

CompuTherm Newsletter

December 28, 2016

New Release of Pandat™ Software and Databases Version 2017

CompuTherm is pleased to announce the new release of the Pandat™ software and databases version 2017. We improved most of the functions and implemented a number of new features in Pandat™ 2017. 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 2017 at our website www.computherm.com.

New Features and Improvements of Pandat™ 2017

High Throughput Calculation (HTC) – the purpose of high-throughput calculation is to perform thousands of calculations in the user defined composition space by one simple setting. Alloy compositions that satisfy user defined criteria can then be searched through data mining of the thousands of simulated results. This function allows a user to develop alloys with certain properties through design. The process is mostly automated by the following steps: (1) user sets the composition space and calculation steps, Pandat then generates batch files automatically to perform all the calculations; (2) user sets the criteria of the properties, Pandat then searches all the alloy compositions that satisfy the criteria through data mining from the calculated results. The searched results can be listed in a table or presented as a color map. Figure 1 shows the solidification range in the Al-Mg-Zn system with varying compositions of Mg and Zn. The left figure is calculated by Lever Rule and the right figure by Scheil model.

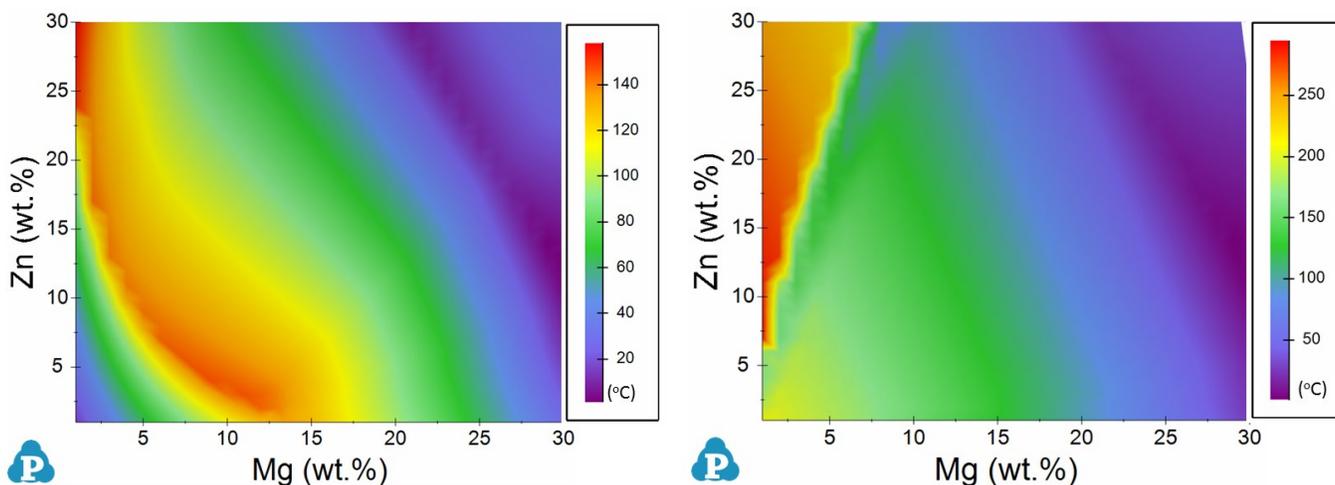


Figure 1: A color map of the calculated solidification range in the Al-Mg-Zn system with varying composition of Mg and Zn. The left figure is by Level Rule, and the right figure by Scheil model

Colormap 3D Diagram – when a property is a function of three variables, it sometimes must be plotted in a 3D space. Pandat™ 2017 can plot any property varying in the three dimensional space as a 3D color map. Figure 2 shows an example of the 3D plot for the liquidus projection of the Al-Mg-Zn system. With the color bar, users can immediately tell the approximate liquidus temperature at a composition and the composition regime with the highest liquidus or lowest liquidus temperature.

