C6730 Phase equilibria

1. Basic terms. Thermodynamic functions of pure substance and several component mixtures. Standard state. Phase nomenclature. Gibbs-Duhem equation. Gibbs energy of real system. Excess functions. 2. Phase structures and their crystallography. **Lattice defects.** Thermodynamics of stoichiometry and non-stoichiometry phases and chemical compounds. Conservation laws of mass, charge, and stoichiometry in thermodynamic systems. Phase rule and phase stability. 3. Gibbs energy of system. Chemical potential and activity. **Differential equations of phase equilibrium**, integral equation of phase equilibrium. Phase equilibrium formation. 4. Mathematical solution of phase equilibrium. Calculations and predictions of phase diagrams. Methods, programs and thermodynamic databases for phase equilibrium calculations. CALPHAD approach. 5. Phase diagrams. **Fundamental types of phase diagrams,** visualization, possible phase boundaries, and phase diagram cross-sections. Use of phase diagrams. 6. Experimental methods of phase equilibria study. Gain of phase data and thermodynamic data. Measurements of thermodynamic functions. Thermal analysis (**cooling curves**, DTA, DSC, ...). Data sources and their accuracy. 7. Real phase equilibria. Unary systems, binary systems (coexistence of gas, liquid, and solid phases; mixture of volatile liquids; **distillation; sublimation;** dissolutions). Phase diagrams of several component systems (coexistence of solid phases; **extraction**; purification; chemical compounds inside phase diagram; intermetallics). 8. Examples of phase equilibrium and phase diagram calculations for systems. Relationship between phase, physical, and mechanical properties. 9. Phase transformations. Stable and metastable phase equilibria. **Diffusion-less phase transformations**. Role of diffusion and nucleation at equilibrium establishing. 10. Diffusion. Essentials. Atomic mechanisms of diffusion. Fick's laws of diffusion. Boundary conditions. Analytical and numerical solutions of diffusion equations. 11. Diffusion in real systems. Atomic mobility. Mass fluxes. Kinetic and thermodynamic factors of diffusion. 12. Diffusion controlled phase transformations. Heterogeneous real systems. Diffusion and equilibrium at high and low temperatures. Simulation programs (DICTRA). 13. Phase equilibria and diffusion controlled processes in chemical laboratory and technology. Coarsening and dissolving of phases, optimization of material technology treatment, homogenization, nitriding, weld stability, protective layers, transformation diagrams, ...