

PANDAT™ 2012

User's Guide



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1. Pandat Basics

Pandat™ software is an integrated computational tool developed on the basis of the CALPHAD (CALculation of PHase Diagram) approach for multi-component phase diagram calculation and materials property simulation. It has a robust thermodynamic calculation engine, a friendly graphical user interface, and a flexible post-calculation table editing function which allows user to plot variety types of diagrams. The software is designed to create a working environment that allows variety of calculation modules be integrated in the same workspace. It currently includes three modules: **PanPhaseDiagram** (phase diagram and thermodynamic property calculation), **PanPrecipitation** (precipitation simulation) and **PanOptimizer** (property optimization). Other modules, such as PanDiffusion (diffusion simulation), can be easily integrated into the workspace for extended applications. The architecture of Pandat™ software is schematically shown in the Figure 1.1.

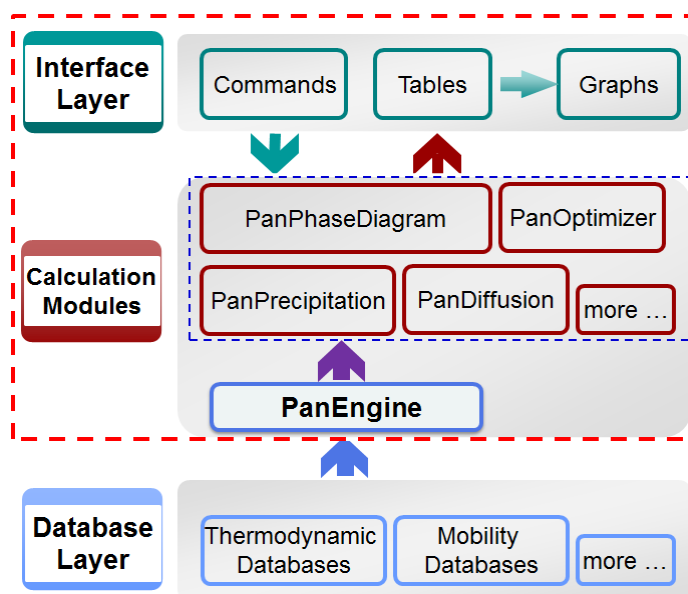


Figure 1.1 The architecture of Pandat™ software

In addition to the functionalities provided by Pandat™ as a stand-alone program being demonstrated in this example book, its calculation/optimization engine (**PanPhaseDiagram**, **PanOptimizer** and **PanPrecipitation**) are built as shared libraries and enable their integration with broader applications in the field of Materials Science and Engineering. More detailed information about Pandat software can be found in [2002Che, 2003Che, 2009Cao].

The **PanGUI** (user interface of the Pandat workspace) consists of six components: **Menus**, **Toolbars**, **Statusbar**, **Explorer window**, **Property window** and **Main display window** as shown in Figure 1.2.

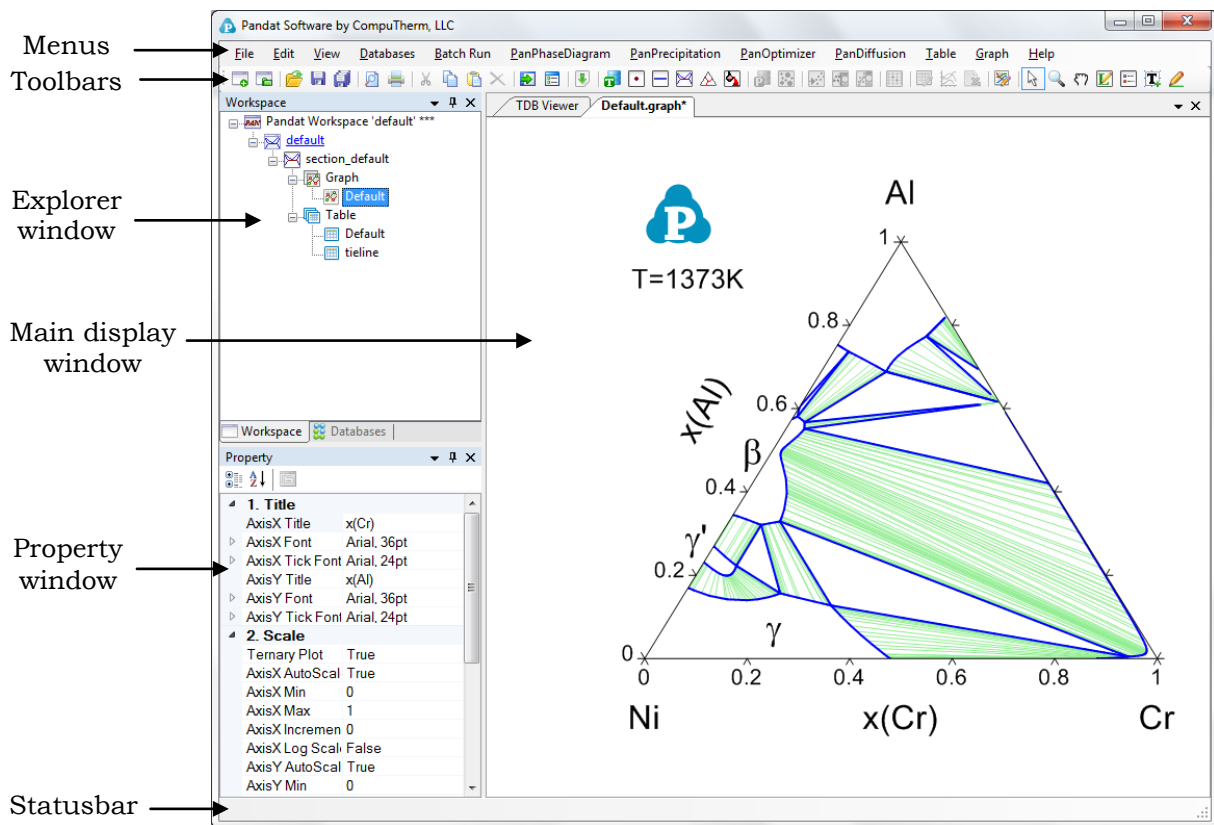


Figure 1.2 The components of the PanGUI

1.1 Menu

Pandat menus provide commands for performing operations on the active window and other general operations such as opening and saving a workspace file (*.pndx) or turning on the display of a toolbar. The menus are context sensitive; that is, they change as the context in Pandat Main display window changes. This ensures that only Context-relevant menus and menu commands are displayed.

1.2 Toolbar

Pandat™ provides toolbar buttons for the frequently used menu commands. Like the menu commands, toolbar buttons are also context-sensitive.

When a toolbar button is pointed at with the mouse, a "tool-tip" displays the button name. A more detailed button description displays in the statusbar at the bottom of the workspace.

1.3 Statusbar

The Pandat Statusbar is located at the bottom of the workspace and provides a detailed description when the cursor is on the menu or toolbar button. If the cursor is on a graph, the coordinates are displayed in the statusbar.


1.4 Explorer window

The Explorer window lists the contents in the current workspace. The contents are displayed in a tree structure. By clicking each node, the text, graph or table will be displayed in the Main display window of Pandat. A node of a calculation result could be deleted.

1.5 Main display window

The Main display window displays the text, graph or table which corresponds to each node in the Explorer window.

2. Get Started

Pandat™ starts with the following start page as shown in Figure 2.1. The user can open the start page at any time by clicking the icon  on the toolbar. On the start page, there are shortcuts which allow users to create a new workspace and open an existing workspace, link to CompuTherm's webpage for recent updates and for comments and discussions from Pandat™ users. It also lists the most recent workspaces and files the user has created, so that user can reopen them easily.

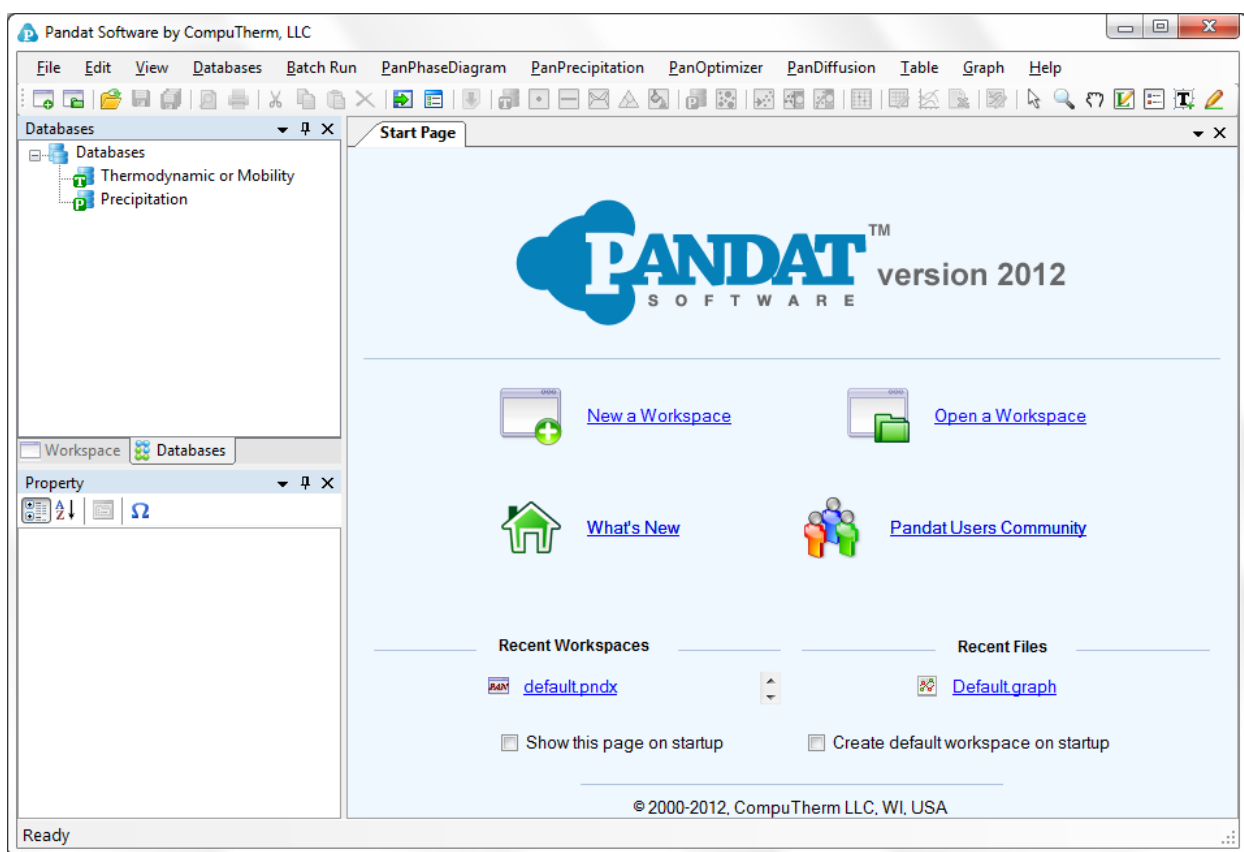







Figure 2.1 The start page of Pandat™ software

2.1 Workspace

The workspace provides a space for user to perform Pandat calculations and organize the calculated results. It must be created before any Pandat calculation is carried out.

User can create a new workspace by clicking on the “New a Workspace” link on the start page, or the icon  on the toolbar, or go through the menus (**File** → **Create a New Workspace**). A new window will pop out as show in the Figure 2.2. User can define the name of the workspace and select a working directory to put the workspace. User can then select the module from the four icons: Phase diagram calculation () , Optimization () , Precipitation simulation () , or Diffusion simulation () . User can also give a “Project Name” for the calculations to be performed. User may choose to create a default workspace with default project name simply by clicking the “**Create**” button or double click the selected module.

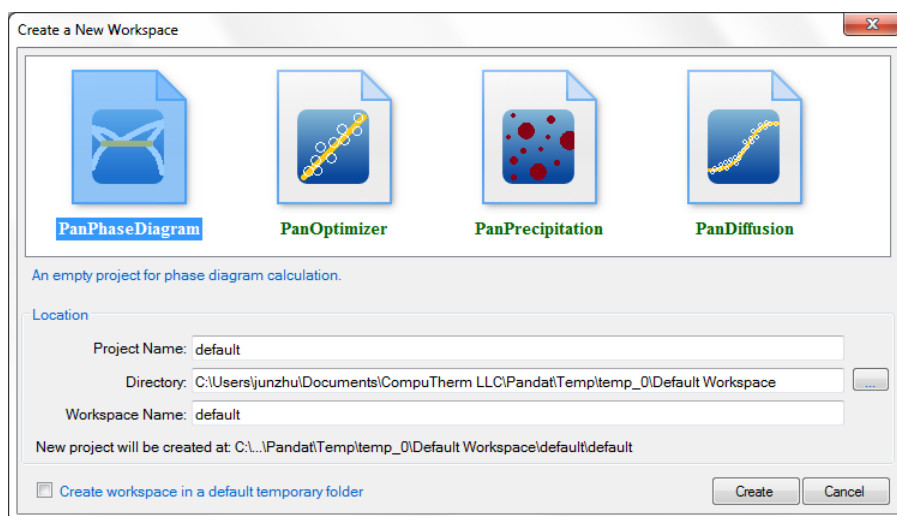



Figure 2.2 Create a new workspace dialog

After using Pandat, user will be given an opportunity to save the workspace that the user has created. The user can open a saved workspace next time by clicking on the “**Open a Workspace**” link on the start page, or the icon  on the toolbar, or go through the menus (**File** → **Open** → **Workspace**). For some very recent workspaces and files, there are shortcuts provided on the start page.

In Pandat™, only one workspace is allowed. When creating a new workspace, the user will be asked if the current workspace needs to be saved. Think twice before clicking the “**Create**” button. The old workspace will be lost if it is not saved when a new workspace is created.

2.2 Project

In the Pandat™, a workspace may contain many projects of different types. For example, a user creates a project for **PanPhaseDiagram** module which contains all calculations for phase diagrams. User can then create a new project of precipitation simulation in the same workspace using menus (**File → Add a New Project**). In this case, the workspace name and the working directory cannot be changed, but the user needs to give a new project name. The database file, table, graph and other data associated with one project can be viewed in individual tabs in the Display window.

The user can move these windows to different positions for his/her convenience. The following Figure 2.3 shows how to move these windows. Hold the left button of the mouse on the window and move the mouse, then a relative position dialog will show up. Release the left button of the mouse when the mouse has moved to the relative position dialog following the red arrow in the figure. The windows of Pandat™ will be rearranged as shown in Figure 2.3.

When more than one project are created in one workspace, only one project will be activated at one time, and only those functions and toolbar icons associated with the activated project are available to the user at the time.

The name of the activated project will be highlighted with blue and have an underline. To select a project as the activated project. right click the mouse on the project name in the explore window and choose "**Set as Active Project**" in the popup dialog as shown in Figure 2.4.

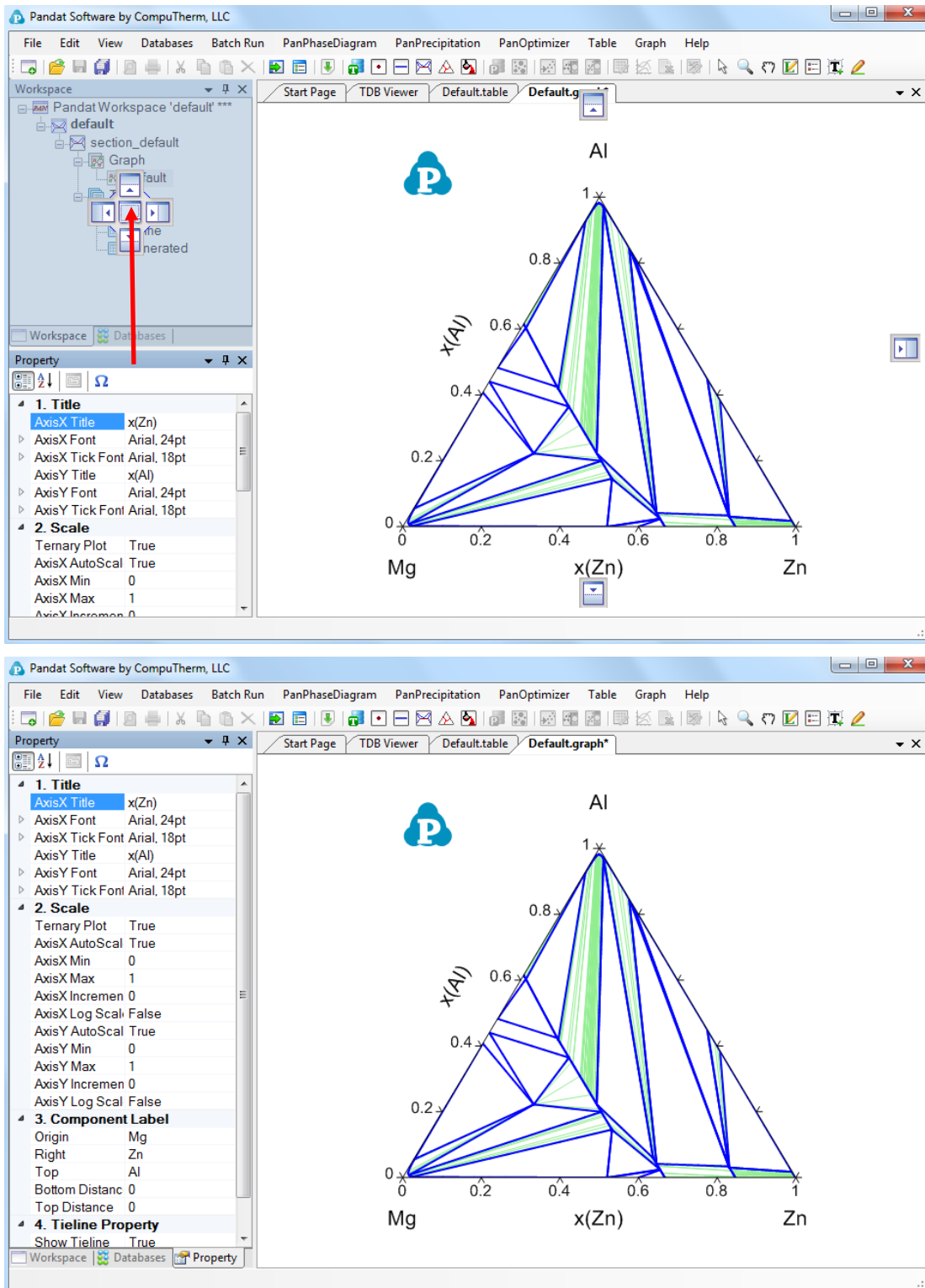


Figure 2.3 Rearrange the windows of Pandat™, before and after

When switching between projects, the user may also need to switch between different databases so that the right database is used for the calculation. In the Databases view dialog in explore window, all the loaded databases are listed and the name of currently activated database is also highlighted with blue and has an underline. To activate another database, right click the mouse on the database name and choose “**Set as Active TDB**” as also shown in Figure 2.5. Inside one project, the user may also load several databases and carry out different calculations of the same type. The user need to make sure that the correct database is activated when performing a calculation.

