

Specification for computational thermodynamic material software and databases

NASA LaRC is seeking software and database applications for computational thermodynamic material modeling. The software required:

- Software for thermodynamic and phase diagram calculation for multi-component systems
- Software for detailed simulation of diffusion controlled phase transformations for multi-component alloys
- Aluminum alloy thermodynamic database
- Titanium alloy thermodynamic database
- Aluminum alloy mobility database

The software is required to:

- be based on the CALPHAD method
- be capable of calculations of:
 - phase diagrams for multi-component multi-phase systems
 - stable and meta-stable phase equilibria
 - amounts of phases and their compositions
 - thermochemical data such as enthalpies, heat capacity and activities
 - driving forces and transformation temperatures
 - liquidus and solidus temperatures
 - solidification simulations with the Scheil-Gulliver model
- have available databases in ferrous, magnesium, and nickel alloys
- run on a standard desktop PC with Windows operating system.