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CompuTherm Newsletter

February 24, 2023

New Release of Pandat™ Software and Databases Version 2023

CompuTherm is pleased to announce the new release of Pandat™ software and databases version 2023. The newly released PanEvolution module, which is extended from previous PanPrecipitation module, enables concurrent simulation of dislocation density, recrystallization, grain growth and coarsening, and precipitation. A new PanPhaseField plugin (PPF-SolidificationCA) is released for solidification simulation using Cellular Automata method. A number of new features and improvements were also implemented in the PanPhaseDiagram and PanDiffusion modules, as well as in the PanPhaseField SDK. This newsletter provides you a quick glance of the highlights. Further details can be found in the User's Guide of Pandat software and Database Manuals version 2023 at our website www.computherm.com

New Features and Enhancements of Pandat™ 2023

PanEvolution Module – The PanEvolution module enables concurrent simulation of dislocation density, recrystallization, grain growth and coarsening, and precipitation. One of the unique features is the plug-in function that provides users with the flexibility to implement user-defined models for recrystallization and grain growth and coarsening simulation.

Figure 1 shows the experimentally measured and predicted flow stress curves for a Ni-based superalloy (52.82Ni–18.96Cr–5.23Nb–3.01Mo–1.00Ti–0.59Al–0.01Co–0.03C–Fe in wt%) at the deformation temperature 1253K and four strain rates (1, 0.1, 0.01, and 0.001s^{-1}) with the initial grain size (75 μm). This alloy has been previously investigated by Lin [2016Lin]. In general, the predicted true stresses well agree with the measured data (symbols). In the early stage of the deformation process, the flow stress increases due to the work hardening effect and then decreases due to dynamic recovery and recrystallization behavior. Eventually, it reaches a steady state if the dynamic recrystallization process is completed under certain conditions.

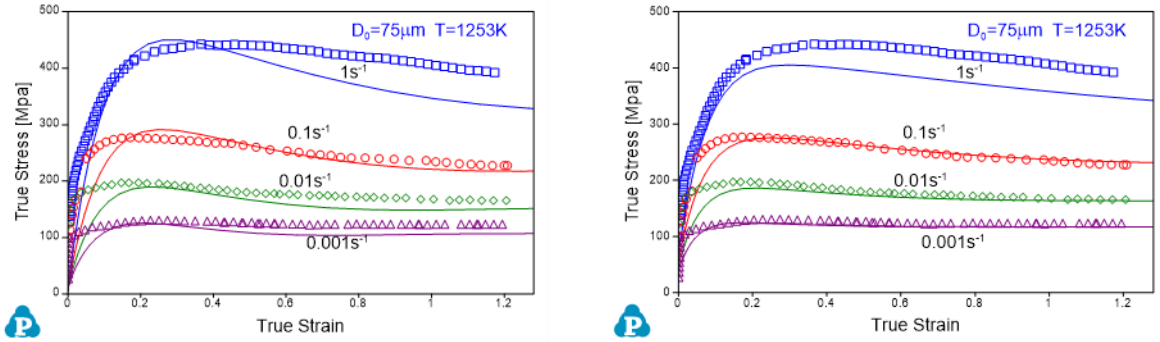

Figure 1: Predicted (lines) and experimentally determined (symbols) true stresses at the deformation temperature 1253 K with the initial grain size of 75 μm using the JMAK model (left) and the Fast-acting physical model (right)

[2016Lin]: Lin, Y. C. et. al., Applied Physics A: Materials Science & Processing, vol. 122, no. 9, 2016.

Main features of the PanEvolution module

Convenient model replacement: PanEvolution allows users to simulate dislocation density, recrystallization, grain growth and coarsening, and precipitation using the built-in models or replacing them with other models. This design enables users to simply type in their user-defined models in the kinetic parameter database file (kdb) without the need of going through the complicated programming/compiling process.

Friendly graphical user interface: A graphical user interface (kdb editor), which allows users to easily create a new kdb or edit an existing kdb, was developed as shown in Figure 2. From the interface, a user can choose to use the recommended kinetic parameters to perform the simulations, modify certain parameters, and save the parameters into a kdb file. The saved kinetic parameters can be easily loaded back for future simulations. As listed in the dialog, we have developed several sets of kinetic parameters for some pre-defined alloys from various groups. One can load a kdb file from the list and apply the kinetic parameters directly to an alloy with similar composition, or edit these parameters to develop a kdb for a new alloy.

