating the energetics of metastable and unstable bulk phases. To illustrate the predictive capabilities of this approach, we applied it to various planar defects in Mg and Fe-based alloys. The results demonstrate the efficacy of this approach in predicting defect behavior in complex alloys and its potential for facilitating the design of novel materials with tailored properties.

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