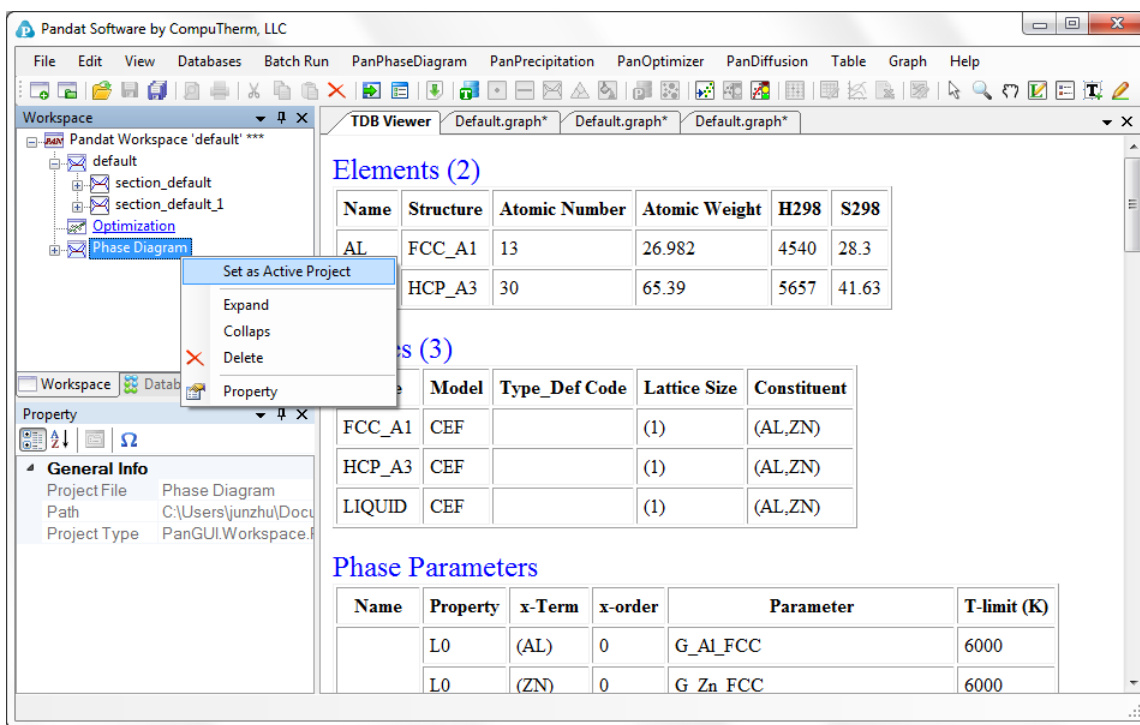


Figure 2.4 Set an active project

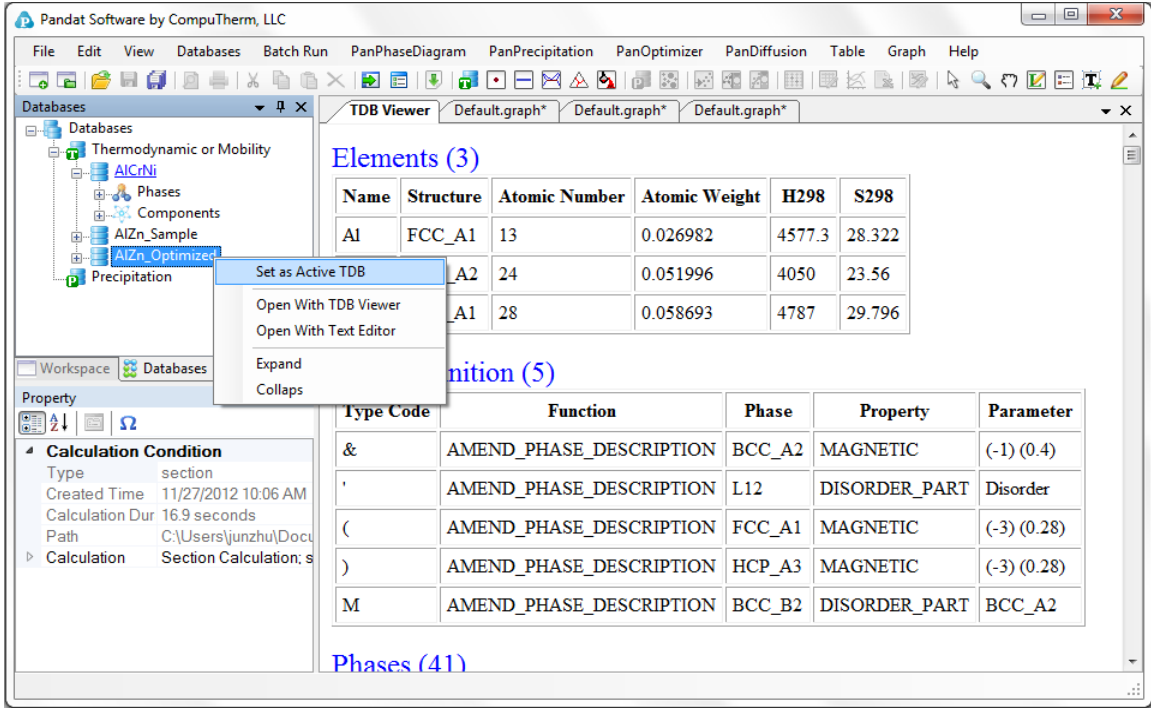


Figure 2.5 Set an active database

2.3 Graph

In each project, the calculated results are presented in two different formats: Graph and Table. Graph is one of the most important parts in Pandat interface. A typical Pandat graph includes at least three elements: a set of X and Y coordinate axes, one or more data plots and associated text and drawing objects. Each graph can have one or more data plots and these data plots can be configured individually. Each data plot corresponds to each data set which can be obtained from either calculation or experiments.

The graph is plotted in the main display window with Pandat logo. The Property window defines the properties for all the elements in the graph in detail. When a typical element is selected, the property of this element will be displayed in the Property window and the user may modify the graph through the Property window.

2.3.1 Property

The overall property of the graph consists of four categories: **Title**, **Scale**, **Component Label** and **Tieline Property**, as shown in the red box area in Figure 2.6. All four categories will be shown in Property window when the whole graph is selected. The Title property defines the title, title font size and tick font size for both X axis and Y axis. The Scale property defines the minimum and maximum values for both X and Y axes and a flag of Ternary Plot. If this flag is set as "True", the figure is plotted as Gibbs triangle as a normal isothermal section. If the flag is set as "False", a Cartesian coordinate figure will be plotted. The Component label defines the labels on the origin, right corner and Top corner of the graph. The Tieline Property defines whether to show the tie-lines and the density of the tie-lines. The other properties of

these tie-lines, such as the color, the style, are defined by individual property window associated with these tie-lines. These properties can be modified when only the tie-lines on the Main Display window are selected and highlighted.

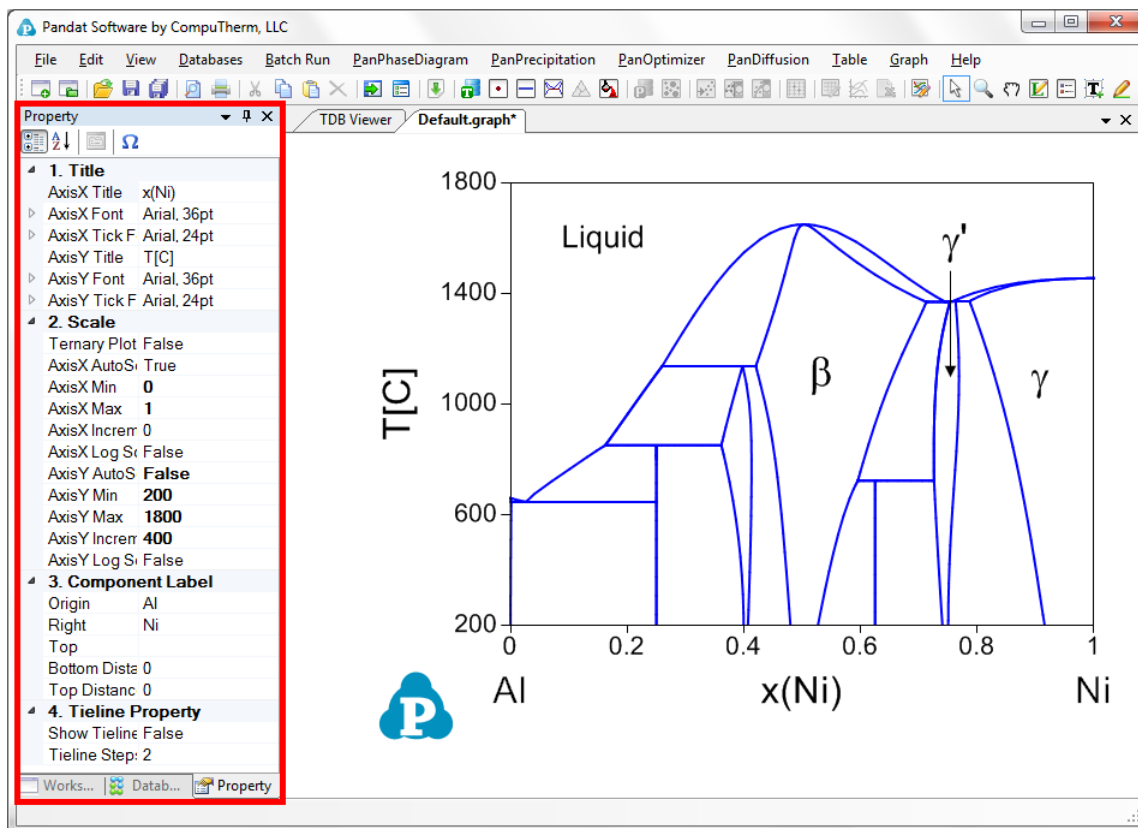


Figure 2.6 Graph property window

User can change the appearance of a particular line or a set of lines belong to the same group by selecting this line (or a group lines) only. The properties for such data plots, such as the line color, thickness, marker type, will show up in the Property window for user to modify. The data points and lines selected will be highlighted in the graph while the other will be grey. As shown in Figure 2.7, the **Plot Property** defines the plot type of the data to be Line or Point. The **Line Property** defines the property of the line and the **Marker Property** defines the property of the point on the graph.

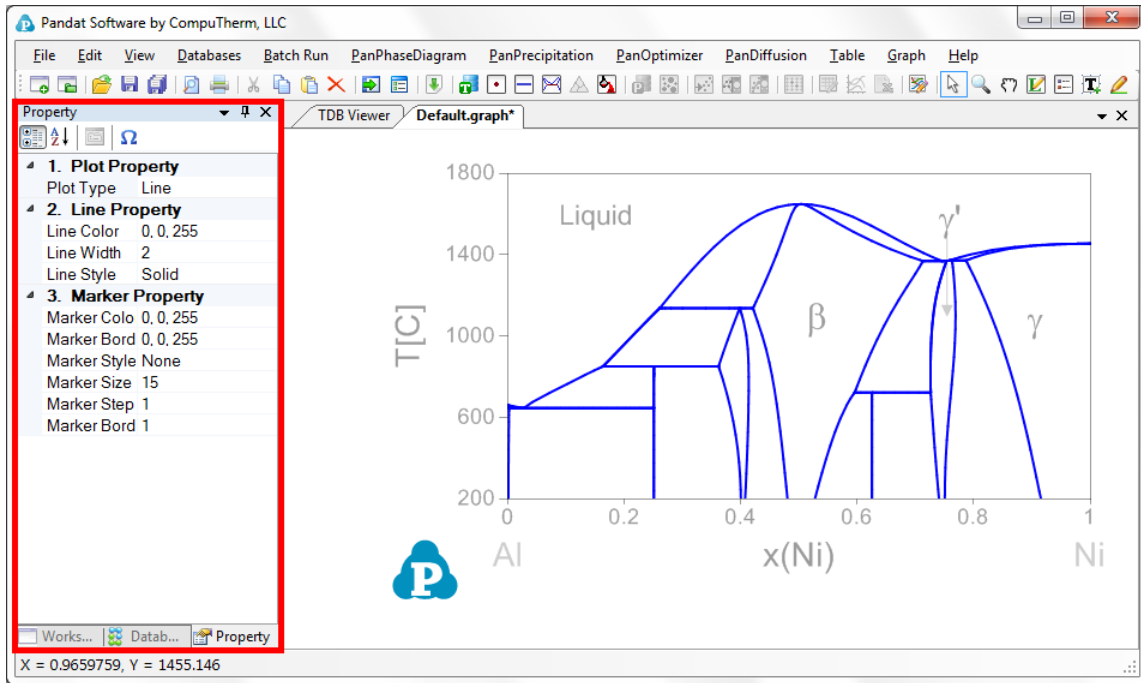


Figure 2.7 Plot property window

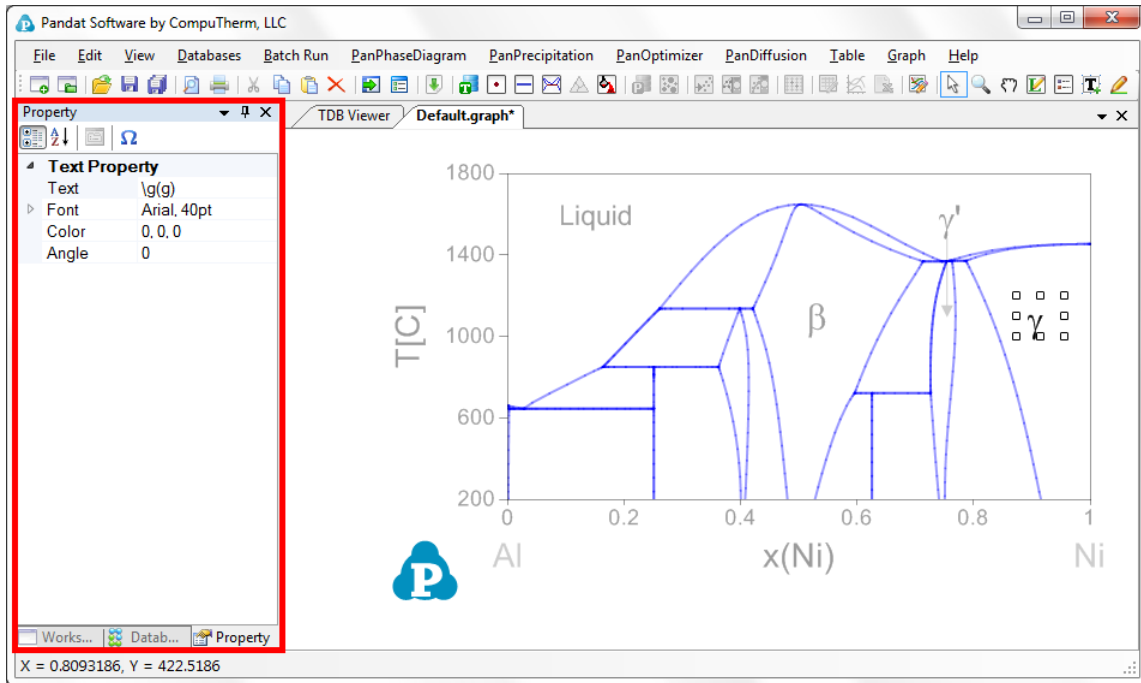


Figure 2.8(a) Text Property window

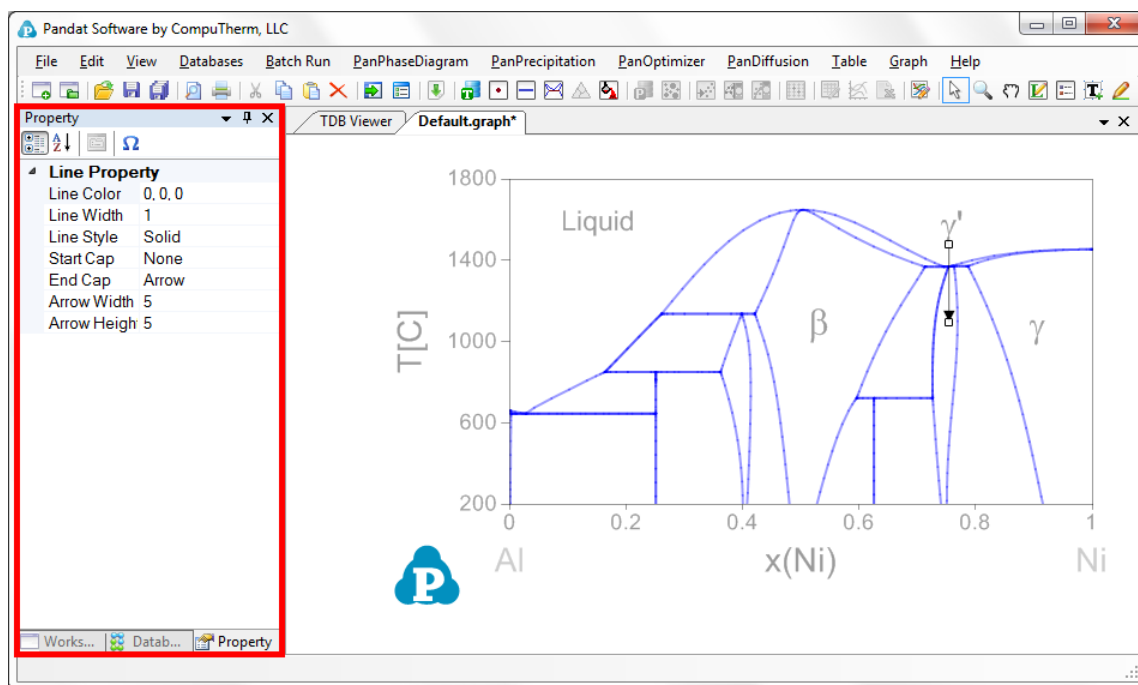



Figure 2.8(b) Line Property window



The user can add texts and lines freely to the graph. The **Text Property** defines the content of the text, font size, color and rotating angle. The **Line Property** defines the color, width, start cap and end cap of the line. Both **Text Property** and **Line Property** are shown in the red box areas in Figure 2.8.

2.3.2 Export the graph to other format

The user can output the Pandat graph to other popular formats such as emf, bmp, jpg, png, gif and tif. The command is located on the menus: **Graph** → **Export**, or right click the mouse on the graph and choose “Export” from the popup menu.

