

References CALPHAD

CALculation of PHAse Diagrams

Books

- CALPHAD (Calculation of phase diagrams): A comprehensive guide, N. Saunders en A.P. Miodownik, Pergamon 1998, ISBN 0-08-0421296

- Computational thermodynamics: The Calphad Method, H.L. Lukas, S.G. Fries and B. Sundman, Cambridge 2007, ISBN 978-0-521-86811-2
 - Two standard works on computational thermodynamics and the CALPHAD method
 - Describe the thermodynamic models, concept and determination of lattice stabilities, experimental techniques, the optimization procedure, applications, ...

- Materials Thermochemistry, O. Kubaschewski, C.B. Alcock en P.J. Spencer, 6th edition, Pergamon Press, 1993, ISBN 0-08-0418880

- Experimental and theoretical techniques for the determination of thermochemical data, such as calorimetry, vapor pressures, EMF, table of Pettifor
...
- Phase equilibria, phase diagrams and phase transformations, Their thermodynamic basis, M. Hillert, Cambridge University press, 1998, ISBN 0-521-56584-7
 - Solution thermodynamics, solution models, types and topologies of phase diagrams, ...
 - The approach is slightly different from that in classical textbooks on thermodynamics
 - The SGTE casebook, thermodynamics at work, K. Hack, Materials modelling series, The institute of materials, 1996, ISBN 0-901716-74-X
 - * Examples of applications of the CALPHAD method in alloy development
 - Pearson's handbook
 - * Information on the crystal structure of elementary phases and compounds

Review Articles

- R. Schmidt-Fetzer et al. Assessment techniques, database design and software facilities for thermodynamics and diffusion. CALPHAD:

Comp. Coupl. of Phase Diagrams and Thermochemistry, 2007, 31:38-52.

- P.E.A Turchi et al. Interface between quantum-mechanical-based approaches, experiments, and CALPHAD methodology. CALPHAD: Comp. Coupl. of Phase Diagrams and Thermochemistry, 2007, 31:4-27.
- A. Costa e Silva et al. Applications of computational thermodynamics – the extension from phase equilibria to phase transformations and other properties. CALPHAD: Comp. Coupl. of Phase Diagrams and Thermochemistry, 2007, 31:53-74.
- In-Ho Jung. Overview of the applications of thermodynamic databases to steelmaking processes. CALPHAD: Comp. Coupl. of Phase Diagrams and Thermochemistry, 2010, 34:332-362.

Links

- website CALPHAD organization:
<http://www.calphad.org/>
- website Thermo-Calc:
<http://www.thermocalc.com/>
 - manual, book with examples, description of available databases

- website PANDAT (computer program for the calculation of phase diagrams, mostly for metallic systems):
<http://www.computherm.com/>
- website FactSage (computer program for the calculation of phase diagrams, mostly for oxidic systems):
<http://www.factsage.com/>
- website SGTE consortium:
<http://www.sgte.org/>
- NIST information on Material Thermodynamics:
<http://www.ctcms.nist.gov/kattner/>
- NIST Diffusion Data Center:
<http://patapsco.nist.gov/diffusion/>
- NIST information on diffusion:
<http://www.ctcms.nist.gov/ce-camp/Present.html>