New Release of Pandat™ Software and Databases Version 2019

CompuTherm is pleased to announce the new release of the Pandat™ software and databases version 2019. Many new features have been implemented and improvements have been made for the PanPhaseDiagram, PanPrecipitation, PanDiffusion and PanOptimizer modules in Pandat™ 2019. 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 2019 at our website www.computherm.com.

New Features of PanPhaseDiagram Module

- **Append database:** User can append a custom-made database (tdb) to an original database (either tdb or pdb). This allows user to modify/replace the model parameters, add new parameters, or add new phases to the original database. More importantly it allows user to calculate any property of interest by defining the property models and model parameters in the custom-made database (tdb). The user defined property can be a function of any thermodynamic properties that can be obtained from the original thermodynamic database. Figures 1-3 show the calculated T₀ curve, lattice parameter, and thermoconductivity using this function.

- **Local equilibrium calculation:** User can calculate local equilibrium by considering coexisting phases having the same chemical potential of every component. A local equilibrium could be stable, metastable or unstable. Figure 4 shows an example calculation of local equilibrium in Al-Zn system.
New Features of PanPrecipitation Module

- **Interfacial energy estimation:** A model based on the generalized broken bond (GBB) method has been implemented to estimate interfacial energy between matrix and precipitate phases. User can now choose to use the instant estimated interfacial energy during particle evolution instead of giving a constant value.

- **Models for heterogeneous nucleation:** Theoretical models have been implemented to consider heterogeneous nucleation at grain boundary/edge/corner or at dislocations. Figure 5 shows an example calculation of carbides precipitation in steel alloys considering heterogeneous nucleation at various locations.

- **Evolution of aspect ratio:** A new model has been implemented to simulate the evolution of aspect ratio due to direction dependent interfacial energy and anisotropic misfit strain energy. The effect of shape factor is taken into account for previously developed growth models. Figures 6-7 show an example calculation for AZ91 with shape evolution during the precipitation process.

- **Strength model:** Strength model has been developed for nickel-based alloys considering particles with multiple particle size groups with weak/strong pair coupling or bowing mechanisms. Figure 8 shows an example of calculated critical resolved shear stress for a nickel alloy Nimonic 105.

- **Input and output:** New features for input and output are available to allow user's input of initial particle size distribution (PSD) for precipitation simulation and output of PSD at user pre-defined times.
New Features of PanDiffusion Module

- **Carbonization simulation:** Users can now simulate carbonization under three types of boundary conditions: fixed carbon composition, assigned environmental carbon activity, and customized carbon flux at boundary. Figure 9 shows an example calculation for the case of given carbon activity.

- **Particle dissolution:** A new feature has been developed to simulate particle dissolution. Figure 10 shows an example of $\gamma'$ dissolution in Ni-Al binary system. Figure 11 compares the simulated and experimentally determined dissolution of Si particle in Al-Si binary system.

- **Phase transformation:** A new function has been developed to simulate phase transformation and interface movement between a stable phase and a metastable phase. Figure 12 shows an example calculation of $\gamma$ transformed to $\alpha$ in Fe-Si-C system.

- **Geometry:** More geometry features can be considered including planar, cylinder, sphere, tube, and shell.

Other New Features of Pandat 2019

- **Memory management:** Memory management is enhanced to allow large number of calculations via batch calculation or high throughput calculation (HTC).

- **HTC loading of compositions:** HTC function is improved to allow efficient loading of imported alloy compositions and composition range setting for the balanced component.

- **Export of tables:** A new function is developed to allow export of all tables for the selected projects.

- **PanOptimizer:** A new function is developed to automatically plot experimental data on the calculated diagram for PanOptimizer.

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New Feature of Databases

- **Thermodynamic and mobility databases**: Improvements have been made for the existing thermodynamic and mobility databases, such as PanAl, PanCo, PanFe, PanHEA, PanMg, PanMo, PanNb, PanNi, PanTi and PanNoble.

- **Database for titanium alloys**: PanTiAl database has been combined with PanTi database. The PanTi2019 thermodynamic database can now be used to simulate both Ti-rich alloys and TiAl-based alloys.

- **Database for steel alloys**: Significant improvement has been made for PanFe thermodynamic database. Figures 13-14 show two examples.

- **Molar volume databases**: Molar volume databases have been developed for PanAl, PanCo, PanFe, PanHEA, PanMg, PanMo, PanNb, PanNi, PanTi, and MDTCu. Figures 15-18 show some examples.

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