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Grain boundary segregation in binary alloys: Prediction of thermodynamic characteristics and interaction coefficients

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Grain boundary segregation is a phenomenon studied both experimentally and theoretically for decades. The interest in this phenomenon is evoked not only by its close relationship to temper embrittlement but also by its ability to stabilize nanocrystalline structures by solute segregation in the concept of Grain Boundary Engineering.

A full description of the exact temperature and solute concentration dependence of grain boundary segregation requires reliable values of segregation enthalpy and –entropy as well as solute interaction coefficients. However, experimental studies of all these values are rather limited, and theoretical studies are usually restricted to segregation energy at zero Kelvin. It is obvious that such a database does not allow a full description of the grain boundary segregation in most systems of interest.

In this contribution we present a semi-empiric method enabling prediction of all required thermodynamic parameters –ideal enthalpy, ideal entropy and real binary interaction (Fowler) coefficient –which, in combination, describe fully the segregation of any segregant at any temperature and at individual grain boundaries. This method is based on the relationship between the segregation enthalpy and the solid solubility limit, and on the enthalpy-entropy compensation effect. The data for numerous solutes in alpha iron are predicted and they are compared to available data in the literature.

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