2.3.3 Useful icons for Graph on Toolbar

Edit Plots for the Current Graph button , allow the user to modify the plots, such as add data plots with mouse drag and drop to set up x and y of the

new plot as shown in Figure 2.9, delete data plots using button , exchange x and y of the plots using button . The available columns can be imported from a file or from Clipboard if the check box in front is selected.

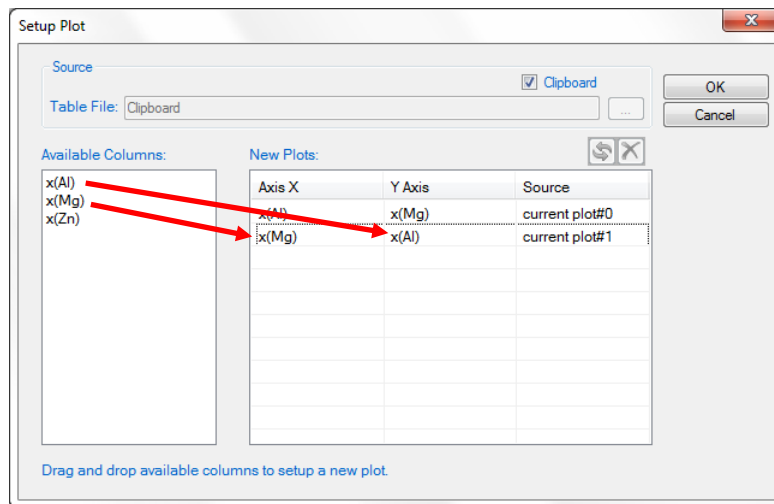





Figure 2.9 Set up data for X and Y for a plot


The table file to be imported can be Pandat table format or ASCII text format. For a general Microsoft Excel table, the user can copy the selected columns in the Excel file and check the Clipboard option, and then the column names will show up in the “Available Columns” dialog for the user to select, which is also shown in Figure 2.9. The copy operations also work for the table columns in the Pandat calculation results.


Select Objects button , allow the user to select drawing elements in a graph such as line, arrow or text.


Zoom Mode button , use the Zoom mode to enlarge a small part of a graph. Hold the left button of the mouse and move the mouse to select a rectangular area on the graph to enlarge. The graph will zoom in to the selected area when


the left button of the mouse is released. Double click this button will bring the zoom image back to the whole diagram again.

Pan Mode button , when this mode is on, put the cursor on the plot and roll the mouse wheel to enlarge or shrink the graph, keeping the current center of the graph unchanged. Hold the left button of the mouse on the graph and move the mouse, the user can move the whole graph.

Label Phase Region button , label the graph with text. Pandat can not only label the normal T-x or x-x phase diagrams from calculations, but also label those user generated graphs using the table data from calculation, i.e., G-x and μ -x diagrams. The user can modify the labeled text like normal text.

Add Legend for Graph button , add legend to the graph. The user can modify the legend using the Property window, as shown in Figure 2.10(a). Double click on the inserted legend will open a new Text Editor window as shown in Figure 2.10(b), and the user can input complex text, such as symbol, superscript and subscript in this windows.

Add Text or Label button , add text to the graph. Change the text content, size, color and rotating angle in the Property window. Double click on the text also open the Text Editor window which allows user to input complex text in it as shown in Figure 2.10(b).

Add Line button , add line or arrow to the graph. Change the line or arrow width and color in the Property window. The default line has no arrows at either end of the line. User can set the start cap and end cap in the Line Property window.

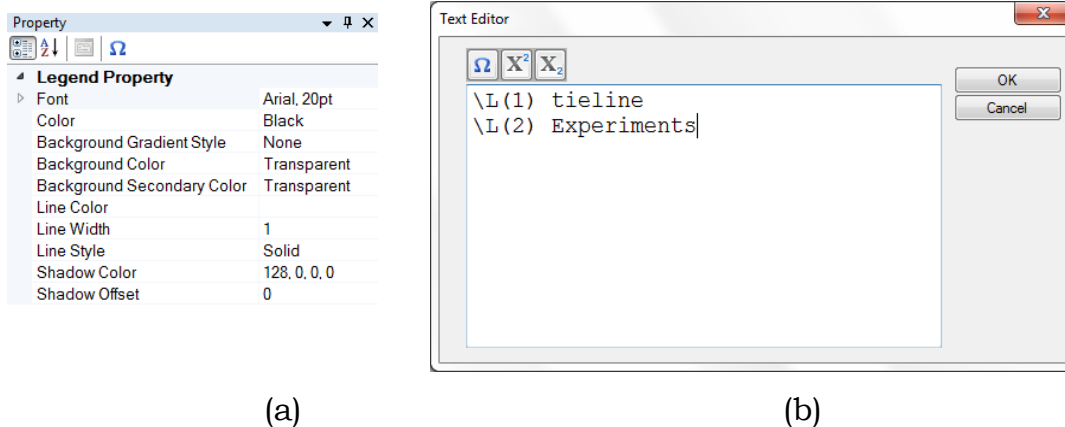
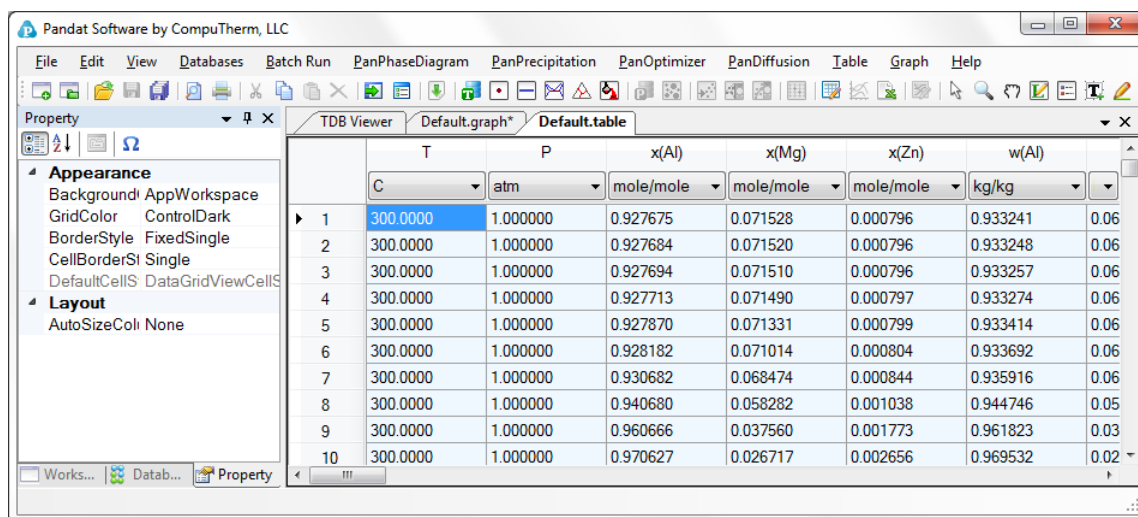


Figure 2.10 (a) Legend property window and (b) Text editor window

2.4 Table


The menu of Pandat **Table** includes: **Add a New Table**, **Create Graph**, and **Export to Excel**. A typical table is shown as Figure 2.11. Each column of data is associated with a corresponding unit. The user can change the unit of each column and observe the instant change of the table values.



	T	P	x(Al)	x(Mg)	x(Zn)	w(Al)	
	C	atm	mole/mole	mole/mole	mole/mole	kg/kg	
1	300.0000	1.000000	0.927675	0.071528	0.000796	0.933241	0.06
2	300.0000	1.000000	0.927684	0.071520	0.000796	0.933248	0.06
3	300.0000	1.000000	0.927694	0.071510	0.000796	0.933257	0.06
4	300.0000	1.000000	0.927713	0.071490	0.000797	0.933274	0.06
5	300.0000	1.000000	0.927870	0.071331	0.000799	0.933414	0.06
6	300.0000	1.000000	0.928182	0.071014	0.000804	0.933692	0.06
7	300.0000	1.000000	0.930682	0.068474	0.000844	0.935916	0.06
8	300.0000	1.000000	0.940680	0.058282	0.001038	0.944746	0.05
9	300.0000	1.000000	0.960666	0.037560	0.001773	0.961823	0.03
10	300.0000	1.000000	0.970627	0.026717	0.002656	0.969532	0.02

Figure 2.11 Table view of the calculation results in Pandat™

2.4.1 Useful icons for Table on Toolbar

Add a New Table button , click this button will pop out a window of Table Editor as shown in Figure 2.12, create a new table by dragging and dropping the available properties in the left dialog to the Property dialog on the right as shown by the red arrow in Figure 2.12, and then click “**OK**” to generate a new table for the selected properties.

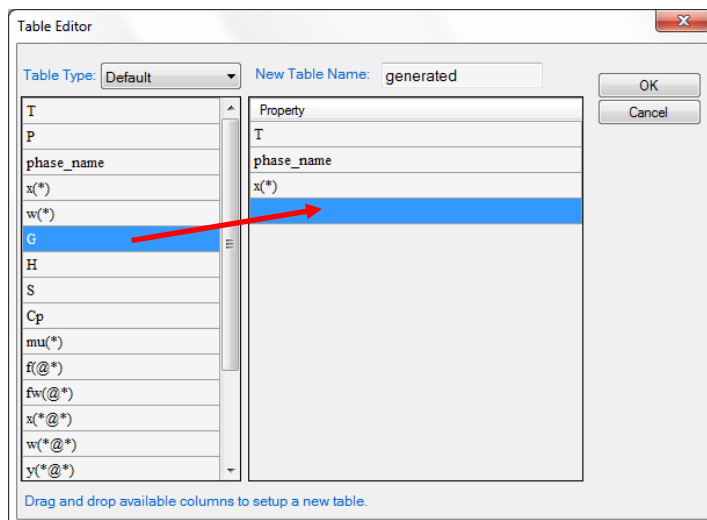




Figure 2.12 Table Editor

Create Graph button , create a new graph for the selected properties. Use the <ctrl> key and the left button of the mouse to select multiple columns in the table as shown in Figure 2.13. The first selected column will be the x and the other columns will be the y's for the new plots. After click on the  button, a graph will then be displayed in the Pandat main display window as shown in Figure 2.14.

	T	P	x(Al)	x(Mg)	x(Zn)	w(Al)
	C	atm	mole/mole	mole/mole	mole/mole	kg/kg
1	300.0000	1.000000	0.927675	0.071528	0.000796	0.933241
2	300.0000	1.000000	0.927684	0.071520	0.000796	0.933248
3	300.0000	1.000000	0.927694	0.071510	0.000796	0.933257
4	300.0000	1.000000	0.927713	0.071490	0.000797	0.933274
5	300.0000	1.000000	0.927870	0.071331	0.000799	0.933414
6	300.0000	1.000000	0.928182	0.071014	0.000804	0.933692
7	300.0000	1.000000	0.930682	0.068474	0.000844	0.935916
8	300.0000	1.000000	0.940680	0.058282	0.001038	0.944746
9	300.0000	1.000000	0.960666	0.037560	0.001773	0.961823
10	300.0000	1.000000	0.970627	0.026717	0.002656	0.969532

Figure 2.13 Select data for creating a new graph

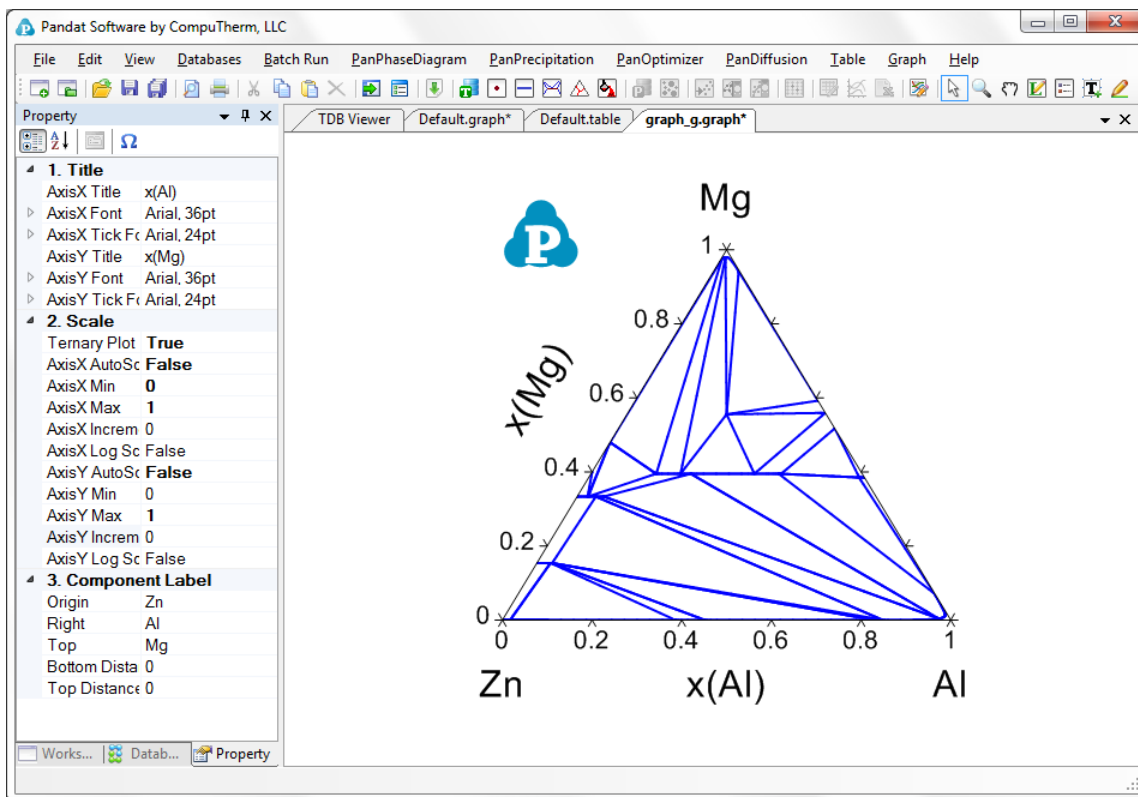



Figure 2.14 A new graph created from selected columns in the table

Export to Excel button  , allow user to export the table of interest directly to a Microsoft Excel file. Excel must be pre-installed in the user's computer.

3. PanPhaseDiagram

3.1 Thermodynamic Database

PanPhaseDiagram is for phase diagram and thermodynamic property calculation. Thermodynamic database is the prerequisite to fulfill such calculations. A thermodynamic database represents a set of self-consistent Gibbs-energy functions with optimized thermodynamic-model parameters for all the phases in a system. The advantage of CALPHAD method is that the separately-measured phase diagrams and thermodynamic properties can be represented by a unique “thermodynamic description” of the materials system in question. More importantly, on the basis of the known descriptions of the constituent lower-order systems, the thermodynamic description for a higher-order system can be obtained via an extrapolation method [1989Cho]. This description enables us to calculate phase diagrams and thermodynamic properties of multi-component systems that are experimentally unavailable.

In the following, thermodynamic models used to describe the disordered ordered phases, and stoichiometric phase are presented. The equations are given for a binary system, and they can be extrapolated to a multi-component system using geometric models [1989Cho, 1975Mug].

The Gibbs energy of a binary solution phase can be written as:

$$G_m^\varphi = \sum_{i=A,B} x_i \cdot G_i^{\varphi,o} + RT \sum_{i=A,B} x_i \ln x_i + x_A \cdot x_B \sum_v L_v \cdot (x_A - x_B)^v \quad (3.1)$$

where the first, second and third terms on the right hand of the equation represent, respectively, the reference states, the entropy of ideal mixing, and the excess Gibbs energy of mixing. Here x_i is the mole fraction of a component i , $G_i^{\phi,o}$ is the Gibbs energy of a pure component i , with an ϕ structure, R is the gas constant, T is the absolute temperature, L_v is the interaction coefficient at the polynomial series of the power v . When $v = 0$, it is a regular solution model, and when $v = 0$ and 1, it is a sub-regular solution model. Equation 3.1 can be extrapolated into a multi-component system using geometric models, such as the Muggianu model [1975Mug]. Ternary and higher-order interaction parameters may be necessary to describe a multi-component solution phase.

An ordered intermetallic phase is described by a variety of sublattice models, such as the compound-energy formalism [1979Ansara, 1988Ansara] and the bond-energy model [1992Oates, 1995Chen]. In these models, the Gibbs energy is a function of the sublattice species concentrations and temperature. The Gibbs energy of a binary intermetallic phase, described by a two-sublattice compound-energy formalism, $(A,B)_p : (A,B)_q$, can be written as:

$$\begin{aligned}
 G_m^\phi = & \sum_{i=A,B} \sum_{j=A,B} y_i^I y_j^{II} G_{i,j}^\phi + RT \left[\frac{P}{p+q} \sum_{i=A,B} y_i^I \ln y_i^I + \frac{q}{p+q} \sum_{i=A,B} y_i^{II} \ln y_i^{II} \right] \\
 & + \sum_{j=A,B} y_A^I y_B^I y_j^{II} \sum_v (y_A^I - y_B^I)^v L_{A,B;j}^v + \sum_{i=A,B} y_i^I y_A^{II} y_B^{II} \sum_v (y_A^{II} - y_B^{II})^v L_{i,A,B}^v \\
 & + y_A^I y_B^I y_A^{II} y_B^{II} L_{A,B:A,B}
 \end{aligned} \tag{3.2}$$

where y_i^I and y_i^{II} are the species concentrations of a component, i , in the first and second sublattices, respectively. The first term on the right hand of the equation represents the reference state with the mechanical mixture of the stable or hypothetical compounds: A, $A_p B_q$, $B_p A_q$, and B. $G_{i,j}^\phi$ is the Gibbs energy of the stoichiometric compound, $i_p j_q$, with an ϕ structure. The value of $G_{i,j}^\phi$ can

be obtained experimentally, if $i_p j_q$ is a stable compound, or it can be a model parameter obtained by optimization using the experimental data related to this phase. The second term is the ideal mixing Gibbs energy, which corresponds to the random mixing of species on the first and second sublattices. The last three terms are the excess Gibbs energies of mixing. The "L" parameters in these terms are model parameters whose values are obtained, using the experimental phase-equilibrium data and thermodynamic-property data. These parameters can be temperature dependent. In this equation, a comma is used to separate species in the same sublattice, whilst a colon is used to separate species belonging to different sublattices. The compound-energy formalism can be applied to phases in a multi-component system by considering the interactions from all the constituent binaries. Additional ternary and higher-order interaction terms may also be added to the excess Gibbs energy term.

