Dr. Patrice Chartrand  
Department of Chemical Engineering, Ecole Polytechnique, Montreal, Canada

A Thermodynamic and Phase Equilibrium Database for Mg-Alloys

Over the last 10 years, a large thermodynamic and phase equilibrium database for Mg-alloys has been developed at the Centre for Research in Computational Thermodynamics of the Department of Chemical Engineering of Ecole Polytechnique in Montreal. The project is supported by General Motors of Canada, Alcoa, Rio Tinto Alcan and Hydro Aluminium, together with the National Sciences and Engineering Research Council of Canada. The CALPHAD (CALculation of PHAse Diagrams) technique is used to calibrate thermodynamic models (Compound Energy Formalism and Quasichemical Model in the Pair Approximation). The content of the database will be presented, in parallel with evaluation from other research groups. Strengths and weaknesses of the models will be discussed, specifically in the view of partial properties and activity coefficients, often used for diffusion calculations. Calculation tools were developed, within the FactSage Thermochemical Package, to quickly estimate the microstructure of solidified alloys after short annealing time.

For more information contact Dr. Steffen Brinckmann, steffen.brinckmann@rub.de