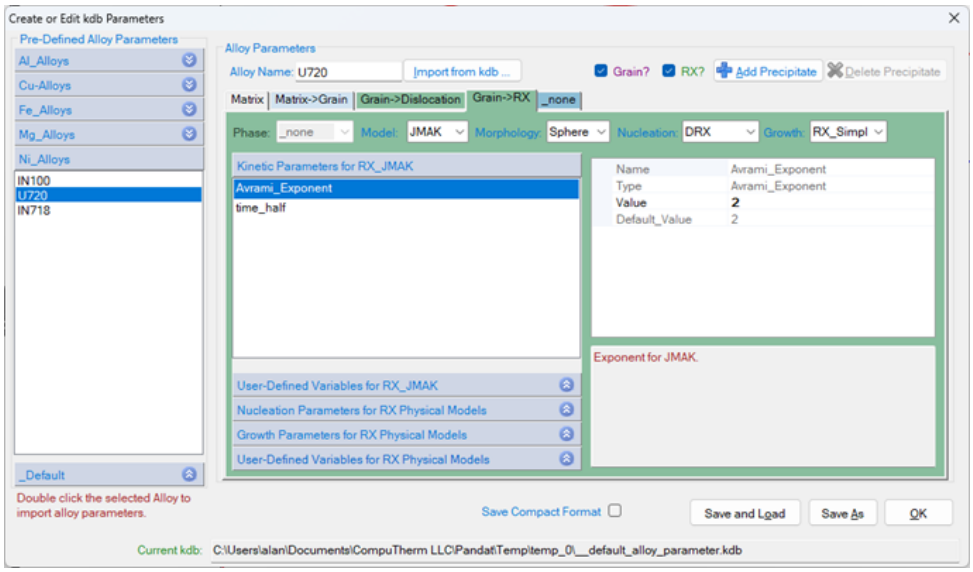

Figure 2: Dialog to create or edit kdb parameters

PanPhaseDiagram Module – Improvements were made for calculating stability diagram, pseudo binary phase diagram, phase equilibria involving phases described by ionic model. Magnetic properties (G, H, and S) are now available from the result table. Gibbs energy Hessian and its eigenvalues and eigenvectors are also available. In addition, extra Gibbs energy can be appended to a phase. Examples are shown in Figures 3 and 4.

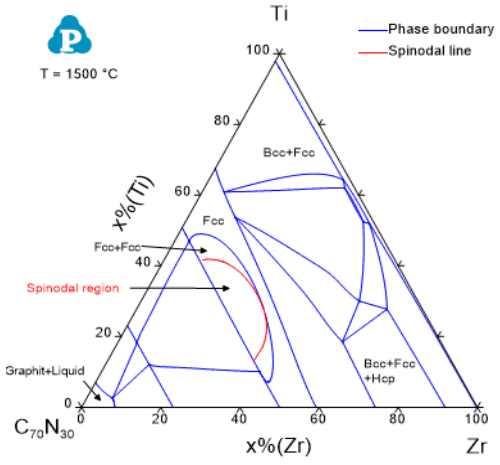

Figure 3: Isothermal section of $C_{70}N_{30}$-Zr-Ti system together with the spinodal line calculated from the eigenvalue of Hessian matrix