The Gibbs energy of a binary stoichiometric compound $A_p B_q$, G_m^φ , is described as a function of temperature only:

$$G_m^\varphi = \sum_i x_i G_i^{\varphi,\circ} + \Delta_f G(A_p B_q) \quad (3.3)$$

where x_i is the mole fraction of component i ($i=p$ if it is A, and $i=q$ if it is B), and $G_i^{\varphi,\circ}$ represents the Gibbs energy of component i with φ structure; $\Delta_f G(A_p B_q)$, which is normally a function of temperature, represents the Gibbs energy of formation of the stoichiometric compound. If $\Delta_f G(A_p B_q)$ is a linear function of temperature:

$$\Delta_f G(A_p B_q) = \Delta_f H(A_p B_q) - T \cdot \Delta_f S(A_p B_q) \quad (3.4)$$

then $\Delta_f H(A_p B_q)$, and $\Delta_f S(A_p B_q)$ are the enthalpy and entropy of formation of the stoichiometric compound. Equation (3.3) can be readily extended to a multi-component stoichiometric compound phase.

The strategy of building a multi-component thermodynamic database starts with deriving the Gibbs energy of each phase in the constituent binaries. There are C_n^2 constituent binaries in an n-component alloy system, where

$$C_n^i = \frac{n!}{i!(n-i)!} \quad (3.5)$$


To develop a reliable database, the Gibbs energies of these binaries must be developed in a self-consistent manner and be compatible with each other. Three binaries form a ternary, and a preliminary thermodynamic description can be obtained by combining the three constituent binaries using geometric models, such as the Muggianu model [1975Mug]. In some cases, a ternary database developed in this way can describe a ternary system fairly well, while in most cases, ternary interaction parameters are necessary to better describe the ternary system. If a new phase appears in the ternary, which is not in any of the constituent binaries, a thermodynamic model is selected for this ternary phase, and its model parameters are optimized using the experimental information for this ternary phase. There are a total of C_n^3 ternary systems in an n-component system. After thermodynamic descriptions of all C_n^3 ternaries for an n-component system are established, the model parameters are simply used to describe quaternary and higher-order systems using an extrapolation approach. High-order interaction parameters are usually not necessary because although interactions between binary components are strong, in ternary systems they become weaker, and in higher-ordered systems they become negligibly weak [1997Kattner, 2004Chang]. It is worth noting that the

term, “thermodynamic database” or simply “database”, is usually used in the industrial community instead of “thermodynamic description”, particularly for multi-component systems.

At CompuTherm, multi-component databases have been developed for variety of alloys, such as for Al-alloys, Co-alloys, Cu-alloys, Fe-alloys, Mg-alloys, Mo-alloys, Nb-alloys, Ni-alloys, Ti-alloys, and solder alloy system.

3.2 Thermodynamic Calculation

3.2.1 Load Database

Pandat can load both PDB and TDB database files. This command can be accessed through the toolbar icon . Or load a database file using the Menu **Database→Load TDB or PDB (Encrypted TDB)** as shown in Figure 3.1. Select a database file from hard drive and click open button, or just double click the database file. Users can store the databases in any directory in the computer.

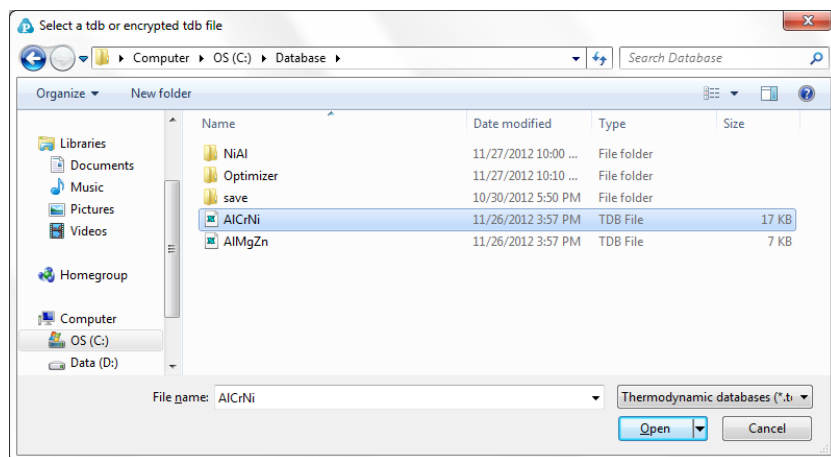
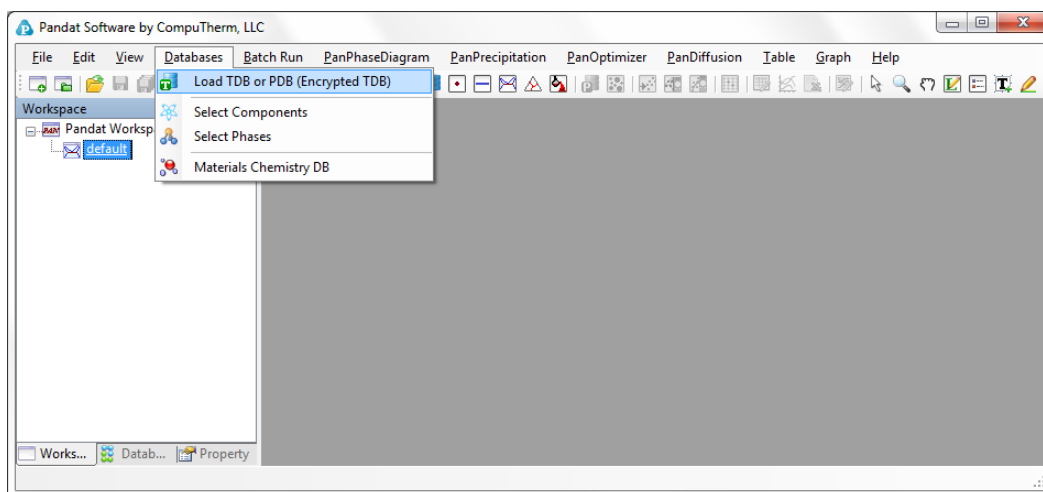




Figure 3.1 Load a database from hard drive through Menu

Immediately after a database is successfully loaded, a popup window shown in Figure 3.2 will ask the user to select the components for subsequent calculations. To add a component to the list of selected components, click on the component on the list of **Available Components** on the left column, and click on the  button to send them to the **Selected Components** on the right column. To select several components at one time, hold the <Ctrl> key and use mouse to select multiple components. To remove a component from selected components list, use mouse to select it, and click the  button.

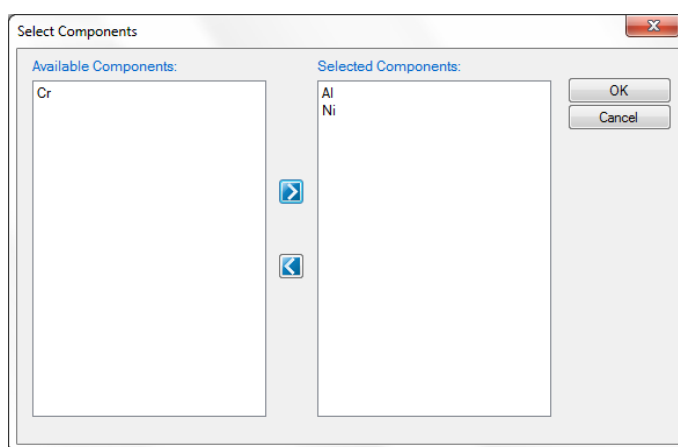


Figure 3.2 Select components for further calculation

While loading a database file, Pandata™ checks the self-consistency of the database. A message will be displayed if the database is not internally consistent such as duplicated definitions of a function, missing definition of components or species in a sublattice, and so on. There are two types of messages: Error and Warning, as shown in Figure 3.3. The warning message can be ignored but the errors must be fixed, otherwise the database cannot be loaded. It is recommended to correct both error and warning before performing calculation. If you have difficulties loading a particular TDB or PDB file, please contact CompuTherm, LLC, and we will help resolve the problem.

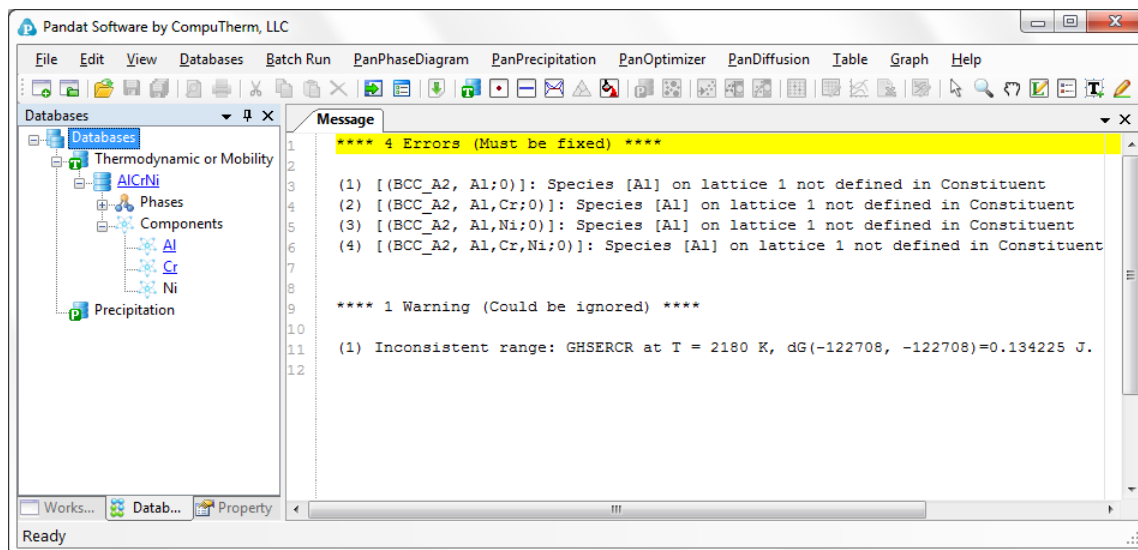


Figure 3.3 A typical message when loading a database

The successfully loaded database will be automatically summarized in the TDB Viewer mode in the main Display window as shown in Figure 3.4. For a TDB format database, the summary includes elements, type definitions, phases with name and thermodynamic model, model parameters and defined functions. For a PDB format database, the model parameters and functions will not be displayed. The user can open a TDB format database with the Text Editor mode to modify the database by right click of the mouse on the database name in the explorer window. The Text Editor is actually a built-in notepad for text files. User can always use his/her favorite text editor to modify the TDB format database.

Multiple databases can be loaded into the same workspace but only one is activated. The current calculation will use the activated database, which is highlighted in the explorer window at Database view. The user may set the inactive database to be active with right click of the mouse as shown in Figure 3.5.

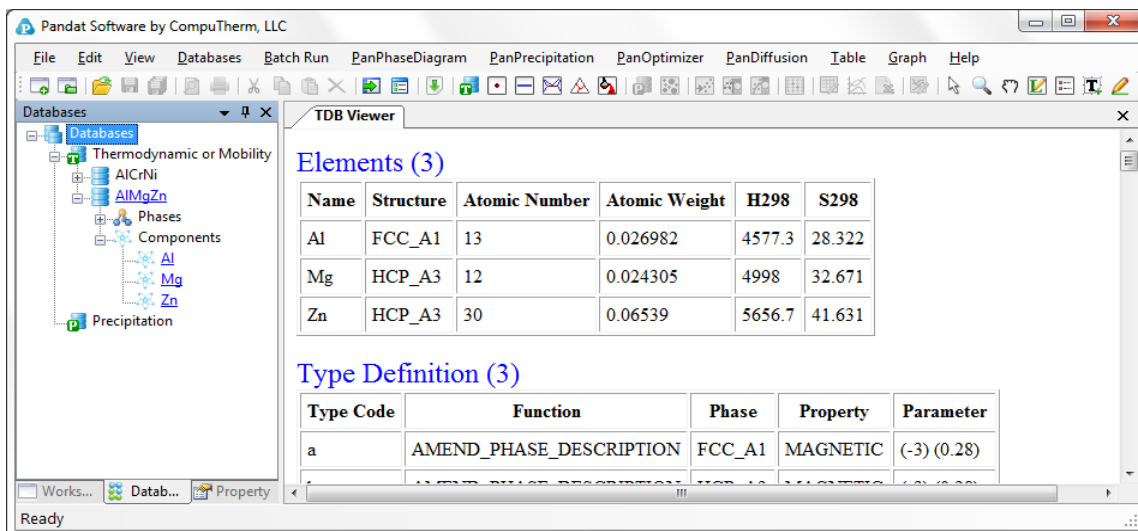


Figure 3.4 The TDB viewer mode for database summary

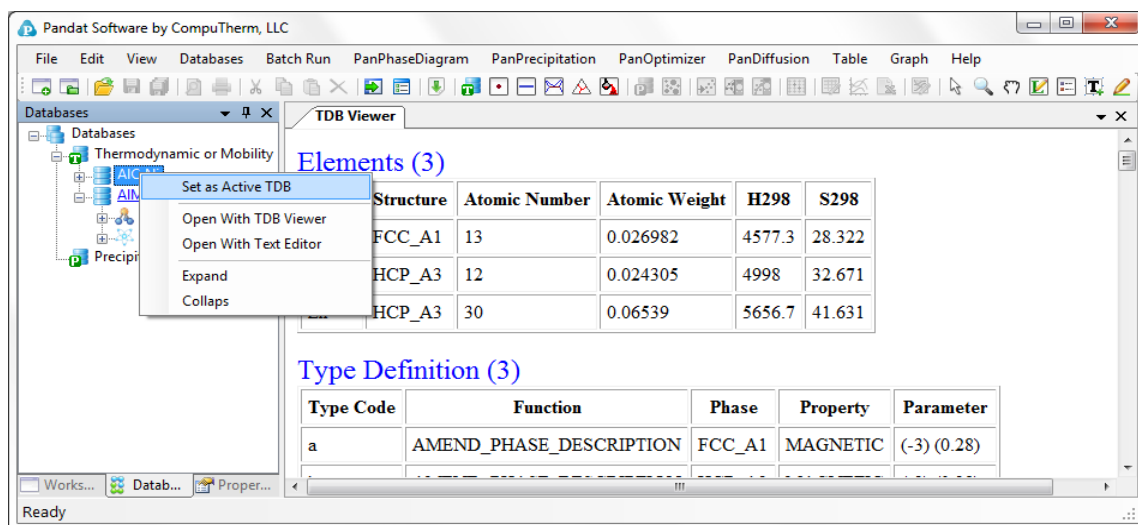



Figure 3.5 Set an inactive database to be active

3.2.2 Options

To configure the calculation options, go through the menus (**View → Options**), or click on the icon  on the toolbar. A pop-up dialog box allows the user to change the units, and output formats of default Table and Graph.

Units: This dialog box allows the user to choose the units to be used in the calculation. Use the mouse left button to select a proper unit for each property and click “OK” to complete the unit setting as shown in Figure 3.6.

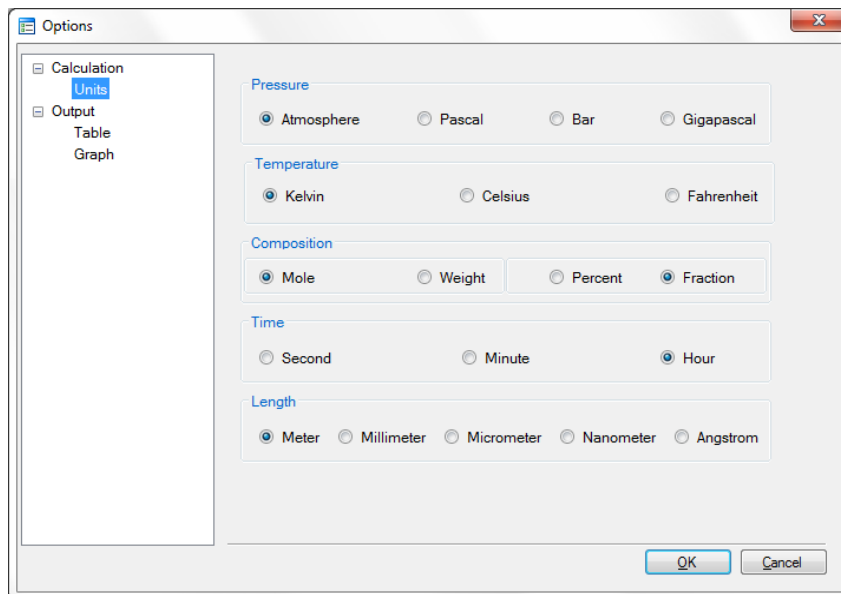


Figure 3.6 Set units for a calculation in Options

Table: This dialog box allows the user to choose user-defined results that will be shown in the output table. As shown in Figure 3.7, the “Choose Table Columns” lists all the possible outputs for each calculation type. The user can check the box in front of each item to select the column to be shown in the output table. The “Default Graphs” dialog defines the X axis and Y axis of the default graph for Pandat calculations. The default graph is the diagram that automatically shows up after a calculation finishes. Through the Default Graphs dialog the user can set up user-defined default graph for each type of calculation.

Graph: This dialog box allows the user to set up the appearance of the output graph. As shown in Figure 3.8, user can set the font and size of the texts, color and weight of the lines, color, shape and size of the symbols and logo size.

