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CompuTherm Newsletter

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New Release of Pandat™ Software and Databases Version 2024

CompuTherm is pleased to announce the new release of Pandat™ software and databases version 2024. New features and functionalities have been developed and implemented in the PanPhaseDiagram and PanEvolution modules. A new PanPhaseField plugin (USER_TI_ALLOYS) has been developed for the simulation of microstructural evolution of multi-component titanium alloys. A new functionality, PyOptimizer, has been implemented in PanPython SDK for optimizing various types of parameters. Thermodynamic databases and mobility databases were enhanced and thermophysical property databases were released for every alloy system. This newsletter provides you with a quick glance of the highlights. Further details can be found in the User's Guide of Pandat software and Database Manuals version 2024 at our website www.computherm.com.

New Features and Enhancements of Pandat™ 2024

PanPhaseDiagram Module – Overall performance has improved for various types of calculations. New functionalities include:

- Molar volume model, $V_m = V_0 e^{V_A}$ with the parameters of V_0 and V_A , was implemented
- Martensite and Bainite transformation temperatures can be calculated for steel alloys
- Four-sublattice permutation models for Fcc and Bcc were implemented
- Effective Bond Energy Formalism (EBEF) was implemented

Figure 1(a) shows the calculated transformation temperatures for the lath and plate types of martensite in the Fe-Ni binary system, which agree with the experimental data well. Figure 1(b) shows a comparison of the calculated and measured martensite transformation temperatures for a large number of steel alloys. For majority of the alloys, reasonable agreement is obtained.

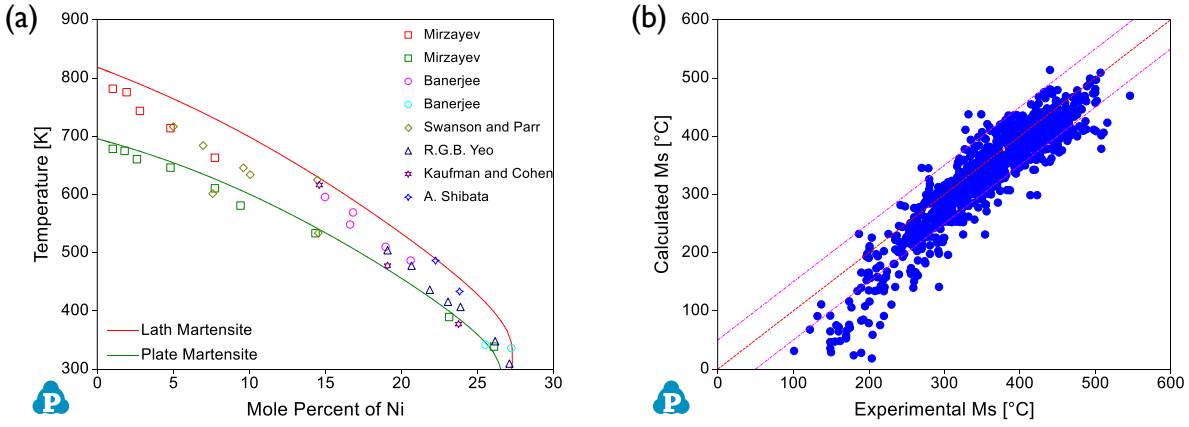

Figure 1:(a) calculated martensite transformation temperature in the Fe-Ni binary system with experimental data.
(b) comparison of calculated and measured martensite transformation temperatures for steel alloys.

PanEvolution Module – Two new functionalities were developed, one for the low/ambient temperature flow stress curve, and the other CCT curve.

The PanEvolution/PanPrecipitation module now incorporates a modified tri-stage model [2023Yan] to estimate Stress-Strain (σ-ε) curves for applications at low/ambient temperatures. Differing from the dislocation theory based on Kocks-Mecking model for hot deformation processes, this tri-stage model adopts empirical equations to describe the stress-strain relationship for elastic, uniform, and non-uniform plastic stages as illustrated in Figure 2 with experimental data [2017Mei].

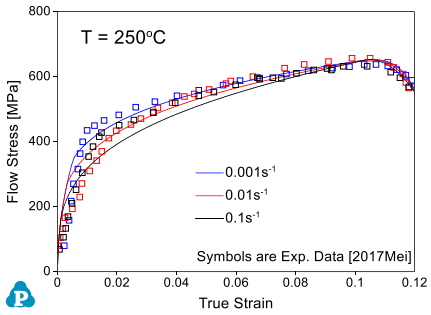

Figure 2: Flow curve of Fe-3.3wt%Si alloy at 250 °C

In this release, we've developed the function for simulating the Continuous Cooling Transformation (CCT) curve, allowing users to explore material transformation behavior under varying cooling rates. Figure 3 presents the Graphical User Interface (GUI) for setting up calculation condition for a model alloy Ni-14Al (at%) with cooling rates ranging from 0.1 to 100 °C/s together with the simulation results.