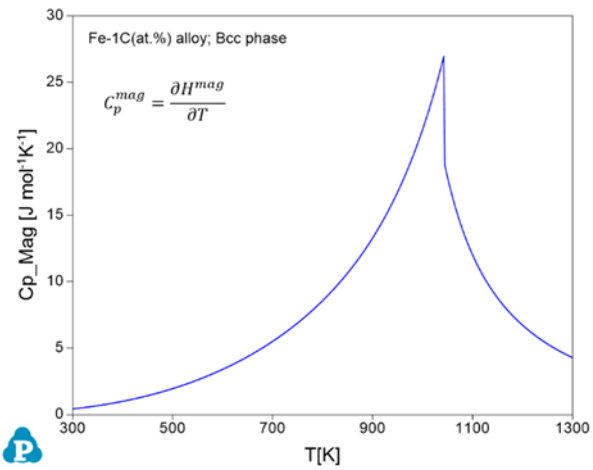

Figure 4: Calculated magnetic contribution for the magnetic specific heat

PanPhaseField Module – A new PanPhaseField plugin (PPF-SolidificationCA) is released for solidification simulation using Cellular Automata method. It can simulate grain growth in Fcc and Bcc alloys during solidification. Given the alloy composition, PPF-SolidificationCA computes grain growth velocity as a function of the local temperature (Figure 5(a)). The grain growth from single nucleation can be simulated, as shown in Figure 5(b), where the <100> crystal directions are the preferred growth directions to form the octahedron shape. User can define the temperature field and nucleation density on the surfaces and the interior of the calculation domain, and the grain growth is initiated upon the temperature dropping below the liquidus temperature. The current capabilities resolve the critical grain growth kinetics, such as the epitaxial growth, the competition and coarsening of columnar grains, and the columnar-to-equiaxed transition. Simulations on the solidification scenarios of welding, directional solidification, and casting are shown in Figures 5(c) – 5(e).

