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CompuTherm Newsletter

February 26, 2018

New Release of Pandat™ Software and Databases Version 2018

CompuTherm is pleased to announce the new release of the Pandat™ software and databases version 2018. A new module, PanDiffusion module, is released. A number of new features were implemented and improvements were made for the PanPhaseDiagram, PanPrecipitation, and PanOptimizer modules in Pandat™ 2018. This newsletter will provide you a quick glance of the highlights. Further details can be found in the User's Guides of Pandat™ software and Thermodynamic Databases version 2018 at our website www.computherm.com.

New Features and Improvements of Pandat™ 2018

PanDiffusion Module – This is a module of Pandat™ software designed to simulate elemental diffusion under a variety of conditions. It is seamlessly integrated with the user-friendly Pandat™ Graphical User Interface (GUI) as well as thermodynamic calculation engine, PanEngine. This module can be used to simulate time evolution of composition profile, phase volume fraction and phase composition of diffusion couples. Variety of thermal history, boundary condition and geometry can be defined. Figure 1 shows an example diffusion simulation between multi-component nickel based superalloys: IN100 and Alloy 718 at 1150°C for 1000 hours. Figure 2 shows an example simulation of a sandwich diffusion couples for the Cr-Fe-Ni system at 1100°C for 1 hour.

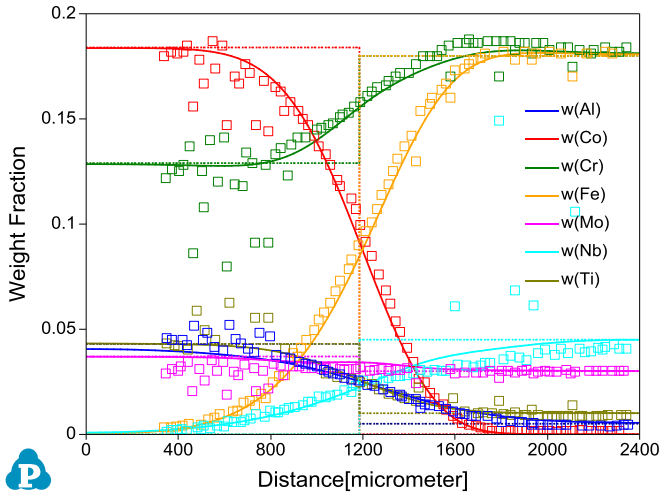

Figure 1: Diffusion between IN100 and Alloy 718 at 1150°C for 1000 hours, experimental data are from Campbell et al., Materials Science and Engineering, A 407 (2005), 135-146.

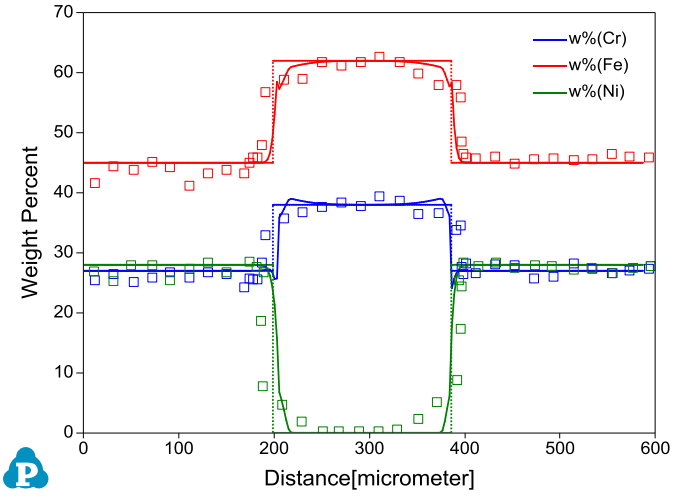

Figure 2: Diffusion of a sandwich diffusion couples for the Cr-Fe-Ni system at 1100°C for 1 hour, experimental data are from Kajihara et al., Acta Metall. Mater., 41(7) (1993), 2045-2059.

