

THERMODYNAMIC EQUILIBRIUM, THERMOCHEMICAL AND PHASE-EQUILIBRIUM DIAGRAM DATA-BASED RESOURCES

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During this reporting period, additional data-based thermodynamic-equilibrium, equilibrium-composition, thermo-chemistry, and phase-diagram resources were acquired that enhance our capabilities (1) for selecting the most appropriate target material for the efficient production and generation of RIBs; (2) for calculating vapor pressures and critical temperatures of selected target materials; (3) for predicting the chemical forms and thermal distributions of RIB specie carrier-compounds released during diffusion and transport to the ionization chamber of the source; (4) for calculating chemical reactions between gaseous reactants and diffusion release products, deliberately introduced into the source to expedite vapor transport of RIB species to the ion source; (5) and for determining eutectic transformations and phase diagrams of high temperature metals and ceramics. In addition to the existing computer codes of *ThermoCalc*,¹ *DICTRA*,² and *HSC*,³ we have acquired the thermo-chemistry code *ChemSage*⁴ and hard-copy library reference material including the following: *Landolt-Börnstein: Diffusion in Solid Metals and Alloys*,⁵ *Binary Alloy Phase Diagrams, Volumes I-III*,⁶ *Thermochemical Data of Pure Substances, Volumes I and II*,⁷ *Phase Equilibrium Diagrams, CD-ROM Database for Ceramics*,⁸ *Metals Handbook, Desk Edition*,⁹ and *Smithells' Metals Reference Book*.¹⁰

¹ *ThermoCalc* is a thermodynamic-equilibrium chemistry computer program developed by the Royal Institute of Technology, Stockholm, Sweden.

² *DICTRA* is a multi-component diffusion computer code developed by the Royal Institute of Technology, Stockholm, Sweden.

³ *HSC* is thermodynamic-equilibrium chemistry computer program marketed by Outokumpu Research, Oy, Pori, Finland.

⁴ *ChemSage* is a computational thermo-chemistry code marketed by GTT Technologies, Herzogenrath, Germany.

⁵ *Landolt-Börnstein: Diffusion in Solid Metals and Alloys*, Edited by H. Mehrer, Springer-Verlag, Berlin, 1990.

⁶ *Phase Equilibrium Diagrams, CD-ROM Database for Ceramics*, Windows version 3.1, The American Ceramic Society, Westerville, OH, 1993.

⁷ *Binary Alloy Phase Diagrams*, second edition, Volumes I, II, and III, editor-in-chief, Thaddeus B. Massalski, American Society for Metals, International, Publisher, William B. Scott, Jr., 1996.

⁸ *Thermochemical Data of Pure Substances*, third edition, editor I. Barin, Volumes I and II, VCH Publishers, New York, 1995.

⁹ *Metals Handbook, Desk Edition*, edited by, H. E. Boyer and T. L. Gall, American Society for Metals, Metals Park, OH, 1997.

¹⁰ *Smithells' Metals Reference Book*, Seventh Edition, Edited by E. A. Brandes and G. B. Brook, Butterworth-Heinemann, Ltd., Oxford, England, 1992.