A General Thermodynamic Model for Crystalline Phases in Multicomponent Materials

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Most materials consist of one or more crystalline phases with several different lattice sites. A very simple model developed to handle interstitial solutions of carbon in steels has gradually been extended to handle intermetallic phases like the sigma, mu and Laves phases, phases with order/disorder transformations like A1/L1_2 in multicomponent superalloys and ionic phases like spinels, pyroxenes, etc. It is now known as the Compound Energy Formalism (CEF) as it includes many models as special cases. CEF provides a closed expression for the Gibbs energy of the phase as a function of temperature, pressure and constitution, i.e. depending on the fraction of each constituent in the sublattices. CEF can take into account the full crystalline complexity with different lattice sites which can be occupied by atoms, molecules, ions or vacancies. This means it can handle long range order but as it assumes random mixing on each sublattice the short range order is modelled as an excess parameter. Each combination of one constituent in each sublattice forms an "em end-member" or compound (which is the origin of the name for the formalism). The contribution to the Gibbs energy due to ferromagnetic transition is modelled with a constitution dependent Curie temperature and the Bohr magneton number. In multicomponent systems a phase with several sublattices will have many end-members that are metastable and lacking experimental data the crystalline structure has often been simplified. However, new possibilities to rapidly calculate the stability of metastable compounds using DFT will make this limitation less critical. The great advantage of CEF is its simplicity and flexibility which makes it easy to extend to multicomponent systems and complex phases which is important in the development of new alloys and materials. Examples will be given how CEF is used for large varieties of crystalline phases like interstitial solutions, carbides and nitrides, intermediate phases with large solubility ranges, superalloys and other materials with order/disorder transformations and multicomponent ionic phases like spinels, pyroxenes etc.

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