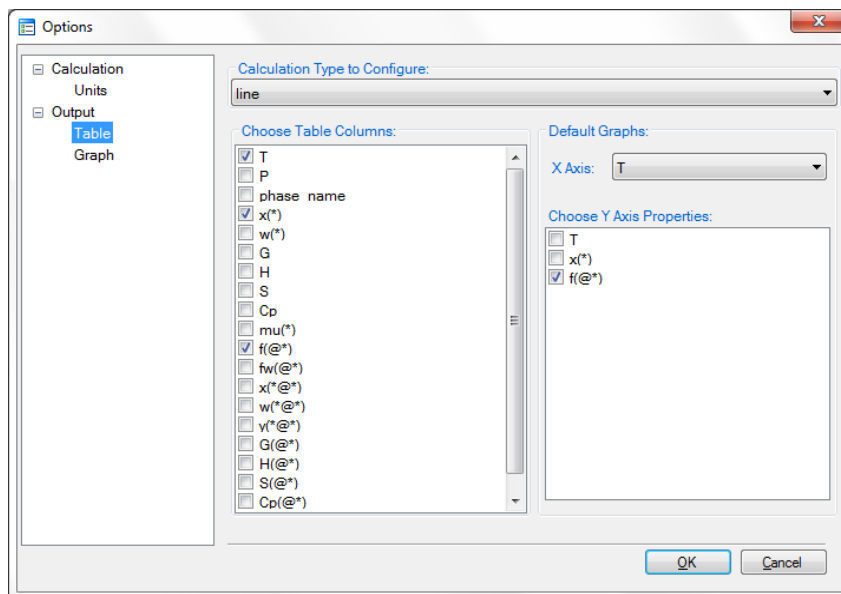


Figure 3.7 Set default table output and default dataset for graph output

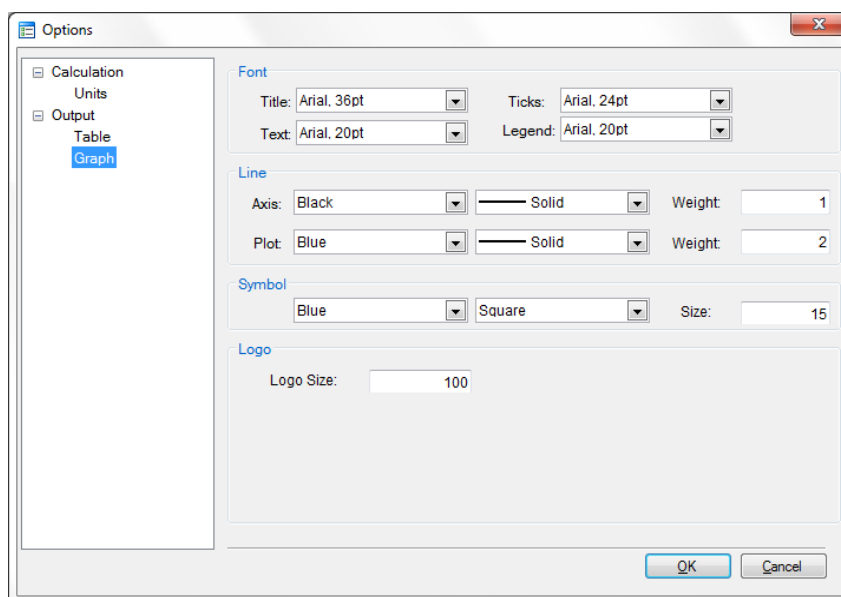




Figure 3.8 Set the appearance parameters for graph

3.3 Tutorial

The Al-Mg-Zn is used as an example for the following calculations. The Al-Mg-Zn.tdb is in the PanPhaseDiagram directory under Pandat examples. Load the database by clicking the  button and select all three components.

3.3.1 Point Calculation (0D)

This function allows the user to calculate the stable phase equilibrium at a single point in a multicomponent system.

Go to **PanPhaseDiagram** on the menu bar and select **Point Calculation** or click the  button on the the tool bar. The dialog box for **Point Calculation** as shown in Figure 3.9(a) allows the user to set up the calculation conditions: composition and temperature. User can always save the current alloy composition in hard disc by clicking **Save Chemistry**. The user can load the alloy composition in the future calculation using the function **Load Chemistry** following Figure 3.9(b).

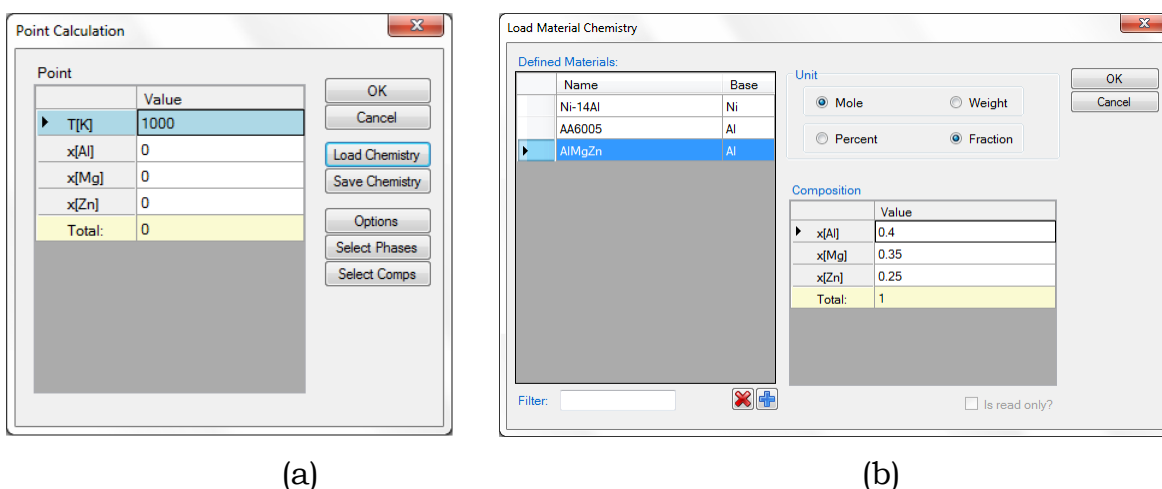



Figure 3.9 Set alloy composition and Temperature for point calculation

The user can access the **Options** window again by clicking **Options** and make any changes for the units. Please refer to the previous section for information on the **Options** window. **Select Phases** button leads the user to a dialog which allows user to select or deselect phases to be involved in the calculation as shown in Figure 3.10. The default setting is that all the phases in the system are selected and listed in the Entered Phases column. User can select the phases that will not participate in the calculation and send them to the Available Phases column using the  key. To select several phases at one time, hold the <Ctrl> key and use mouse to select multiple phases. The **Select Comps** button allows user to make last minute change on the component selection. Please refer to the previous section for information on the **Select Components** window.

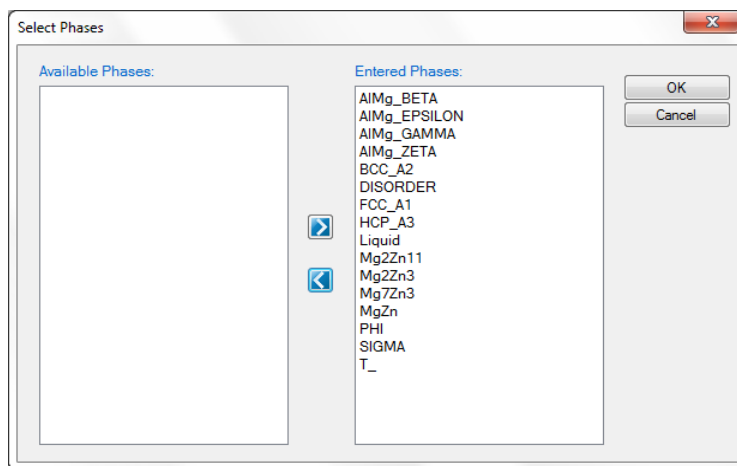



Figure 3.10 Select Phases dialog

After the calculation is completed, the calculated results are displayed in the Pandat main display window as a single row Table. The data in a table may be saved by using the shortcut keys. First use the mouse to select the part to be saved. Then press down the <ctrl> plus the “C” key to make a copy of the selected part. Finally, use the paste option or <ctrl>+“V” to paste the selected

part to another application such as Notepad, Excel or Word. These operations may also be realized through the commands in **Edit** menu.

3.3.2 Line Calculation (1D)

This function allows the user to calculate a series of point calculations along a line in a multicomponent system. Go to **PanPhaseDiagram** on the menu bar and select **Line Calculation** or click the  button on the tool bar. The **Line Calculation** (1D) dialog box allows the user to set the start and end points of the line, and the number of calculations or steps to be performed along the line as shown in Figure 3.11. The user can also access the calculation **Options**, **Select Comps** and **Select Phases** windows through this dialog box. The function **Save Condition** can save the current calculation condition on to disk and be reloaded in the future by using the **Load Condition** button. Note that the line calculation set up in Figure 3.11 is along the line of fixing alloy chemistry with varying temperature.

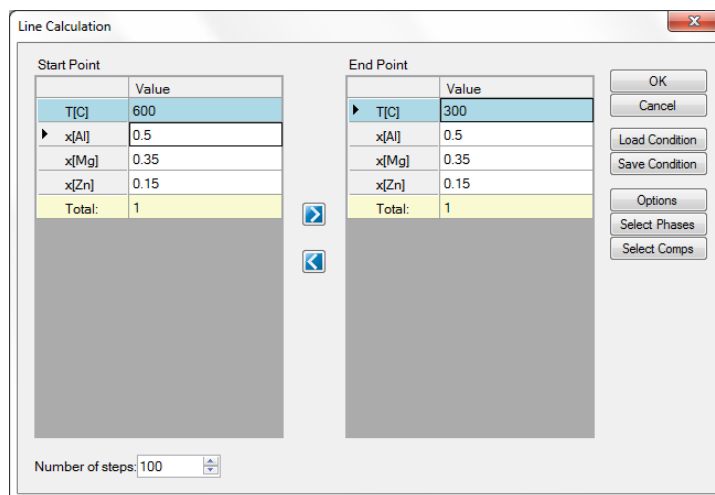


Figure 3.11 Set calculation conditions for a line calculation

The calculated results are stored in graph and table. The default graph plots the variation of fraction of each phase with respect to temperature, as shown in Figure 3.12. The user can modify the figure through the Property window for

the title and legend to get a better view as shown in Figure 3.13, or generate new table and plot other figures as needed.

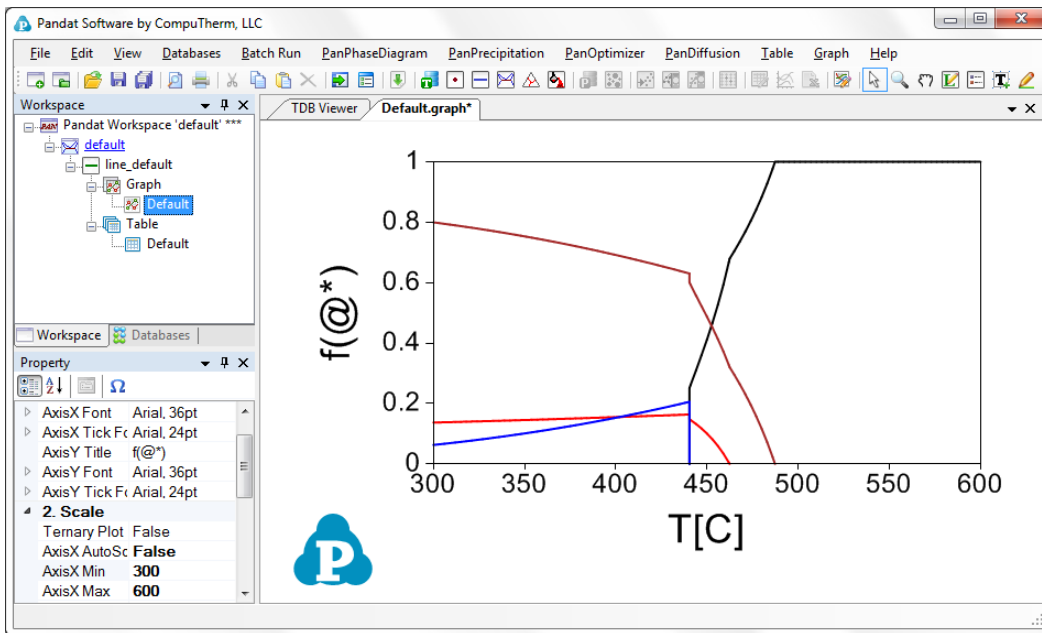


Figure 3.12 Graph view of the line calculation result

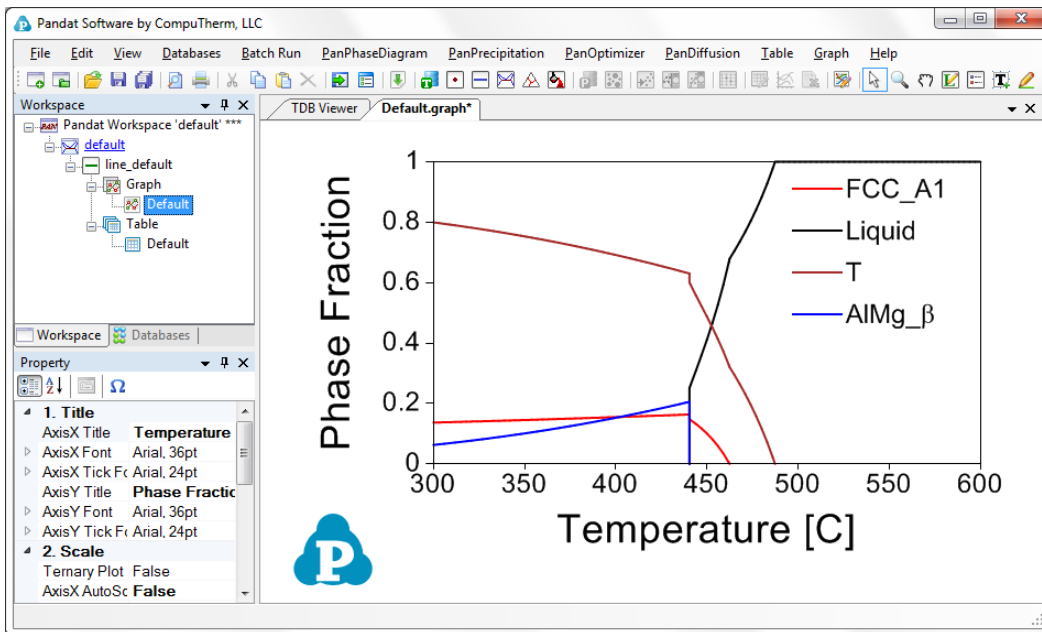



Figure 3.13 Modify the graph with a better view

It should be pointed out that user can certainly choose to fix the temperature and vary the alloy composition for a line calculation.

3.3.3 Section Calculation (2D)

This function allows user to calculate any two-dimensional section of a multicomponent system. Three non-collinear points in the calculation space are required to define a 2D section. Common 2D section diagrams are isotherms and isopleths.

Go to **PanPhaseDiagram** on the menu bar and select **Section Calculation** or click the  button on the the tool bar. The **Section (2D) Calculate** dialog box allows the user to set up the calculation conditions in terms of composition and temperature. Figure 3.14 shows the two most common 2D calculations for a ternary system: (a) Isotherms which is a horizontal section that fixes the temperature and (b) Isopleth which is a vertical section that uses the temperature as the Y axis.

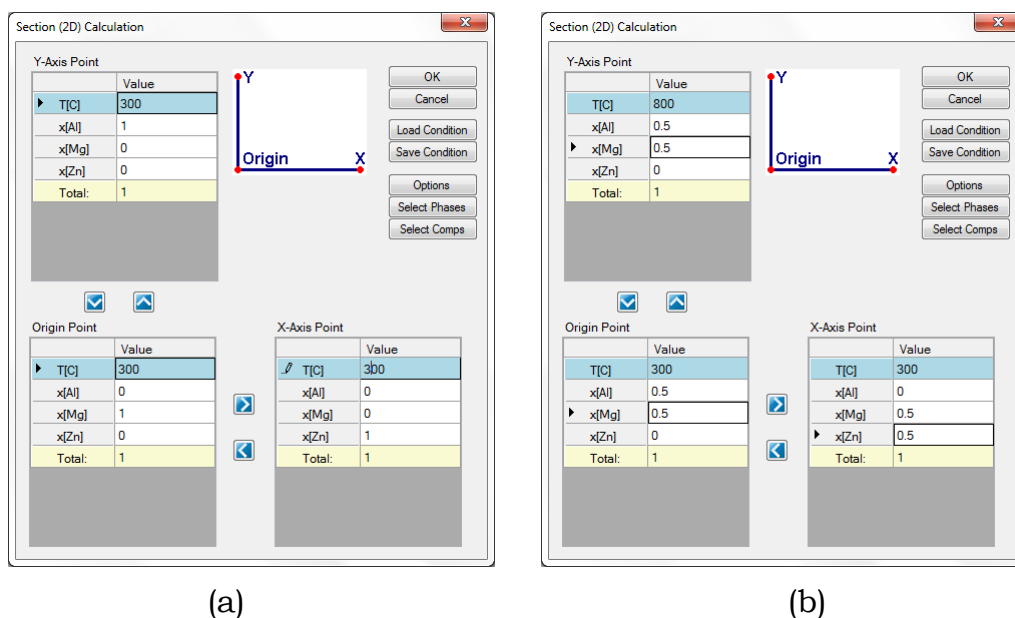


Figure 3.14 Set calculation conditions for section calculation

The composition at each point should be self-consistent. For example, $x(\text{Al})+x(\text{Mg})+x(\text{Zn})=1$ for the Al-Mg-Zn ternary system. It is not necessary to have a correlation between a **Y-Axis** point, the **Origin** point and an **X-Axis** point. The user can also access the **Options**, **Select Phases** and **Select Comps** windows through this dialog box.

The setting on Figure 3.14(a) defines a calculation of an isothermal section for the Al-Mg-Zn ternary at 300°C. The setting on Figure 3.14(b) defines a vertical section calculation from the middle of the Al-Mg binary to the middle of the Mg-Zn binary in the temperature range of 300-800 °C. The results from a Section calculation are displayed in two types of format in the Pandat main window: Graph and Table. Figures 3.15 and 3.16 show the graph view of the two calculation results and Figure 3.17 shows a table view of the isotherm calculation result. Users can switch between Graph view and Table View by clicking “Graph” and “Table” on top of the Pandat Explorer window. Extensive operations on **Graph** and **Table**, such as labeling and adding a legend, have been discussed in details in [Section 2.3](#) and [Section 2.4](#).

