Modeling of Thermo-Physical Properties for Phase Transformations in Metal Systems

John Ågren [C, S]
Materials Science and Engineering/Physical Metallurgy, Royal Institute of Technology (KTH), Stockholm, Sweden
john@kth.se

The performance of materials depend on their internal structure which, in inorganic materials, evolves by means of various phase transformations. In metallurgy phase transformations are analyzed and modelled in terms of their mechanism, driving force and kinetics. The driving force stems from the thermodynamic properties and the kinetics from various transport and interfacial properties. In order to be useful these properties must be accessible for all important conditions under consideration, e.g. composition, temperature etc. It is thus necessary to represent the properties by mathematical models which may be based on of various degree of physical realism, spanning from empirical equations to first-principle calculations. Nevertheless, the computations must be fast enough to allow application to very complex systems. The CALPHAD method, initially developed in the 60s for thermo-chemical properties and calculation of phase diagrams, is a role model for such models and will be briefly discussed. The method was more recently extended to cover also diffusion, viscosity and interfacial properties as well as elastic and mechanical properties. In fact CALPHAD may be regarded as the most efficient way of representing knowledge of very different kind, e.g. experimental, ab-initio calculations and pure guesses. It is an essential part of the materials genome. Some applications to phase transformations in metallic systems will be discussed.