Lecture: Thermodynamics - engineering approach
Course I, summer semester.
prof. Rafał KOZUBSKI

The course covers the following topics:

1. Foundations of statistical thermodynamics.
2. Description of atomic configuration in a multicomponent crystalline system: atomic short- and long-range ordering (LRO and SRO), decomposition.
3. Ising model in configurational thermodynamics. Characteristics of necessary approximations.
4. Cluster Variation Method (CVM).
5. Bragg-Williams method as the "zeroth" CVM approximation.
6. Basic conditions controlling the occurrence of atomic ordering and decomposition processes.
7. Chemical ordering: characteristics of "order-disorder" transitions
8. Decomposition: lever rule, miscibility gap, kinetics of spinodal decomposition.
9. Monte Carlo techniques in configurational thermodynamics: simulation of Markov chains as a key for the simulation of equilibrium states and relaxation phenomena.
10. Metropolis-type and "residence time" algorithms for atomic ordering simulation.
11. Monte Carlo simulation of phase equilibria

Questions concerning phase equilibria and structural phase transitions in multicomponent crystalline systems are discussed. The lecture covers both static and kinetic aspects of the phenomena.

Literature:

R.H. Fowler, E.A. Guggenheim "Statistical Thermodynamics" Cambridge 1956
R.E. Smallman "Modern Physical Metallurgy" Butterworths 1985
D. de Fontaine, Solid State Physics, Vol. 34, 73, (1979)
R. Kozubski, "Metody Monte Carlo w badaniach przemian strukturalnych w stopach i związkach międzymetalicznych w skali atomowej", *Inżynieria Materiałowa* Nr 2, **XXX**, 108-117, (2009).