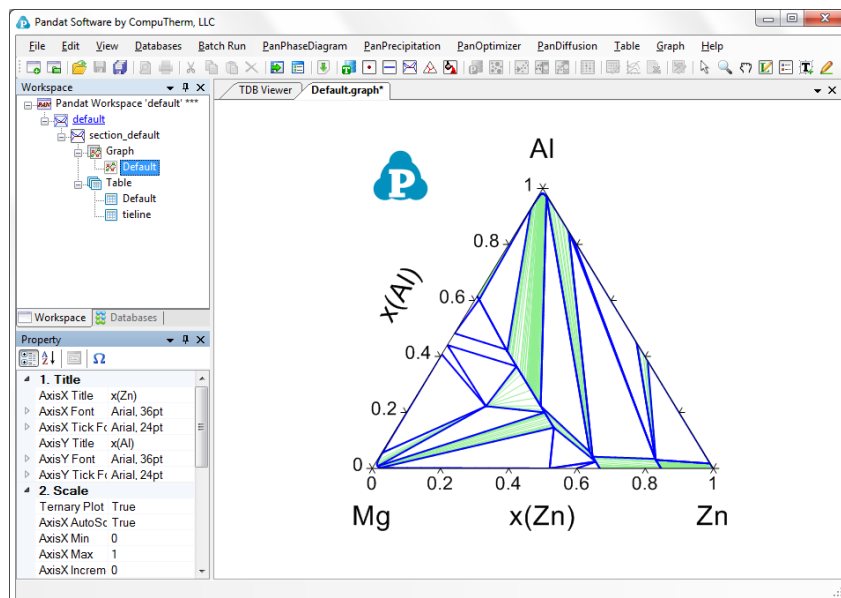


Figure 3.15 Isothermal section of the Al-Mg-Zn ternary system at 300 °C

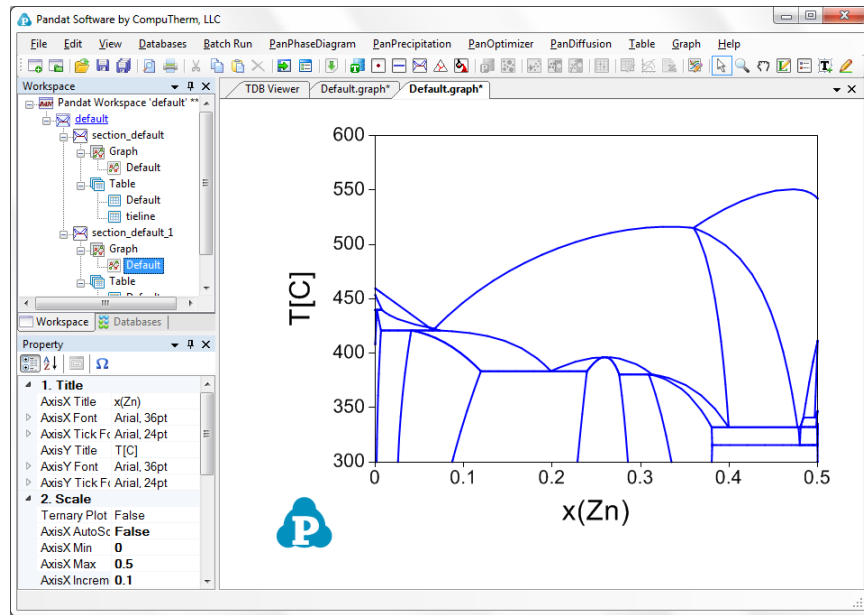



Figure 3.16 Isopleth of the Al-Mg-Zn ternary system at 50 at.% of Mg

	T	P	x(Al)	x(Mg)	x(Zn)	w(Al)	
	atm	mole/mole	mole/mole	mole/mole	mole/mole	kg/kg	
1	300.0000	1.000000	0.927675	0.071528	0.000796	0.933241	0.06
2	300.0000	1.000000	0.927684	0.071520	0.000796	0.933248	0.06
3	300.0000	1.000000	0.927694	0.071510	0.000796	0.933257	0.06
4	300.0000	1.000000	0.927713	0.071490	0.000797	0.933274	0.06
5	300.0000	1.000000	0.927870	0.071331	0.000799	0.933414	0.06
6	300.0000	1.000000	0.928182	0.071014	0.000804	0.933692	0.06
7	300.0000	1.000000	0.930682	0.068474	0.000844	0.935916	0.06
8	300.0000	1.000000	0.940680	0.058282	0.001038	0.944746	0.05
9	300.0000	1.000000	0.960666	0.037560	0.001773	0.961823	0.03
10	300.0000	1.000000	0.970627	0.026717	0.002656	0.969532	0.02
11	300.0000	1.000000	0.975548	0.020910	0.003542	0.972661	0.01
12	300.0000	1.000000	0.977936	0.017781	0.004283	0.973717	0.01
13	300.0000	1.000000	0.979073	0.016125	0.004802	0.973973	0.01
14	300.0000	1.000000	0.980121	0.014395	0.005484	0.973909	0.01
15	300.0000	1.000000	0.980582	0.013512	0.005906	0.973702	0.01
16	300.0000	1.000000	0.980977	0.012633	0.006390	0.973344	0.01
17	300.0000	1.000000	0.981284	0.011782	0.006934	0.972818	0.01
18	300.0000	1.000000	0.981398	0.011377	0.007225	0.972494	0.01
19	300.0000	1.000000	0.981546	0.010622	0.007833	0.971736	0.00
20	300.0000	1.000000	0.981580	0.010277	0.008143	0.971312	0.00
21	300.0000	1.000000	0.981501	0.009108	0.009391	0.969419	0.00

Figure 3.17 Table view for the 300 °C isotherm calculation results

3.3.4 Liquidus Projection

This function permits the calculation of a liquidus projection diagram for a system with more than two components. PanEngine automatically searches the univariant liquidus lines.

Go to **PanPhaseDiagram** on the menu bar and select **Liquidus Projection** or Click the  button on the the tool bar. The **Liquidus Projection** dialog box shown in Figure 3.18 allows the user to calculate univariant liquidus lines, i.e., liquidus projection for a multicomponent system. Isothermal curves involving the liquid phase in a ternary system can also be calculated by checking the box **Calculate Isotherms**. The density of isothermal curves depends on the scale of **Temperature Interval**. A larger value for the temperature interval leads to fewer isothermal curves but with increased speed of calculation. The default **Compositional Range** is full range for each component. The user can also access the calculation **Options** and **Select Phases** windows through this dialog box.

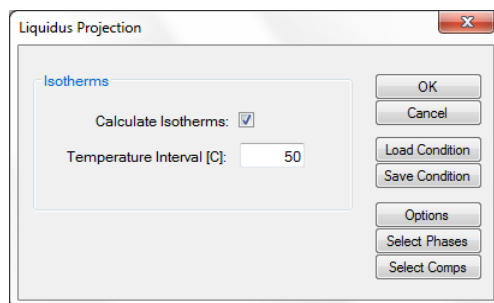


Figure 3.18 Liquidus calculation setting dialog

The results from a liquidus projection calculation are displayed in two types of format in the Pandat main window: Graph and Table. Figures 3.19, 3.20 and 3.21 show the graph view, default table and isotherm table for the liquidus projection calculation results, respectively. Users can switch between Graph view to Table View by clicking “Graph” and “Table” in the Pandat Explorer

window. Extensive operations on Graph and Table, such as labeling and adding legend, have been discussed in details in [Section 2.3](#) and [Section 2.4](#).

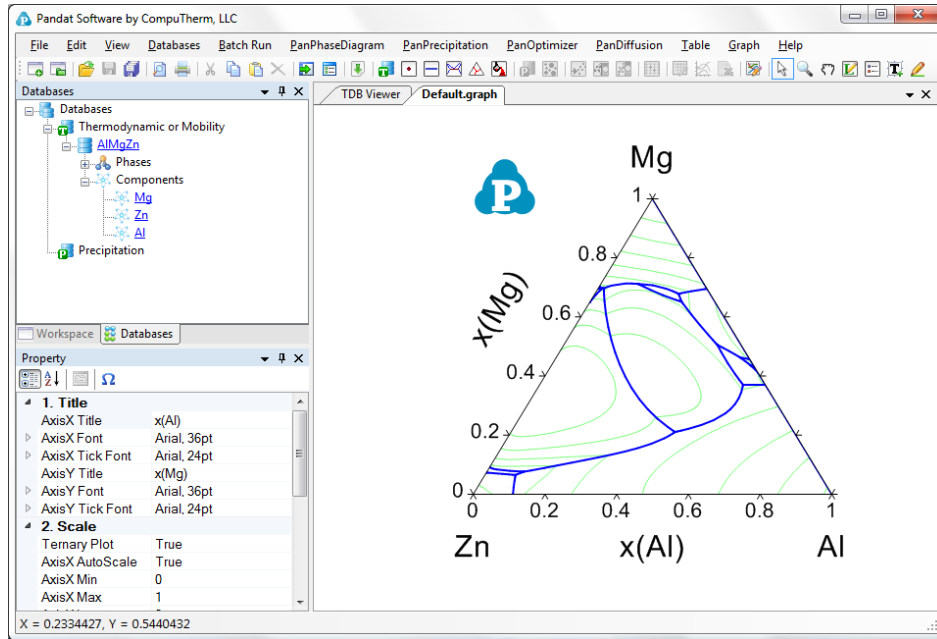


Figure 3.19 Liquidus projection of the Al-Mg-Zn ternary system

	T	P	x(Al)	x(Mg)	x(Zn)	w(Al)
C	atm	mole/mole	mole/mole	mole/mole	kg/kg	
1	332.0880	1.000000	0.012734	0.696849	0.290417	0.009473
2	332.3050	1.000000	0.012406	0.696987	0.290607	0.009227
3	332.5320	1.000000	0.012062	0.697131	0.290807	0.008970
4	332.9840	1.000000	0.011375	0.697419	0.291206	0.008455
5	333.8830	1.000000	0.010000	0.697993	0.292007	0.007427
6	334.7750	1.000000	0.008625	0.698564	0.292810	0.006401
7	334.9970	1.000000	0.008282	0.698707	0.293012	0.006145
8	335.0650	1.000000	0.008176	0.698750	0.293073	0.006066
9						
10	335.0650	1.000000	0.008176	0.698750	0.293073	0.006066
11	335.3140	1.000000	0.007836	0.698871	0.293293	0.005812
12	335.8100	1.000000	0.007155	0.699111	0.293734	0.005305
13	336.7970	1.000000	0.005794	0.699590	0.294616	0.004292
14	338.7450	1.000000	0.003073	0.700541	0.296387	0.002272
15	340.6580	1.000000	0.000353	0.701482	0.298165	0.000261
16	340.7770	1.000000	0.000183	0.701541	0.298276	0.000135
17	340.8950	1.000000	0.000013	0.701599	0.298387	0.000010
18	340.9020	1.000000	0.000003	0.701603	0.298394	0.000002
19	340.9020	1.000000	0.000001	0.701603	0.298395	0.000000


Figure 3.20 Default table view for the liquidus projection calculation results

	T	x(AI)	x(Mg)	x(Zn)	w(AI)	w(Mg)
	C	mole/mole	mole/mole	mole/mole	kg/kg	kg/kg
1	600.0000	7.153650E-007	0.936090	0.063909	7.167280E-007	0.844823
2	600.0000	0.000002	0.936090	0.063908	0.000002	0.844823
3	600.0000	0.000007	0.936088	0.063905	0.000007	0.844826
4	600.0000	0.000018	0.936085	0.063898	0.000018	0.844831
5	600.0000	0.000039	0.936078	0.063883	0.000039	0.844841
6	600.0000	0.000124	0.936050	0.063826	0.000124	0.844883
7	600.0000	0.000208	0.936022	0.063770	0.000209	0.844924
8	600.0000	0.000547	0.935911	0.063542	0.000548	0.845089
9	600.0000	0.005955	0.934182	0.059863	0.006000	0.847832
10	600.0000	0.008653	0.933347	0.058000	0.008741	0.849273
11	600.0000	0.010000	0.932938	0.057062	0.010115	0.850011
12	600.0000	0.011346	0.932533	0.056121	0.011491	0.850761
13	600.0000	0.014034	0.931738	0.054228	0.014252	0.852293
14	600.0000	0.019397	0.930203	0.050399	0.019804	0.855492
15	600.0000	0.030068	0.927350	0.042582	0.031042	0.862417
16	600.0000	0.051181	0.922442	0.026378	0.054100	0.878327
17	600.0000	0.071970	0.918531	0.009498	0.078026	0.897019
18	600.0000	0.082231	0.916949	0.000820	0.090345	0.907473
19	600.0000	0.082869	0.916859	0.000772	0.091122	0.908159

Figure 3.21 Isotherms table for the liquidus projection calculation results

3.3.5 Solidification Simulation

Two simple property models, equilibrium solidification and Scheil solidification, have been integrated into Pandat for calculating solidification pathways. The equilibrium model, also called the lever rule model, assumes that complete diffusion occurs in both liquid and solid phases, and the compositions of solid and liquid always follow the phase boundaries defined by the equilibrium phase diagram. The fractions of liquid and solid can be calculated through the lever rule. In contrast, Scheil solidification assumes that no diffusion occurs in the solid phases, that the composition of liquid phase is uniform (infinite diffusivity in liquid) and that local equilibrium at the solid-liquid interface is always maintained. The **Solidification Simulation** function calculates the solidification path of an alloy using either the lever rule or Scheil model as being decided by the user.

Go to **PanPhaseDiagram** on the menu bar and select **Solidification Simulation** or click the  button on the tool bar. The dialog box as shown in Figure 3.22 allows the user to set up alloy compositions of interest and the estimated temperature of the liquidus surface. The user can choose the simulation under either **Non-Equilibrium(Scheil)** or **Equilibrium (Lever Rule)** condition. The maximum temperature step size and the minimum of mole fraction of liquid phase can be adjusted in the input dialog.

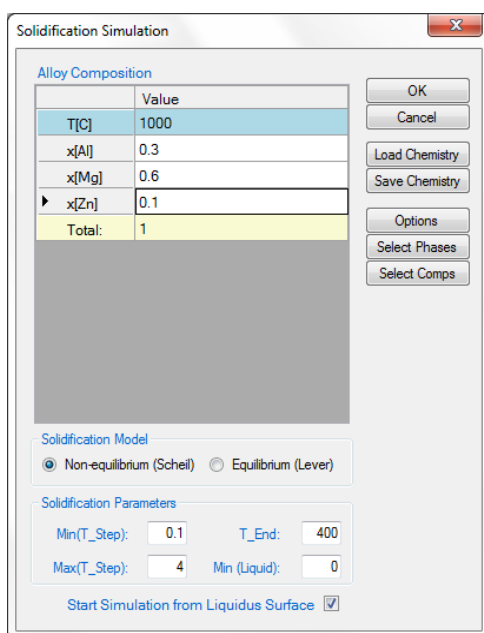


Figure 3.22 Set calculation conditions for solidification simulation

The results are displayed in either Graph View or Table View. Figures 3.23 and 3.24 show the graph view and table view for the solidification simulation results with the calculation condition shown in Figure 3.22. Extensive operations on Graph and Table, such as labeling and adding legend, have been discussed in details in [Section 2.3](#) and [Section 2.4](#).

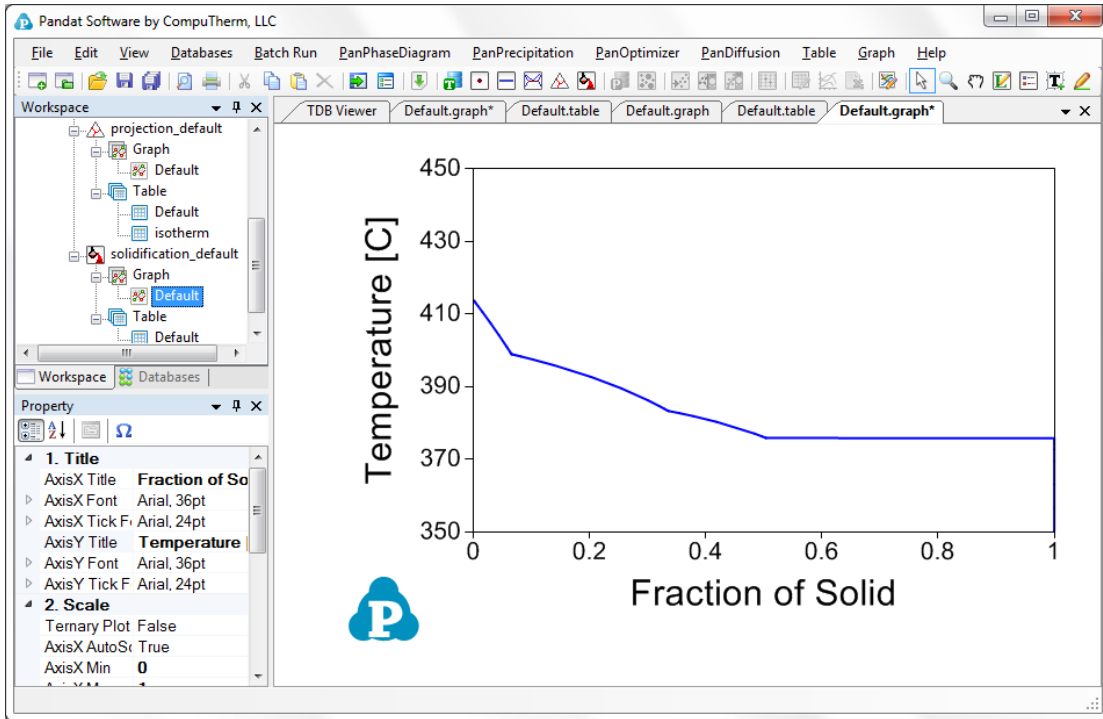


Figure 3.23 Graph view of the solidification simulation result

	T	P	x(Al)	x(Mg)	x(Zn)	w(Al)	
	C	atm	mole/mole	mole/mole	mole/mole	kg/kg	
1	413.7410	1.000000	0.300000	0.600000	0.100000	0.277055	0.49
2	413.6410	1.000000	0.299983	0.600098	0.099919	0.277071	0.49
3	413.4410	1.000000	0.299949	0.600295	0.099757	0.277103	0.49
4	413.0410	1.000000	0.299879	0.600687	0.099433	0.277167	0.50
5	412.2410	1.000000	0.299739	0.601471	0.098790	0.277292	0.50
6	410.6410	1.000000	0.299448	0.603035	0.097517	0.277528	0.50
7	407.4410	1.000000	0.298832	0.606144	0.095024	0.277951	0.50
8	404.2410	1.000000	0.298185	0.609221	0.092594	0.278324	0.51
9	401.0410	1.000000	0.297507	0.612268	0.090225	0.278647	0.51
10	399.4410	1.000000	0.297162	0.613778	0.089060	0.278796	0.51
11	399.0410	1.000000	0.297076	0.614153	0.088771	0.278832	0.51
12	398.9780	1.000000	0.297062	0.614213	0.088725	0.278838	0.51
13	398.9410	1.000000	0.296945	0.614316	0.088739	0.278725	0.51
14	398.7410	1.000000	0.296306	0.614876	0.088818	0.278111	0.51
15	398.3410	1.000000	0.295040	0.615988	0.088972	0.276894	0.52
16	397.5410	1.000000	0.292547	0.618180	0.089273	0.274500	0.52
17	395.9410	1.000000	0.287709	0.622448	0.089843	0.269863	0.52

Figure 3.24 Table view of the solidification simulation result

4. PanOptimizer

PanOptimizer is a module of Pandat™ software designed for optimizing thermodynamic, kinetic and thermo-physical model parameters using experimental data. The module allows users to develop their own databases or model parameters for customized applications. This module is also easy to master by students who want to learn thermodynamic modeling.

4.1 Features of PanOptimizer

4.1.1 Normal Optimization

Derived from the maximum likelihood principle, when the discrepancies between model-calculated and experimental values are assumed to be independent, identically distributed with a normal distribution function, a set of model parameters with the best fit to the given experimental data can be obtained by the least square method. In the real world the experimental data may come from different sub-populations for which an independent estimate of the error variance is available. In this case, a better estimate than the ordinary least squares (OLS) can be obtained using weighted least squares (WLS), also called generalized least squares (GLS), then the sum of the squares can be written as

$$\frac{1}{2} \sum_{j=1}^m w_j [y_j - \phi(x; T_j, c_j)]^2 \quad (4.1)$$

The idea is to assign each observation a weight factor that reflects the uncertainty of the measurement. According to our previous experiences this

method is efficient and reliable in the optimization of model parameters and develop variety of databases.

