Thermodynamic Optimization of Alkaline-Earths in Aluminum - Magnesium Alloys

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Abstract

The purpose of this project is to obtain a thermodynamic model for the Mg-Al-**X** systems (**X** is an alkaline-earth). Because of their high creep resistance, these new alloys are very interesting for the car industry. The liquid alloy Gibbs energy is represented by the modified quasichemical model which takes into account the short-range-order amount first-nearest-neighbor atoms according to the following atomic pair reactions :

$$[Al\text{-}Al] + [X\text{-}X] = 2\,[Al\text{-}X] \quad \Delta g_{Al\text{-}X} << 0$$
$$[Mg\text{-}Mg] + [X\text{-}X] = 2\,[Mg\text{-}X] \quad \Delta g_{Mg\text{-}X} << 0$$
$$[Al\text{-}Al] + [Mg\text{-}Mg] = 2\,[Al\text{-}Mg] \quad \Delta g_{Al\text{-}Mg} \approx 0$$

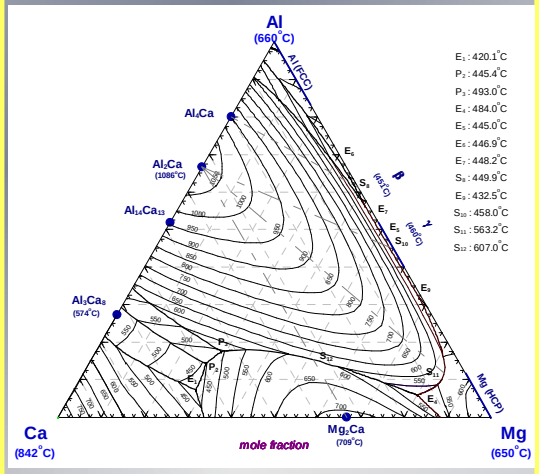
Δg being very negative for these systems (except Al-Mg), the equilibrium is shifted to the right promoting Al-X and Mg-X pairs to the detriment of X-X, Mg-Mg and Al-Al pairs. This short-range-order tendency can be seen by the « **V-shape** » of the mixing enthalpy curves and by the « **m-shape** » of the mixing entropy curves. The thermodynamic model can be summarized by a Gibbs energy formulation for example for the ternary Mg-Al-Sr, which contains the values of Δg_{AlMg}, Δg_{AlSr} and Δg_{MgSr} :

$$G = n_{Al} g^{o,L}{}_{Al} + n_{Mg} g^{o,L}{}_{Mg} + n_{Sr} g^{o,L}{}_{Sr} - T\Delta s^{config} + \tfrac{1}{2} n_{AlMg} \Delta g_{AlMg} + \tfrac{1}{2} n_{AlSr} \Delta g_{AlSr} + \tfrac{1}{2} n_{MgSr} \Delta g_{MgSr}$$

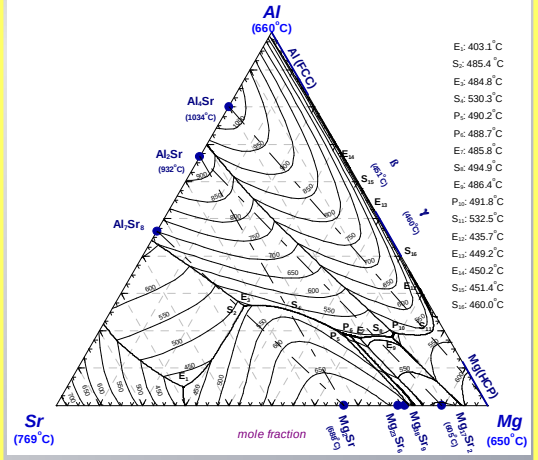
where T is the temperature (K), n_i the number of moles of the *i* element, n_{ij} the number of moles of *i-j* nearest-neighbors pairs and Δs^{config} the configuration quasichemical entropy. The equilibrium amount of the different pairs is obtained by Gibbs energy minimization at constant T and P with respect with the elemental mass balances (which involve coordination numbers relating amounts of pairs to amounts of elements). To better represent the compositional variations of the thermodynamic properties and the phase equilibria, the values of Δg_{ij} are expressed as T and n_{ij} functions. The parameters of these functions are obtained by optimization of the experimental data found in literature: ΔH^{mix}, ΔH^{form}, C_p, activity of components, partial pressures, and liquidus temperatures are related to derivatives of the Gibbs energy functions for the phases. Model parameters are stored in databases as part of the ***FactSage*** software. Finally, it is possible to simulate industrial process relative to those new Al-Mg-Ca-Sr-Ba alloys as for example treatment of liquid metal and Scheil cooling. Thermodynamic properties (melting points, eutectic, conditions of stability of phases, density, surface tension, etc.) can also be calculated from the results of the present optimizations.