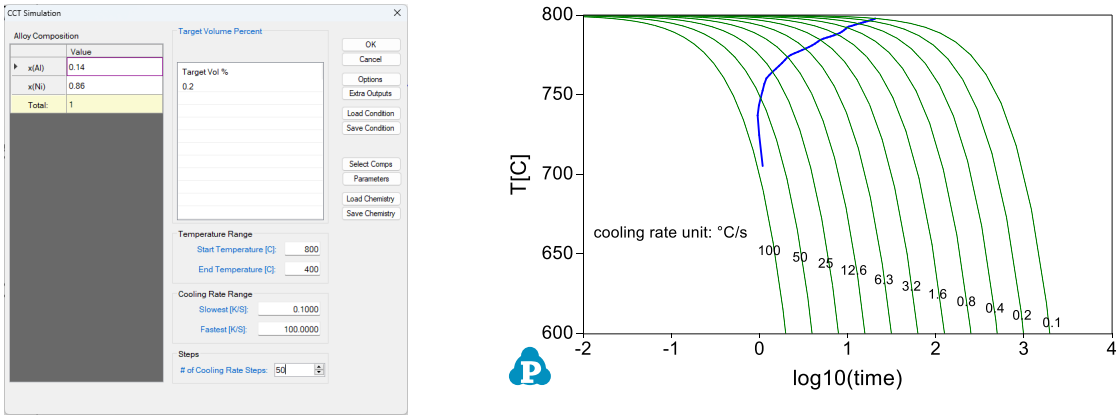

Figure 3: The user-interface and the calculated CCT curve (blue line) together with cooling curves (green lines) for the Ni-14Al (at%) alloy

PanPhaseField Module – A new PanPhaseField plugin (USER_TI_ALLOYS) has been developed for simulating microstructural evolution in Ti-alloys based on multi-phase field model which considers:

- Burgers orientation relationships between α and β phases
- Interfacial energy anisotropy of α phase
- Effect of applied stress

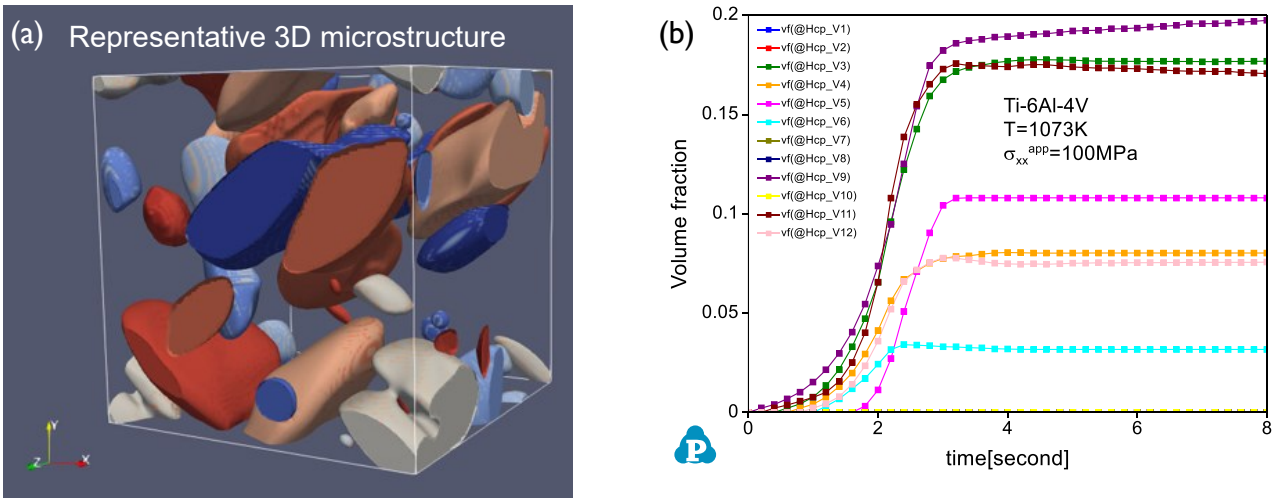

Figure 4: (a) Simulated 3D α/β microstructure of Ti-6Al-4V. (b) Volume fraction of different α variants (i.e. α phase with different orientations) as a function of time under tensile stress σ = 100 MPa, at T = 1073 K in Ti-6Al-4V.

New Features in PanPython SDK

- An optimizer, PyOptimizer, has been developed within PanPython SDK, which can optimize parameters used in the kinetic models adopted in PanEvolution module. Users can now optimize kinetic parameters using a large number of experimental data from multiple experimental conditions simultaneously and the optimization process can be observed through real time Python generated plots.
- The "Run All Batch Files" feature in PanPython was further enhanced to produce a summary of successful and failed calculations. Furthermore, a new mode, "Pandat Command", was introduced, which significantly improves the efficiency of point calculations by at least one order of magnitude.