4.1.2 Rough Search

“Rough Search” is used to obtain a rough topology of a phase diagram based on the given experimental data. It is useful for quickly estimating the initial values of the model parameters at the beginning stage of the optimization procedure. The algorithm implemented in PanOptimizer for a rough search is based on the condition of equilibrium between any two specified phases in a closed system at constant P and T:

$$\mu_c(i) = \mu_c(j) \text{ for any component C in any two phases } i, j \quad (4.2)$$

For a given two-phase equilibrium between phase i and j , their chemical potential $\mu_c(i)$ and $\mu_c(j)$ can be calculated at the given equilibrium compositions measured experimentally. A set of model parameters can thus be obtained by minimizing the chemical potential differences between any two phases in equilibrium. The least square problem is then written as:

$$\frac{1}{2} \sum_{k=1}^m w_k \sum_C \left[\frac{\mu_c(i) - \mu_c(j)}{RT_k} \right]^2 \quad (4.3)$$

where w_k is a weight factor that reflects the uncertainty of the measurement for equilibrium k , and i and j represent any two phases in equilibrium k .

The idea of rough search is now illustrated using the Al-Zn system as an example. Figure 4.1(a) is the calculated phase diagram using random assigned model parameters for Liquid, FCC_A1, HCP_A3, and Figure 4.1(b) is the phase

diagram calculated after the rough search. Figure 4.1(c) and Figure 4.1(d) show the Gibbs energy curves for phases i =FCC_A1 and j =HCP_A3 at 500K calculated by the model parameters used to calculate phase diagrams in Figure 4.1(a) and Figure 4.1(b), respectively. The compositions of experimental tie-line between these two phases are also highlighted in the phase diagrams for comparison. The chemical potentials for both Al and Zn are quite different in the two phases before the rough search as is seen in Figure 4.1(c). This is due to the fact that the calculated equilibrium between these two phases at 500K using the initial assigned parameters is off from the given experimental tie-line composition as demonstrated in Figure 4.1(a). After rough search, the chemical potential differences between Fcc_A1 and Hcp_A3 become almost zero for both Al and Zn as shown in Figure 4.1(d) and the calculated phase diagram agrees with the experimental data very well as shown in Figure 4.1(b). It should be pointed out that equilibrium at 500K is used in this example for the purpose of illustration. In the real case, tie-line compositions at different temperatures should be used for optimization.

In the rough search, in addition to minimize chemical potential difference of two phases, the differences between the calculated and measured thermodynamic properties, such as the enthalpy or entropy data, for a given single phase can also be minimized to obtain the best set of model parameters. Therefore, the final least square problem for rough search is then written as:

$$\frac{1}{2} \sum_{k=1}^m w_k \sum_C \left[\frac{\mu_C(i) - \mu_C(j)}{RT_k} \right]^2 + \frac{1}{2} \sum_{j=1}^n w_j [y_j - \phi(x; T_j, c_j)]^2 \quad (4.4)$$

The meaning of the second term in equation (4.4) is the same as that in equation (4.1) except that it only describes the thermodynamic properties of a single phase.

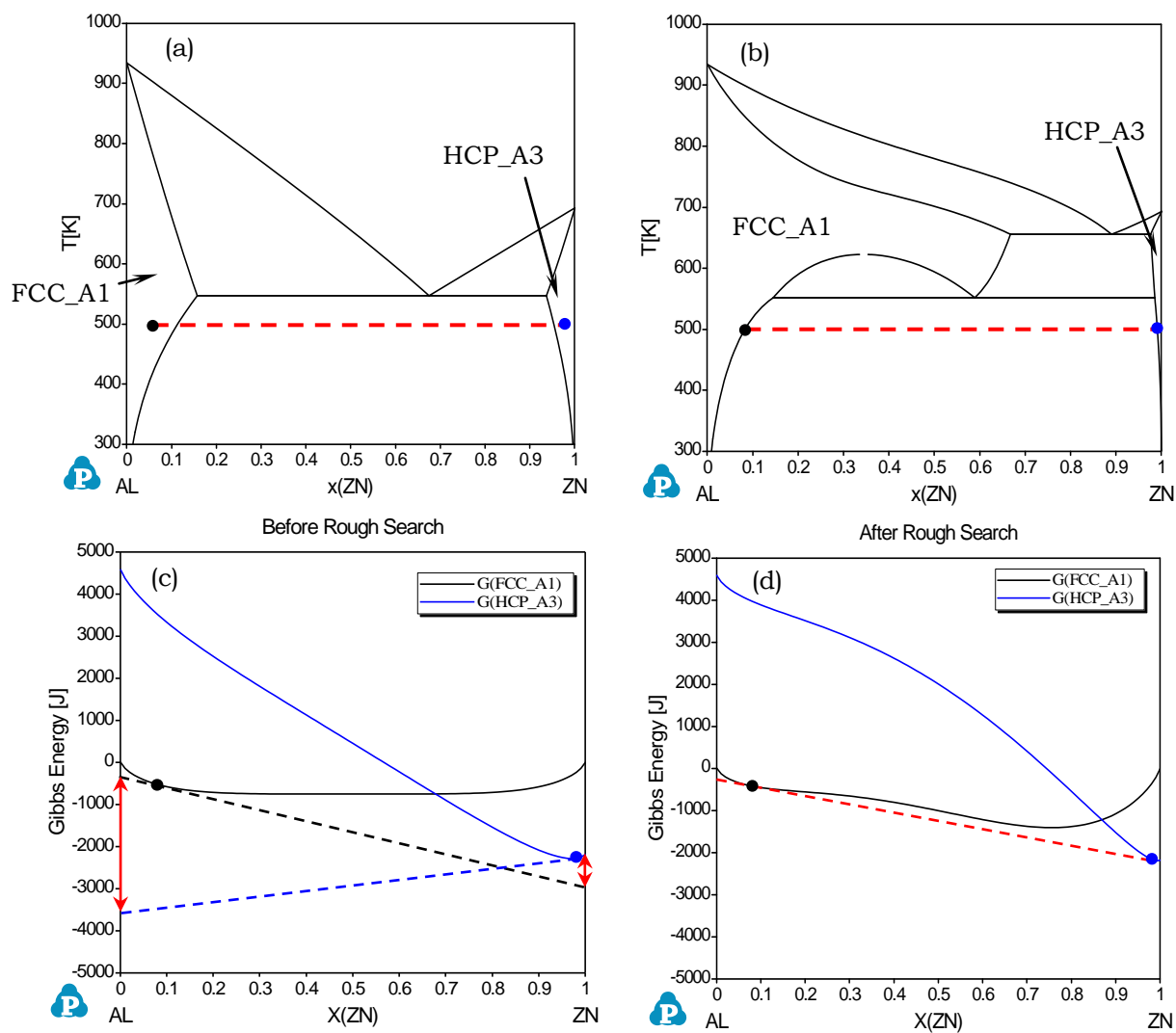


Figure 4.1 (a) Calculated Al-Zn phase diagram before the rough search
 (b) Calculated Al-Zn phase diagram after the rough search
 (c) Calculated Gibbs energy curves before the rough search
 (d) Calculated Gibbs energy curves after the rough search

4.2 PanOptimizer Functions

The major functions included in the PanOptimizer menu are shown in Figure 4.2:

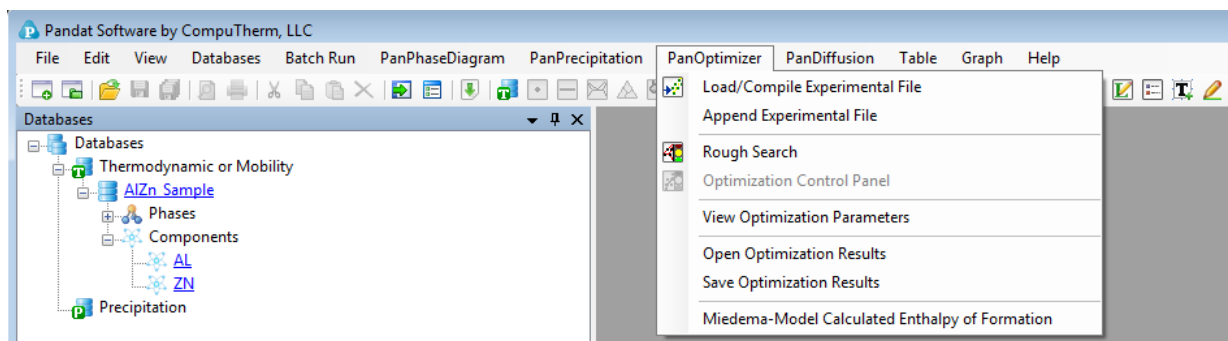


Figure 4.2 The PanOptimizer Menu

The shortcut of the three commonly used functions **Load/Compile Experimental File**, **Rough Search** and **Optimization Control Panel** are also displayed in the Toolbar as shown in Figure 4.3.

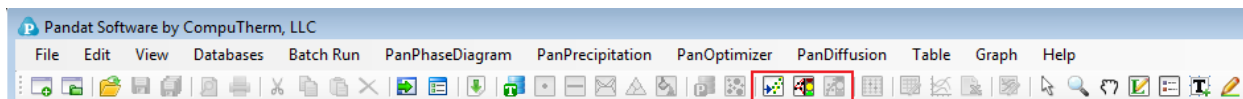


Figure 4.3 PanOptimizer toolbar

The functionality of each function is given below:

- **Load/Compile Experimental File**: Load/Compile experimental data file for model parameter optimization
- **Append Experimental File**: Append more experimental data from different data file

- **Rough Search**: Global/Local search of initial values of model parameters for obtaining the phase diagram topology of a system

- **Optimization Control Panel**: Allow user to set boundaries for the model parameters to be optimized, select experimental data to be used, and assign weight to each set of experimental data

- **View Optimization Parameters**: View/Edit model parameters to be optimized

- **Open Optimization Results**: Open the saved intermediate optimization results including the model parameters and experimental data

- **Save Optimization Results**: Save the intermediate optimization results during the optimization process including the model parameters and experimental data

4.3 Step by Step Instruction for Normal Optimization

In general, user should follow a few steps below to perform the model parameter optimization.

4.3.1 Step 1: File preparation

- Prepare the thermodynamic database file (.TDB)

In order to do the optimization, user must first define the model parameters to be optimized in the thermodynamic database (.tdb). The model parameters to be optimized can be defined in Pandat™ workspace where all the built-in keywords are automatically highlighted. It can also be done through outside text editor such as “Notepad”. Each model parameter that needs to be optimized is defined by the keyword “OPTIMIZATION”. The format of defining a model parameter is:

```
Optimization [parameter name][low bound][initial value][high bound] N !
```

A definition sample for liquid phase in binary Al-Zn system is given as follows

// Keyword	Name	Low Bound	Init. Value	High Bound	
Optimization	LIQ_AA	0	0;	60000	N !
Optimization	LIQ_AAT	-20	0;	20	N !
Optimization	LIQ_BB	-60000	0;	60000	N !
Optimization	LIQ_BBT	-20	0;	20	N !


```
Phase LIQUID % 1 1 !
Constituent LIQUID : AL, ZN : !
Parameter G(LIQUID, AL; 0)      298.15  G_Al_LIQUID;          6000 N !
Parameter G(LIQUID, ZN; 0)      298.15  G_Zn_LIQUID;          6000 N !
Parameter G(LIQUID, AL, ZN; 0) 298.15  LIQ_AA + LIQ_AAT*T;    6000 N !
Parameter G(LIQUID, AL, ZN; 1) 298.15  LIQ_BB + LIQ_BBT*T;    6000 N !
```

Two modes of optimization are allowed in the current version: one is “bounded” optimization and the other one is “no bound” optimization. Even though the low and high bounds will be in effect in the bounded optimization only, they are required for definition of model parameters in a TDB file. The model parameters can be named at users’ choices. It is suggested that the name is related to the phase to be optimized. Note: User may use “%” to denote the major species in a sublattice of a phase in a TDB file. PanOptimizer will automatically assign the initial values for the major species denoted by “%”. The following example means Zn is the major species in the first sublattice of the HCP_A3 phase:

```
Phase HCP _A3 % 2 1 0.5 !
Constituent HCP_A3: AL, ZN%: Va:!
```

- **Prepare the experimental file (.POP)**


Users need to provide their own experimental data file for optimization of model parameters. The most widely accepted format for experimental data file in the CALPHAD society is a POP file. PanOptimizer accepts most of the keywords in the POP format and adds a few special keywords. In a POP file, a phase can have four statuses: ENTERED, FIXED, DORMANT, and SUSPEND. The first

two statuses were used most frequently. When phases are in the ENTERED status, PanOptimizer does not require user to input any initial values for calculation since the truly stable phase equilibria will be found automatically in this case with the built-in global optimization algorithm. On the other hand, for those phases in FIXED or DORMANT status, the initial values should be provided by the user. Example POP files are provided in the installation dictionary of Pandat™.

4.3.2 Step 2: Carry out optimization

Once above files have been prepared, user is ready to carry out optimization:

- **Load thermodynamic database file**

First of all, the database file (.TDB) containing the phases to be modeled is loaded by click the  button. This database file defines the model type and model parameters of each phase in the system. The model definition is consistent with the currently accepted format in the CALPHAD society, and the model parameters can be real numbers or variables to be optimized.

- **Load and compile experimental file**

After loading a TDB file with defined model parameters to be optimized, users should then load and compile the experimental POP file. Go to PanOptimizer menu and choose **Load/Compile Experimental File**, user can then select the POP file already prepared as shown in Figure 4.4. User can also choose **Append Experimental File** to append new experimental data stored in a separate file to the currently opened POP file.

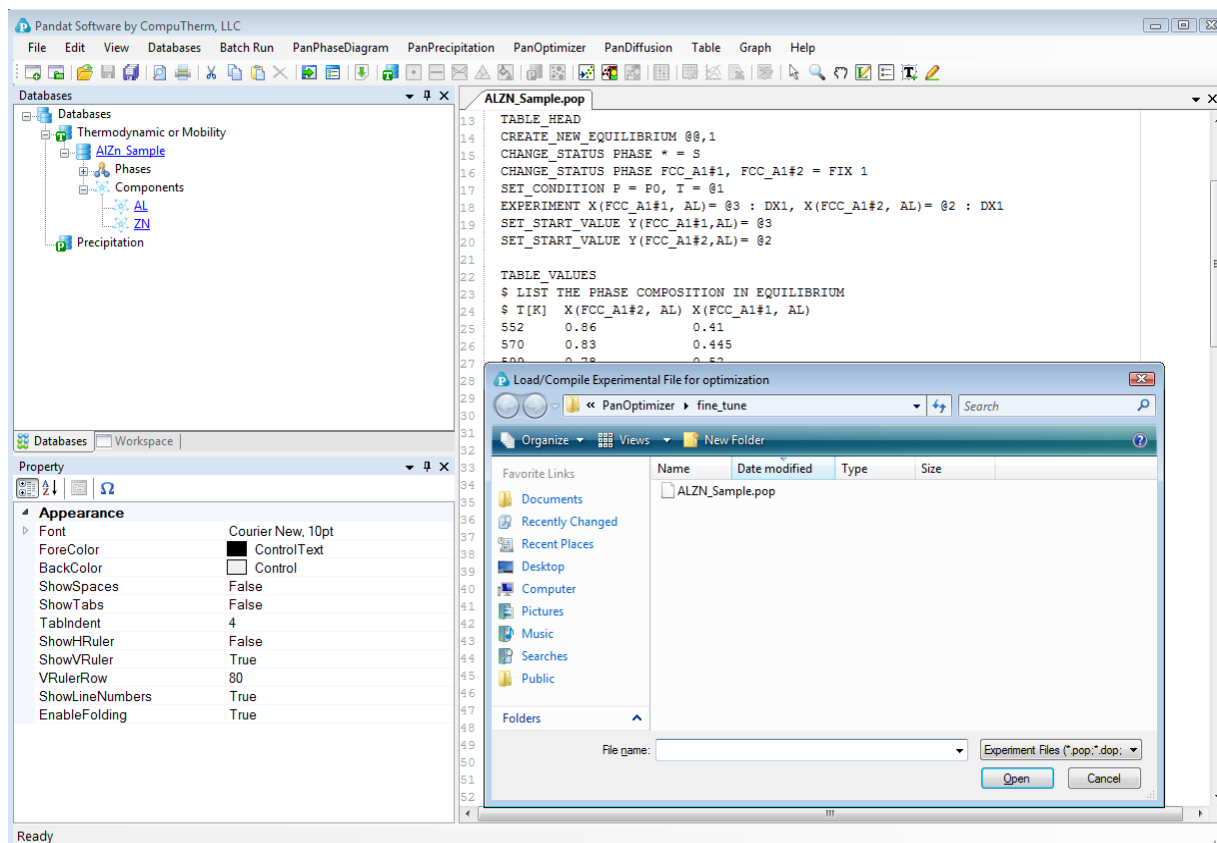


Figure 4.4 Dialog window of loading an experimental file

- **Perform Optimization**

Once the TDB file and the experimental POP file are loaded, user is ready to do the optimization. In the current version of PanOptimizer, the optimization is controlled through the optimization control panel as shown in Figure 4.5.

There are four control areas in the optimization control panel. They are: Histogram (A), Bound/Unbound Variables (B), Optimization (C), and Optimization Results (D).