Calculated Liquidus Surfaces

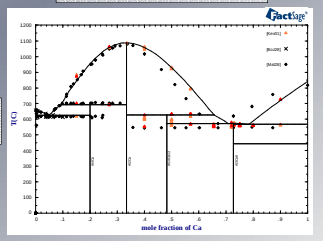
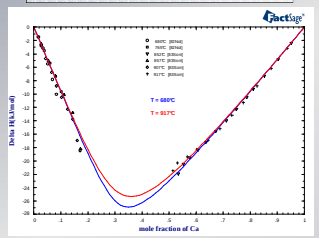
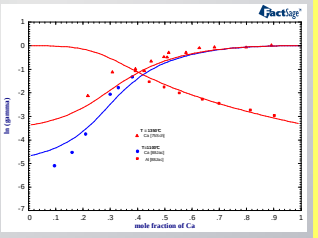
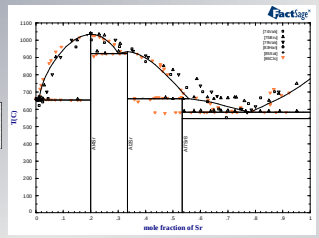
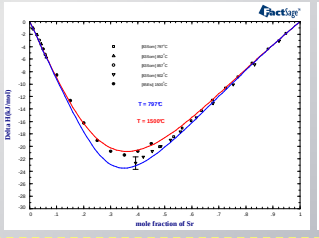
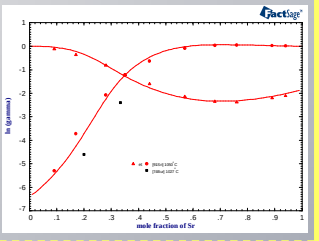
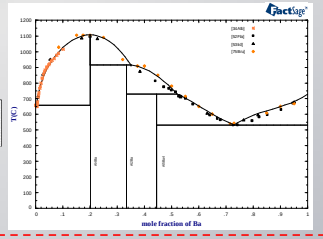
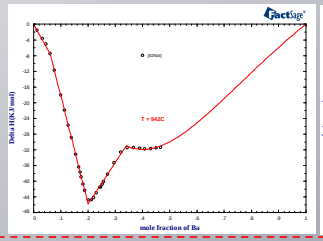
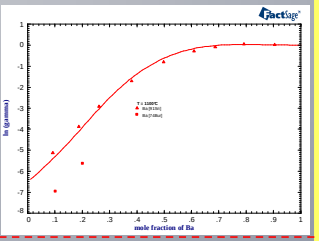
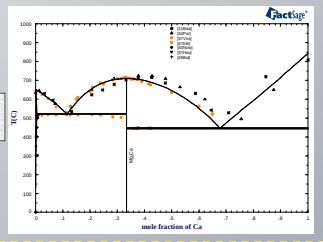
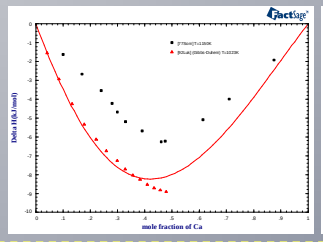
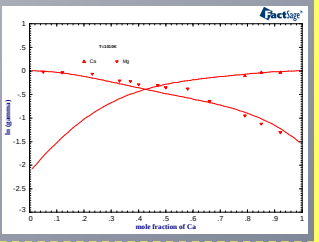
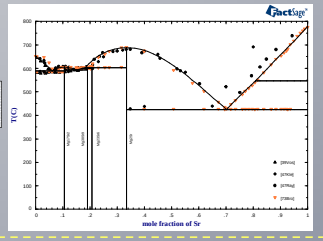
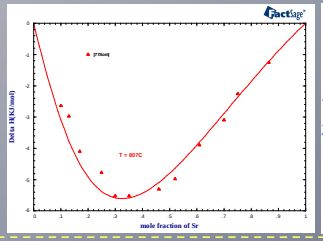
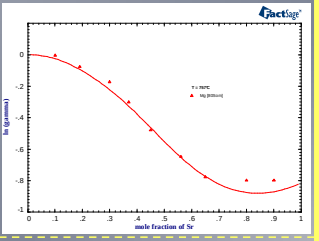
Al-Mg-Ca



Al-Mg-Sr



Binary Systems

	Calculated Phase Diagrams	Calculated Mixing Enthalpy (ΔHmix)	Calculated Activity Coefficient (γ)
Al-Ca			
Al-Sr			
Al-Ba			
Mg-Ca			
Mg-Sr			
Mg-Ba