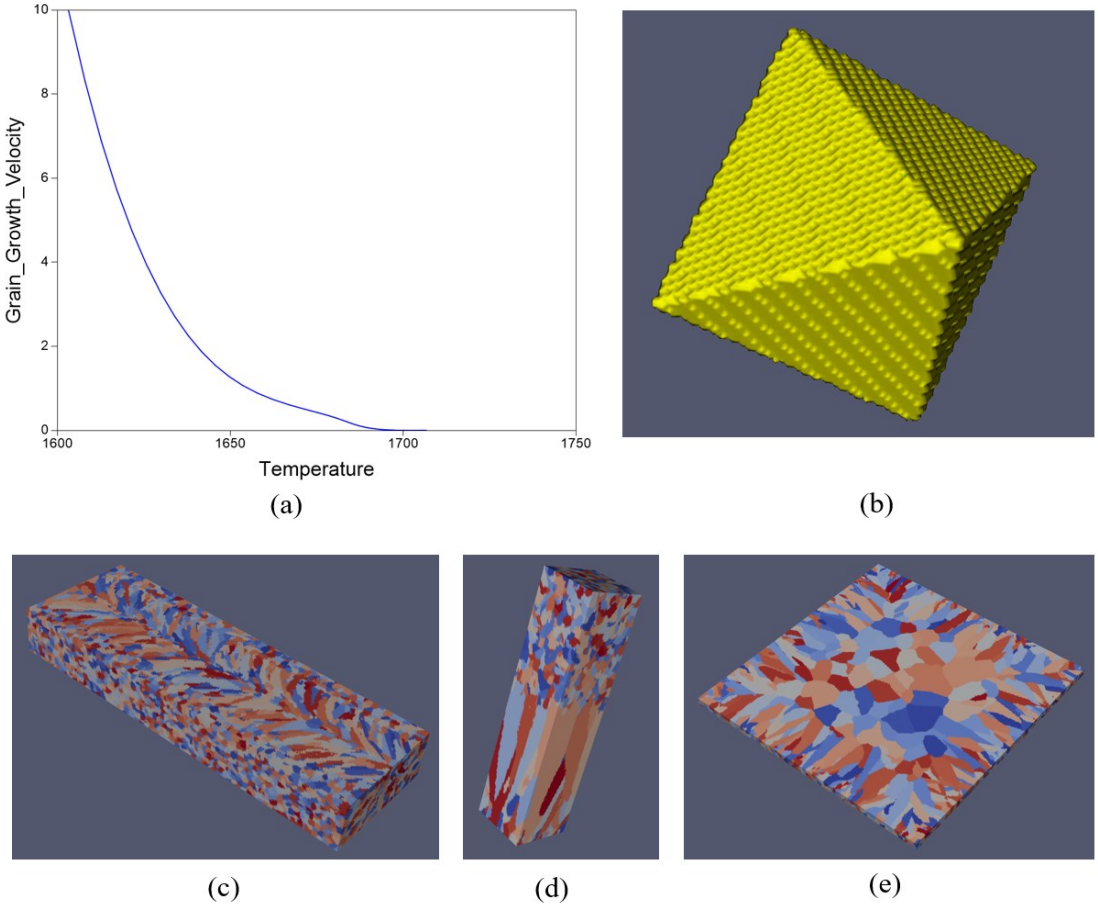

Figure 5: Functionalities of PPF-SolidificationCA plugin. (a) Grain growth velocity computation. (b) Single grain growth. (c) Welding. (d) Directional solidification. (e) Casting.

New features Developed in PanPhaseField SDK

- A function to create the time moments of printing VTK files and output custom properties in the result table.
- Support for user-defined variables and custom parameters for each individual phase in the pfdb.
- A function to obtain extended thermodynamic properties such as thermodynamic factor, liquidus slope, and latent heat.
- An API function to modify the step-size of PanDataNet.
- A USER_PFM_SPINODAL_ADVANCED plugin, an extension of the USER_PFM_SPINODAL, provides more options for customizing simulations. It has the ability to specify the maximum atomic mobility and to print custom fields like chemical potential and Laplacian.

PanDiffusion Module – Major improvement was made in the moving boundary model which now allows the simulation of solid-liquid diffusion couple. Other improvements include an option to specify the number of profile outputs and more options for users to calculate effective mobility. An example of using the moving boundary model on the solid-liquid diffusion couple is given below.

Hot-dip galvanization is an efficient coating method to prevent electrochemical corrosion on steel surface. When hot steel is dipped in liquid Zn, the diffusion of Zn into steel creates a tightly bonded alloy coating. This process can now be simulated with PanDiffusion. The model system Fe-Zn for hot-dip galvanization is simulated with PanDiffusion using the moving boundary model as shown in Figure 6. The figure shows the simulated diffusion couple between Zn and Fe at temperature above 800°C where Zn is in liquid state and Fe is in solid state. The simulated concentration profiles of Zn within Fe agree well with the experimental measurements at various temperatures.

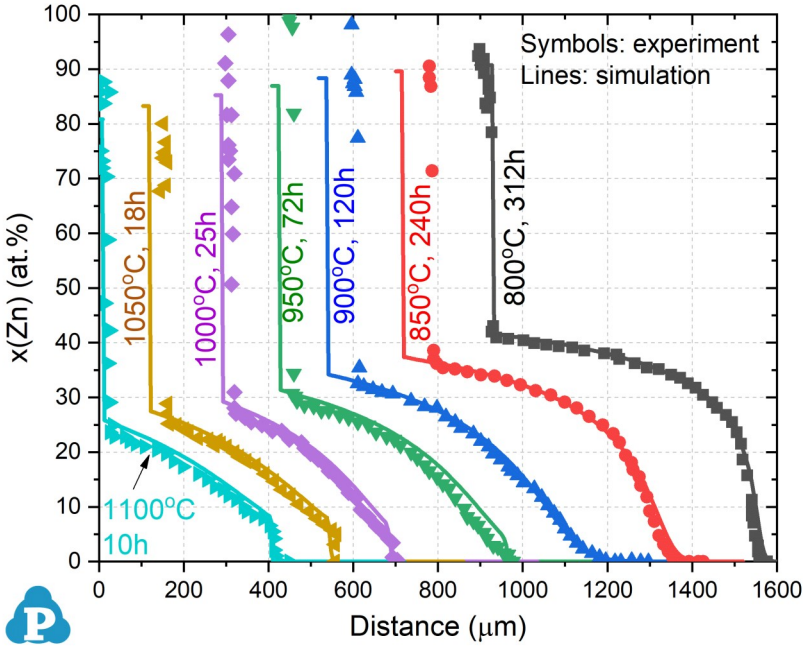

Figure 6: Simulated Fe-Zn diffusion couple using the moving boundary model. Experimental data are from [2020Zhu]

[2020Zhu]: Zhu, Lilong et., al., *Materials & Design* 188 (2020): 108437.