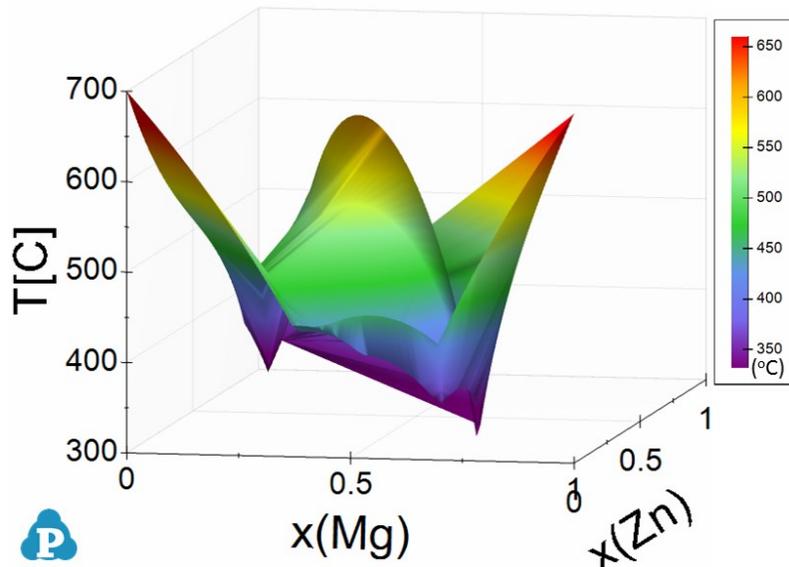


Figure 2: 3D plot for the liquidus projection of the Al-Mg-Zn system

Console Mode – In addition to the GUI mode, Pandat™ 2017 can run in the console mode. The console mode allows users to run Pandat with a batch file without opening Pandat GUI. It is designed for users who want to integrate Pandat calculations (i.e., a line calculation or precipitation simulation) with a third party software (example: iSight) for numerous times. Detailed instruction can be found in Pandat™ 2017 User Guide.

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 TiAl-based thermodynamic database, PanTiAl, is newly released. Figures 3 and 4 are examples of database validation, which compare the calculated and measured liquidus, solidus and γ' solvus for Ni and Co alloys.

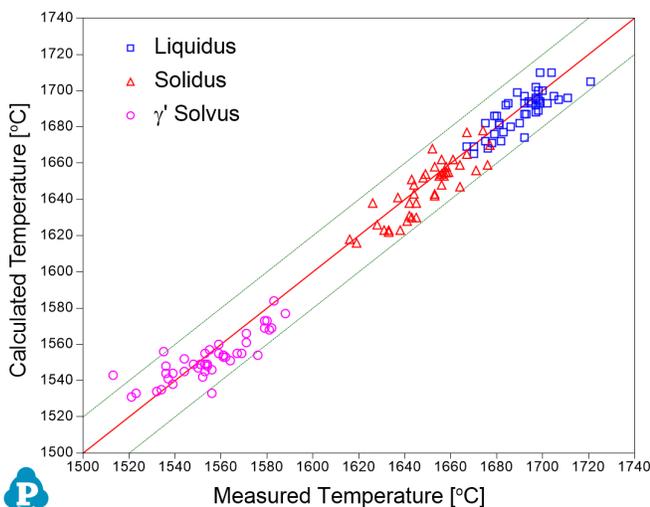


Figure 3: Validation of PanNi2017

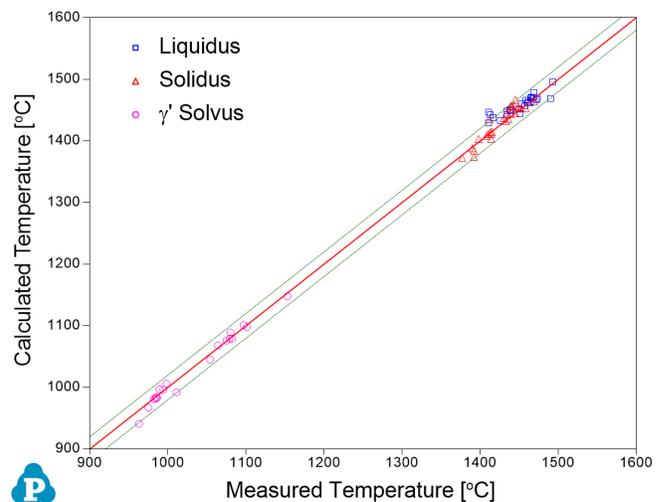


Figure 4: Validation of PanCo2017