Streamlining Predictions of Temperature-Dependent Changes in Defect Properties of Intermetallic Compounds

 Point defects are atomic scale irregularities in crystal structures of solids. These point defects can significantly affect electrical, optical, and mechanical properties of materials. The concentration of a defect depends on temperature, chemical composition, and the difference in enthalpies of the material with and without the defect. Using a thermodynamic model, this study analyzed the temperature and composition dependences of four types of defects in binary intermetallic compounds. It was possible to characterize the enthalpy conditions that lead to temperature- or composition-induced changes in dominant defect concentration. For example, there are ranges of enthalpies for which one type of defect dominates at low temperature and a different type dominates at high temperature for compositions near stoichiometry. The results will allow researchers who calculate defect formation enthalpies using computer simulations to streamline their predictions of temperature-dependent changes in defect-dependent materials properties.

This work is funded in part by the NSF grant DMR 15-08189. We gratefully acknowledge the important contributions of Nicholas Sharp and Yann Couturieux.