New Features and Enhancements of Other Pandat Software Modules

PanOptimizer Module

- Improved functions for optimization of user-defined properties and phase equilibria for entered phases
- Bug fixed for updating optimization parameters when the same tdb is modified and reloaded.

Pandat GUI

- Bug fixed for properly showing Pandat table and property window after certain operations in GUI.
- An improved feature for the legend of contour diagrams in VTK graphs.
- A feature to automatically generate tables and line graphs when creating a result node for phase field simulation.
- A new feature to load conditions from existing calculations in the workspace.

PanPython SDK

- An updated API function for running all types of calculations provided by Pandat.
- New capability of HTC for the following calculation types: solidification, line, grain growth, grain evolution, and microstructure.
- Parallel calculations of batch files listed in a folder or in a *.pbl file.
- Data mining of targeted properties after HTC calculations, such as liquidus, solidus, and phase amounts.
- New capability for optimization of kinetic parameters for PanEvolution simulations.

Databases Development

- A new database for zinc-rich alloys, PanZn, is released. This database includes 13 components and 281 phases. Complete thermodynamic descriptions for 74 constituent binaries and 32 ternaries were developed for this database. This database was validated by published phase equilibrium data of a number of zinc alloys. In addition to the thermodynamic database, mobility database and molar volume database were also released for this alloy system.
- Improvements were made for the existing thermodynamic databases, mobility databases and molar volume databases: PanAl, PanCo, PanFe, PanMg, PanMo, PanNb, PanNi, PanTi, PanTiAl, PanNoble, PanHEA, and PanRHEA. A mobility database can be integrated with the corresponding thermodynamic database of an alloy system to simulate a variety of diffusion-controlled processes, such as precipitation, diffusion and solidification processes. A molar volume database can be integrated with the corresponding thermodynamic database of an alloy system to simulate volume and density related properties.
- New thermophysical property databases for viscosity and surface tension of the liquid phase are released, which can be integrated with the corresponding thermodynamic database of an alloy system to simulate viscosity and surface tension. Example calculations are shown in Figure 7 for aluminum alloys, one on viscosity and the other surface tension.

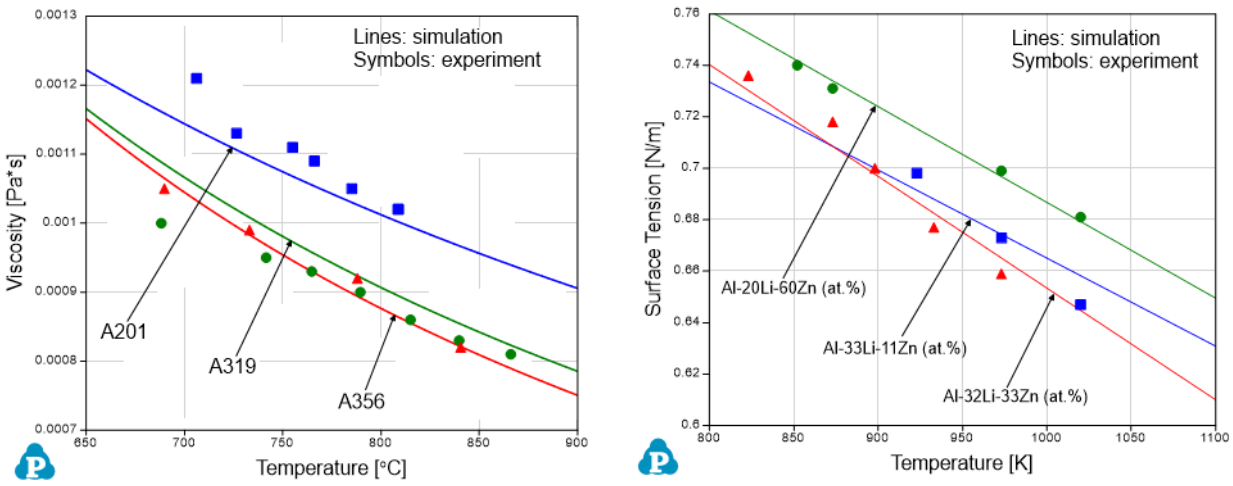

Figure 7: Calculated thermophysical properties of aluminum alloys

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