Figure 5 and Figure 6 demonstrate an example of using PyOptimizer. In this example, PyOptimizer was used to optimize the kinetic parameters in PanEvolution module using the experimental data from [2014Chen] as shown in Figure 5. These optimized kinetic parameters were then used to calculate the volume fraction of the recrystallized grain as shown in Figure 6.

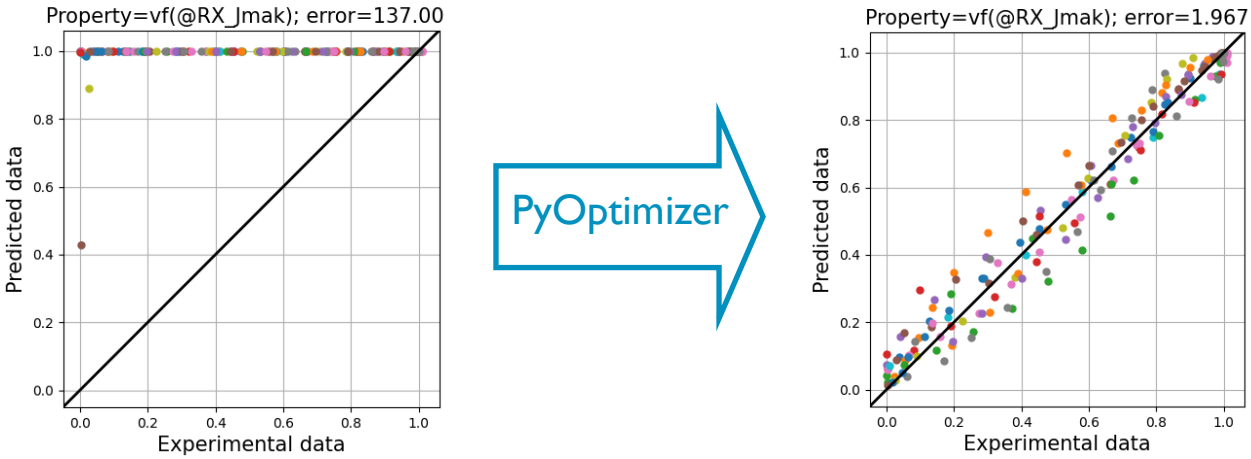

Figure 5: Comparison between the calculated volume fraction of recrystallized grain with those experimentally determined in [2014Chen] before and after using PyOptimizer

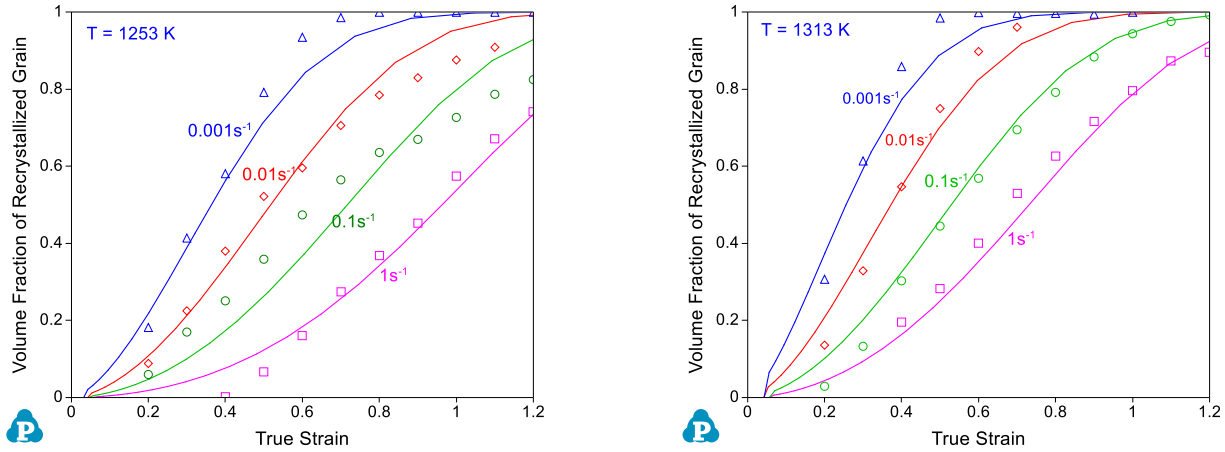

Figure 6: Calculated volume fraction of recrystallized grain using the optimized kinetic parameters in comparison with experimental data [2014Chen]

References:

[2023Yan] Yan, Jia-Bao, et.al., "Stress-strain models and numerical simulations of high-strength steel Q690E and Q960E at low temperatures." Journal of Constructional Steel Research 207 (2023): 107957.

[2017Mei] Mei, Rui-bin, et al. "Tensile flow stress of non-oriented Fe-3.3% Si steel at a wide range of moderate temperatures." Journal of Materials and Applications 6:2 (2017): 100-106.

[2014Chen] Chen, X.-M. et al. , Dynamic recrystallization behavior of a typical nickel-based superalloy during hot deformation, Materials & Design, 57 (2014) 568-577.