

Some basic references about the CALPHAD approach

i. Sub-lattice model: where it all started

1. Hillert, M. and L.-I. Staffansson, *The regular solution model for stoichiometric phases and ionic melts*. Acta Chemica Scandinavica, 1970. **24**: p. 3618-3626.

ii. Sub-lattice model generalized to multi-component multi-lattice

2. Sundman, B. and J. Agren, *A regular solution model for phases with several components and sublattices, suitable for computer applications*. Journal of Physical Chemistry of Solids, 1981. **42**: p. 297-301.

iii. Sub-lattice applied to the liquid: The "ionic" model

3. Hillert, M., B. Jansson, B. Sundman, and J. Agren, *A two-sublattice model for molten solutions with different tendency for ionization*. Metallurgical Transactions A, 1985. **16A**(February): p. 261-266.

iv. A recent view of the properties of the Compound Energy Model

4. Hillert, M., *Some properties of the compound energy model*. CALPHAD, 1996. **20**(3): p. 333-341.

v. Geometric models (Mugiannu, Koehler, etc.)

5. Ansara, I. *Prediction of thermodynamic properties of mixing and phase diagrams in multi-component systems*. in *Metallurgical Chemistry- Proceedigns of a symposium held at Brunel University and the NPL on 14-16 July 1971*. 1971. London: Her Majesty's Stationery Office.
6. Ansara, I., C. Bernard, L. Kaufman, and P. Spencer, *A comparison of calculated phase equilibria in selected ternary alloy systems using thermodynamic values derived from different models*. CALPHAD, 1978. **2**(1): p. 1-15.
7. Hillert, M., *Empirical methods of predicting and representing thermodynamic properties of ternary solution phases*. CALPHAD, 1980. **4**(1): p. 1-12.
8. Chou, K. and Y.A.Chang, *A study of ternary geometrical models*. Ber.Bunsenges. Phys.Chem., 1989. **93**: p. 735-741.

vi. Basic Thermo-calc

9. Sundman, B., B. Jansson, and J.O. Andersson, *The Thermo-Calc databank system*. CALPHAD, 1985. **9**: p. 153-190.
10. Sundman, B., B. Jansson, and J.-O. Andersson. *Thermo-Calc, a databank for calculation of phase equilibria and phase diagrams*. in *Computer calculation of phase diagrams*. 1986. Orlando: ASM International, Materials Park, OH.

(See also the manual at www.thermocalc.se)

vii. How are equilibria calculated?

11. DeHoff, R.T., *Thermodynamics in Materials Science*. 1993, New York: McGraw-Hill, Inc. 532.
12. Ansara, I., *Comparison of methods for thermodynamic calculation of phase diagrams*. International Metals Reviews, 1979. **24**(1): p. 20-53.

viii. Good summaries are given at the Ringberg Workshops, published in CALPHAD Journal. Examples are:

13. de Fontaine, D., S.G. Fries, G. Inden, P. Miodownik, R. Schmid-Fetzer, and S.L. Chen, *Group 4: Lambda Transitions*, in *Workshop on Thermodynamic models and data for pure elements and other endmembers of solution February 26 to March 3, 1995*. 1995: Schloss Ringberg.
14. Pelton, A.D., M. Blander, M.T. Clavaguera-Mora, M. Hoch, L. Holglund, H.L. Lukas, P. Spencer, and B. Sundman, *Thermodynamic modeling of solutions Group 1-Liquids*. CALPHAD, 1997. **21**(2): p. 155-170.
15. Kattner, U., G. Erickson, P. Spencer, M. Schalin, R. Schmid-Fetzer, B. Sundman, B. Jansson, B. Lee, T. Chart, and A.C.e. Silva, *Group 4 & 5: Process Modeling and applications- 1997 Ringberg Workshop*. CALPHAD, 2000. **24**(1): p. 55-94.
16. Hillert, M., B. Burton, S.K. Saxena, S. Degterov, K.C.H. Kumar, H. Ohtani, F. Aldinger, and A. Kussmaul, *Group 4: Modelling of Oxides- 1996 Ringberg Workshop*. CALPHAD, 1997. **21**(2): p. 247-263.