

Calculation and Evaluation of Para-Equilibrium Phase Diagrams*

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A thermodynamic model for the evaluation of compositionally constrained equilibrium has recently been implemented into the MatCalc computer program. The thermodynamic formalism is based on the sublattice model and will be briefly described. The model uses the same free energy models and databases that are used in other, commercially available packages such as ThermoCalc™ and ChemSage™. However, the added flexibility to consider constrained equilibrium allows the user to calculate phase equilibria while holding one or more constituent compositions constant. The model is applied to the calculation of ortho- and para-equilibrium phase diagrams in several ternary model systems Fe-X-C (where X=Mn, Si, Cr, Mo) and a commercial 2¼Cr-1Mo steel. Here, ortho-equilibrium designates the state of full thermodynamic equilibrium, whereas para-equilibrium denotes partial equilibrium conditions, where the chemical potential of all interstitial components is equilibrated while the composition with respect to the substitutional components is the same in all phases. A comparison of the ortho- and para-equilibrium phase diagrams clearly shows the impact of para-equilibrium constraints on the austenite/ferrite transformation temperature. The conditions for forming non-equilibrium cementite with para-equilibrium constraints are identified. The calculations show that in para-equilibrium, the stability of cementite is enhanced with respect to other carbides. The driving forces for precipitation of cementite as well as the complex chromium/molybdenum carbides are evaluated as a function of the precipitate composition. It is shown that the present model is a valuable tool for understanding the phase stability and sequence of transformations that take place in many commercial steels.

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