CALPHAD
Computer Coupling of Phase Diagrams and Thermochemistry

DESCRIPTION

The design of industrial processes requires reliable thermodynamic data. CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) aims to promote computational thermodynamics through development of models to represent thermodynamic properties for various phases which permit prediction of properties of multicomponent systems from those of binary and ternary subsystems, critical assessment of data and their incorporation into self-consistent databases, development of software to optimize and derive thermodynamic parameters and the development and use of databanks for calculations to improve understanding of various industrial and technological processes. This work is disseminated through the CALPHAD journal and its annual conference. Contributions of high quality in these and related fields, especially the fields of first-principles calculations, experimental measurements of thermochemical and phase equilibrium data, phase transformations, and the process and materials designs that the CALPHAD works are based on or used for, are welcome.

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