A CALPHAD-Type Database for Co-Base Superalloys

Ursula R. Kattner[1, S, C] and Julio Cesar Pereira dos Santos[1]

[1]*Material Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*
ursula.kattner@nist.gov

Knowledge of the phase equilibria in materials systems is essential for the identification of promising alloy candidates and their processing requirements. The CALPHAD method is a well-established tool for obtaining such information. As part of the CHiMaD/NIST project, a database for Co-base gamma/gamma' superalloys is being developed. The database includes descriptions of the Gibbs energy and molar volume as functions of temperature and composition. The model parameters are assessed using data from experimental measurements and theoretical predictions, such as density functional theory (DFT). However, DFT data for only the binary endmembers are in general insufficient to predict realistic homogeneity ranges in multi-component systems and the generation of ternary endmember data is an enormous computational effort. The effective bond energy formalism (EBEF) is being explored for the description of complex intermediate phases within the framework of existing descriptions of the binary and ternary subsystems to give better reliability of the predictions of the higher-component systems.