



Invited Talk, Tuesday, May 7, 11:20 a.m. - 12:00, ICAMS² session: T2

Thermodynamic assessment and modelling of ternary Ti–Al systems

Damian Cupid¹, Mario Kriegel², Michele Manuel³, Hans J. Seifert¹

¹Karlsruhe Institute of Technology, Institute for Applied Materials (IAM-AWP), Karlsruhe, Germany

²Technical University of Freiberg, Institute of Materials Science, Freiberg (Saxony) Germany

³University of Florida, Department of Materials Science and Engineering, Gainesville, FL, USA

Titanium aluminides alloyed with Cr, Mo and Nb, respectively, are promising materials for high temperature turbine applications. In comparison to non-alloyed titanium aluminides they show improved high temperature oxidation resistance and good processability. The computer calculations of phase diagrams with consistent thermodynamic databases (CALPHAD approach) can be efficiently used to support such advanced Ti-Al-base alloy development. Additionally, the thermodynamic data are key input for kinetic sharp interface and phase field simulations in ternary systems.

Thermodynamic descriptions for Ti–Al–X ternary systems (X: Cr, Mo, Nb) were developed by thermodynamic assessment and optimization. Experimental data from this work as well as literature data on thermodynamics and phase equilibria were used. Based on this information, analytical descriptions for the Gibbs energies for all stoichiometric and solid solution phases were delivered.

Sublattice models described in the Compound Energy Formalism were applied. In all modeling cases the crystal structures and species site occupancies of the related Wyckoff-positions in dependence on alloy compositions and temperature were taken into account. The methods of thermodynamic dataset development will be presented. The calculated thermodynamic results are shown, e.g. by isothermal sections, isopleths, phase fraction diagrams, and chemical potential diagrams. Additionally, all thermodynamic functions in the ternary system can be calculated. Key thermodynamic experiments were defined and carried out to refine the datasets and confirm calculated results.