New Features of Pandat GUI and PanPhaseDiagram, PanPrecipitation, and PanOptimizer Modules

- Improved Pandat workspace style with saving/loading layout functions;
- Improved graph functions for adding symbols, sub/superscript in graph title and component labels;
- Tooltip function for graphs generated from any table with the "Label" column, such as the default graph from a solidification simulation;
- Faster loading speed for huge Pandat tables;
- New properties including partial molar enthalpy and entropy, ideal and excess Gibbs free energy, enthalpy and entropy of a solution phase;
- Pseudo binary section in a ternary system;
- Loop calculation for Point calculation at various compositions, temperatures, and pressures, and Solidification simulation at multiple compositions;
- Improved PanEngine reliability including numerical derivative, liquidus projection with extreme small amount of a component, extensive search;
- Reciprocal model for phases described by a two-sublattice CEF;
- More reliable PanOptimizer;
- Enhanced HTC functions and new functions for running HTC precipitation simulations in console mode. The console mode allows users to run Pandat with a batch file without opening Pandat GUI;
- Faster and more reliable PanPrecipitation module which increases the calculation speed of multi-component alloys by ~5 times.

Databases – Improvements are available for the existing databases, such as PanAl, PanCo, PanFe, PanMg, PanMo, PanNb, PanNi, PanTi and PanNoble. The PanHEA database for high entropy alloys is significantly enhanced. A 16 components TiAl-based thermodynamic database, PanTiAl, is released. Figures 3 and 4 are examples of database validation of TiAl-based alloys.

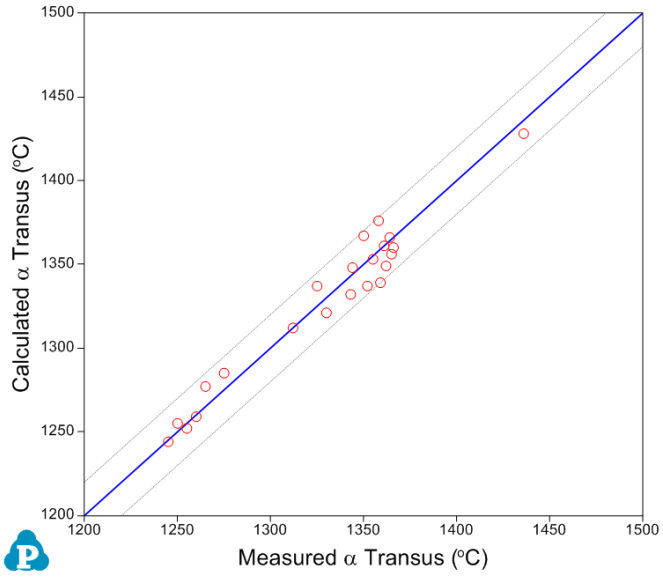

Figure 3: Comparison between calculated and measured α transus temperatures

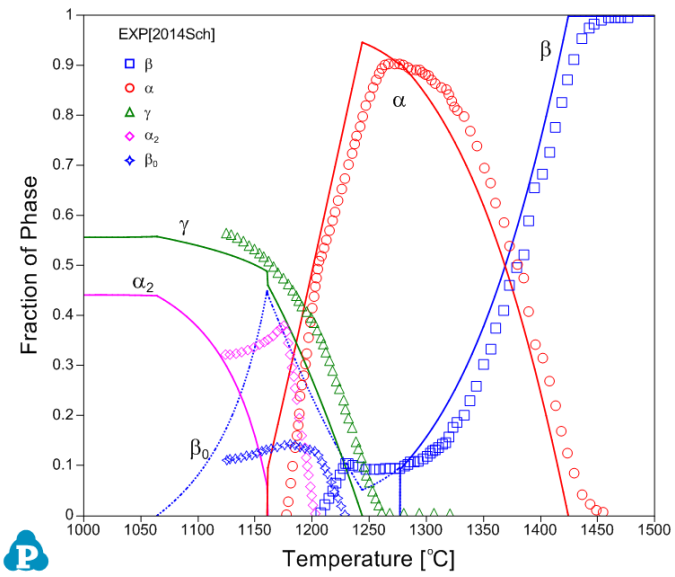

Figure 4: Comparison of calculated and measured phase fractions for alloy Ti-43Al-4Nb-1Mo-0.1B (at.%)