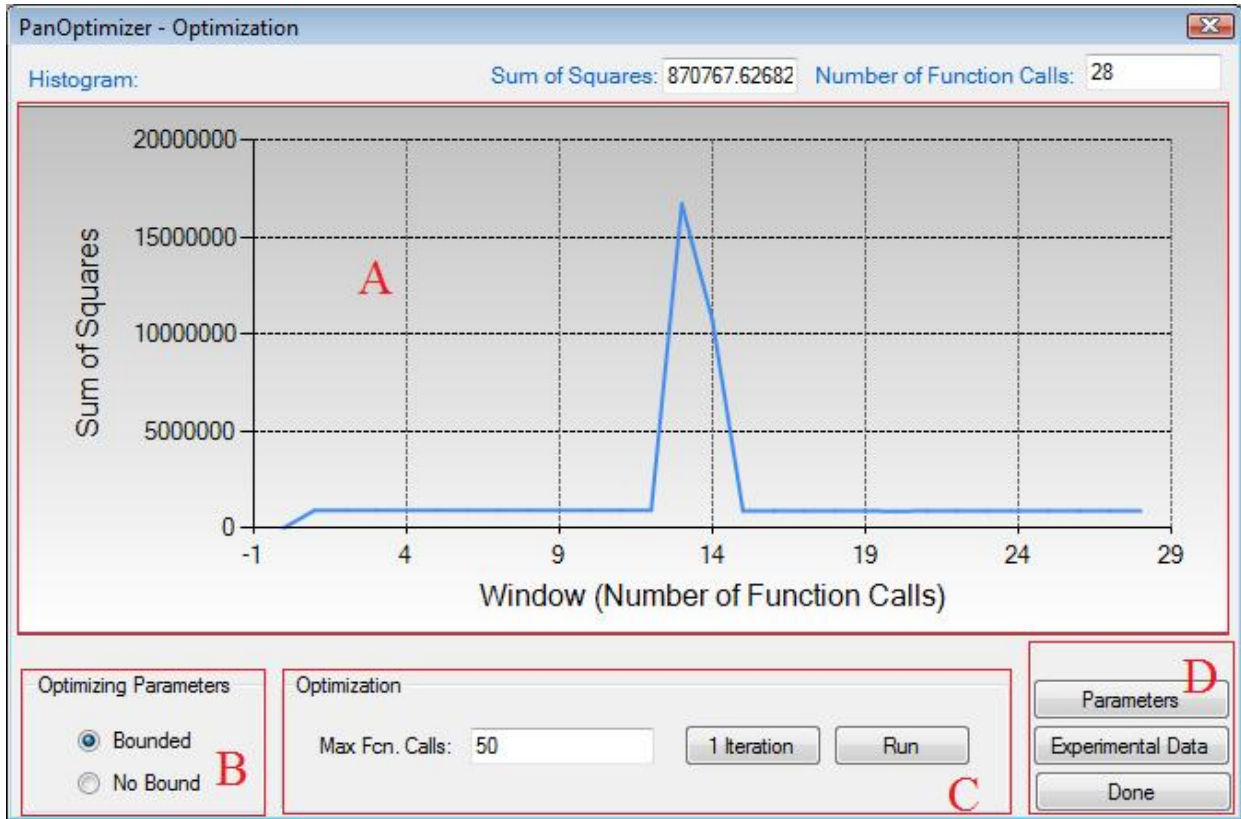


Figure 4.5 The optimization control panel.

- **Histogram (A)**

Histogram is for displaying and tracing the history of the discrepancy between model-calculated values and experimental data, which is characterized by the Sum of Squares displayed during the whole optimization procedure. The histogram plots the sum of squares *vs.* the number of function calls. The exact value of the sum of squares in the current step can be found at the up-right corner of this area.

- **Free Bound/Unbound Variables (B)**

The user can choose the model parameters to be optimized in either the bounded or the unbounded mode. In the bounded mode, the low and high bounds defined in a TDB file will take into effects.

- **Optimization (C)**

The goal of the optimization process is to obtain an optimal set of model parameters so that the model calculated results can best fit the given experimental measurements. The optimization process can be controlled by choosing **1 Iteration** or **Run**. With **1 Iteration**, the maximum number of function calls is set to be $2(N+2)$, where N is the number of model parameters to be optimized. The user can click **Run** mode several times until the optimal solution is found or the designated maximum number of function calls is reached.

Here we take the binary Al-Zn system as an optimization example. The TDB and POP files are available at the installing directory of Pandat “/Pandat_Examples/PanOptimizer/”. In this example, there are totally 11 parameters to be optimized and all the initial values are set to be zero. The available experimental data include:

- mixing enthalpy of liquid phase at 953K
- invariant reaction at 655K: LIQUID → FCC_A1 + HCP_A3
- invariant reaction at 550K: FCC_A1#2 → FCC_A1#1 + HCP_A3
- tie-lines: FCC_A1#1+FCC_A1#2, LIQUID+FCC_A1, LIQUID+HCP_A3 and HCP_A3+FCC_A1

Before the optimization, user may want to check the calculated results using the initial set of model parameters without optimization. Phase diagram calculation can be done through 2-D section calculation, and enthalpy calculation can be done through the 1-D line calculation. The Figure 4.6 shows the calculated Al-Zn phase diagram and enthalpy of liquid phase at 953K along with the given experimental data, respectively. The parameters without optimization result in large discrepancies between the calculated values and the experimental measurements. Optimization of these model parameters (initially set as zero) is needed.

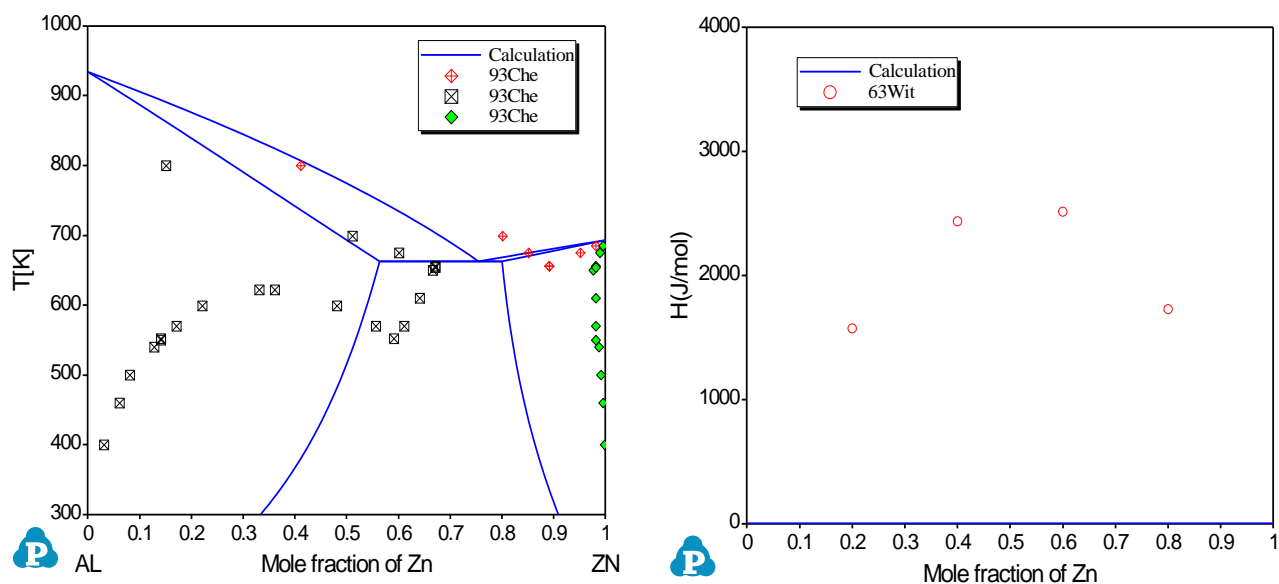


Figure 4.6 Comparisons between calculated results and experimental data before the optimization

By clicking **Run** twice (two rounds), and each run with 50 function calls, the sum of squares decreases from 904896 to 3061 as shown in Figure 4.7. After another two rounds of **Run**, the sum of squares decreases from 3061 to 2.8 as shown in Figure 4.8. Now, we can do the real time calculation using the instantly obtained optimized parameters. The two comparisons in Figure 4.9

show excellent agreements between the calculated results and the measurement data.

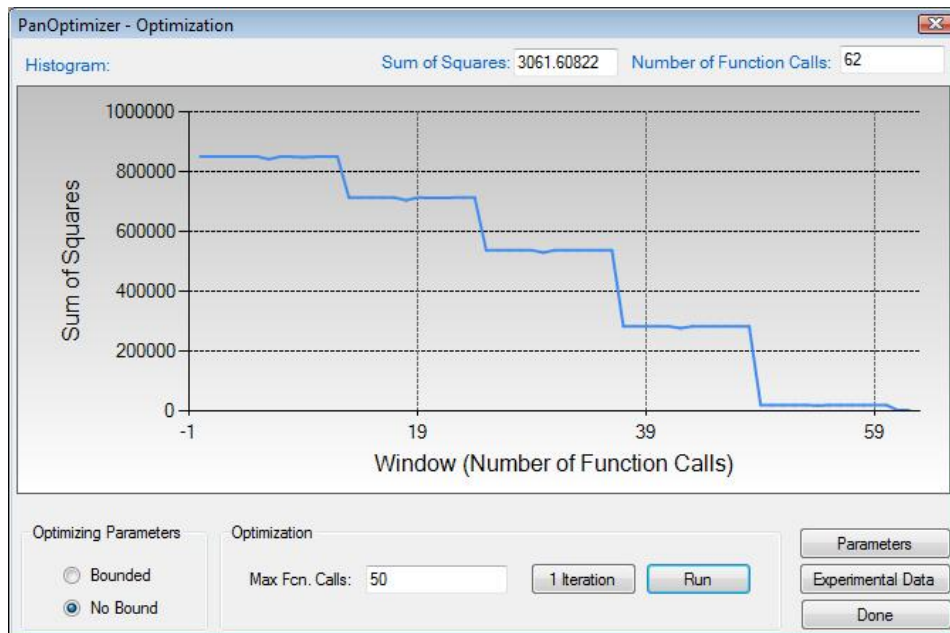


Figure 4.7 The sum of squares after two rounds of optimization

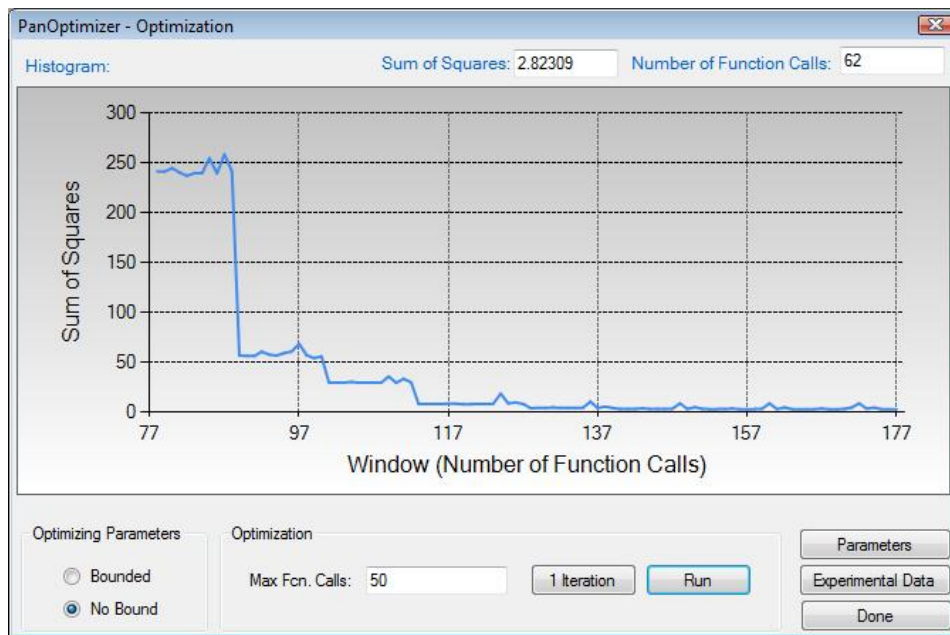


Figure 4.8 The sum of squares after another two rounds of optimization

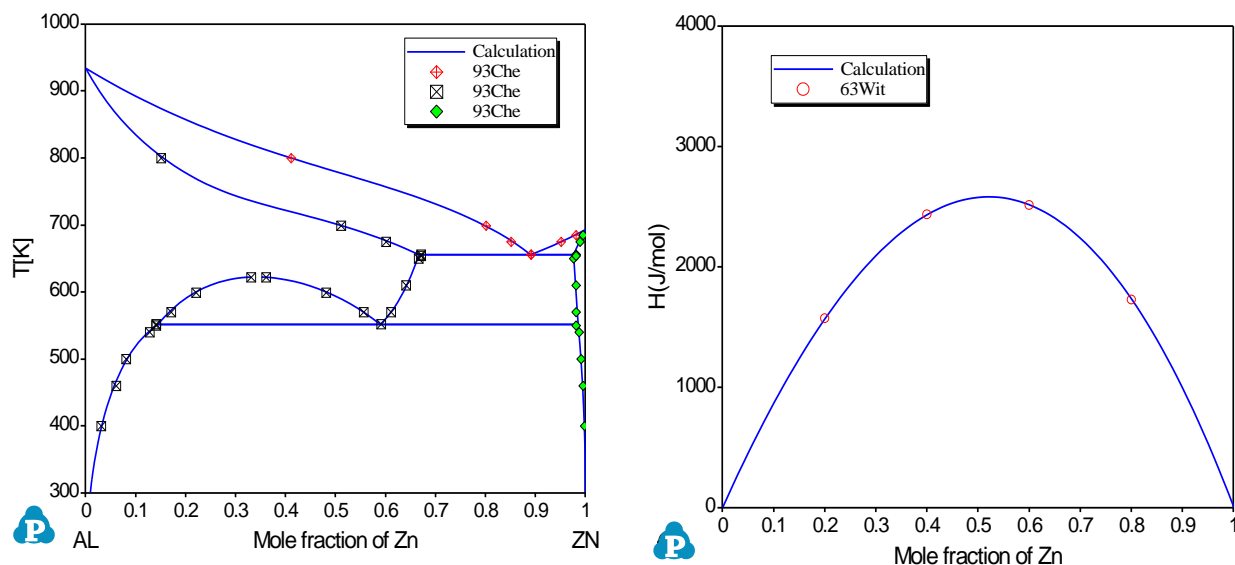


Figure 4.9 Comparisons between the calculated results and the experimental data after optimization

- **Optimization Results (D)**

During optimization, user can check model parameters through the **Parameters** button (see Figure 4.5). For each model parameter, user can change its low bound, upper bound and initial value in the dialog window as shown in Figure 4.10. User can **Include** or **Exclude** a certain parameter in the optimization through the “check box” in front of the parameter. If a set of optimized parameters is satisfactory, user can save this set of values as default ones through **Set Default** shown in Figure 4.10. Otherwise, user can reject this set of values and go back to previous default values through **Get Default**. User also can save the TDB file with the optimized model parameters through **Save TDB**. The standard deviation and relative standard deviation (RSD) of each parameter are computed during optimization. The parameter evolution during the last 100 iterations can be tracked by clicking the parameter name in the table as indicated in Figure 4.10. It should be noted that any changes on model

parameters made by user will take into effect only after the “**Apply**” button is clicked.

By clicking the **Experimental Data** button on Figure 4.8, a table which lists the calculated values and the experimental data for each experimental data set will pop out as shown in Figure 4.11. This table allows user to view how well the current optimized parameters describe each set of experimental data. If the discrepancy is found to be large and not satisfied for a certain set of data, a bigger weight factor for this set of data can be given in the next round of optimization. Through the column of “**Residual**” shown in Figure 4.11, user can see different color after each comparison. The green means satisfactory results are achieved, while the red color means large deviation remaining. Again, user can **Include** or **Exclude** a certain experimental data set for the optimization through the check box in front of each experimental data **Name**. Also, more detailed experimental data information can be viewed by clicking the experimental data ID in the table.

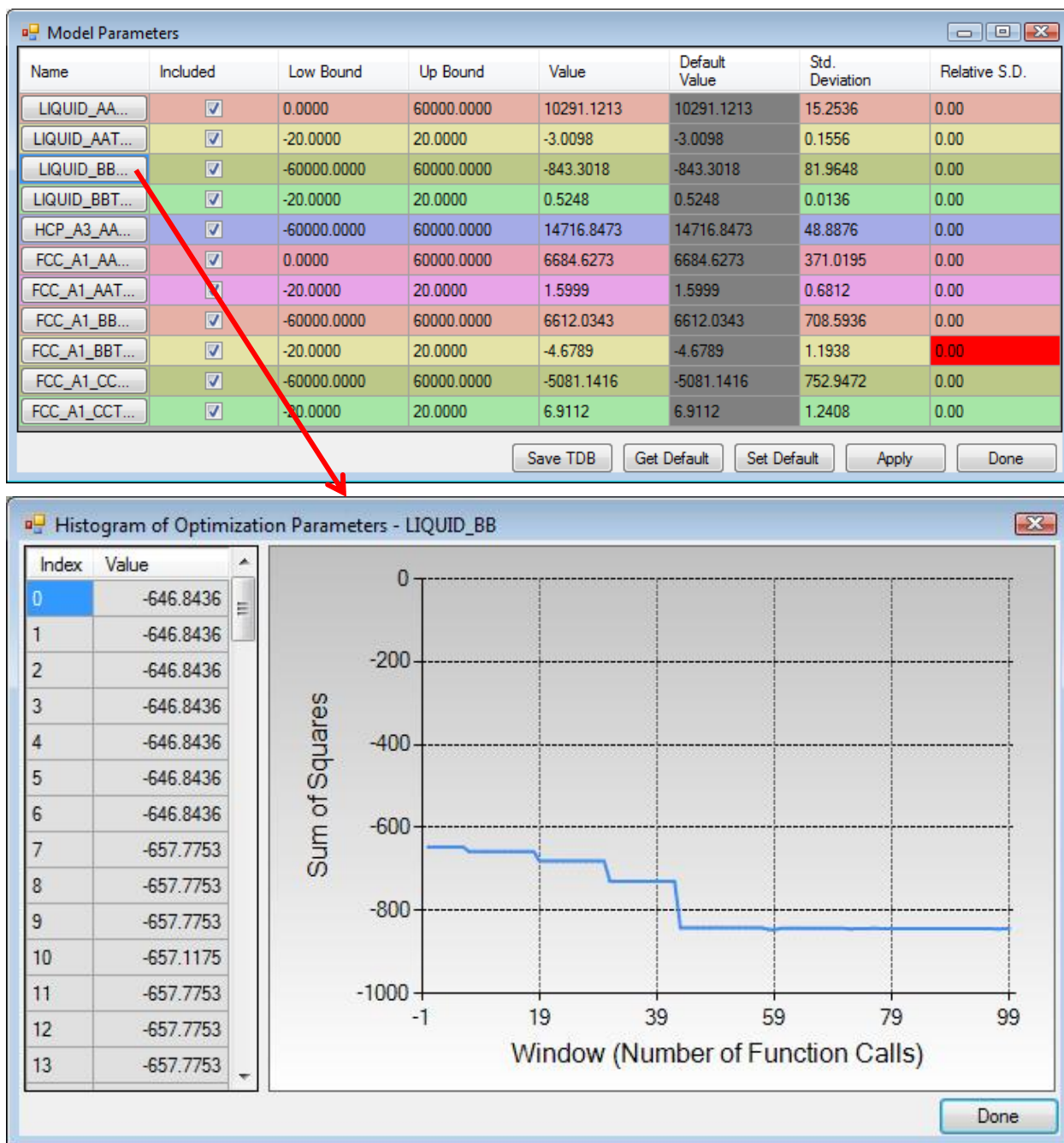


Figure 4.10 Dialog windows of Model Parameters and Histogram of Optimization Parameters

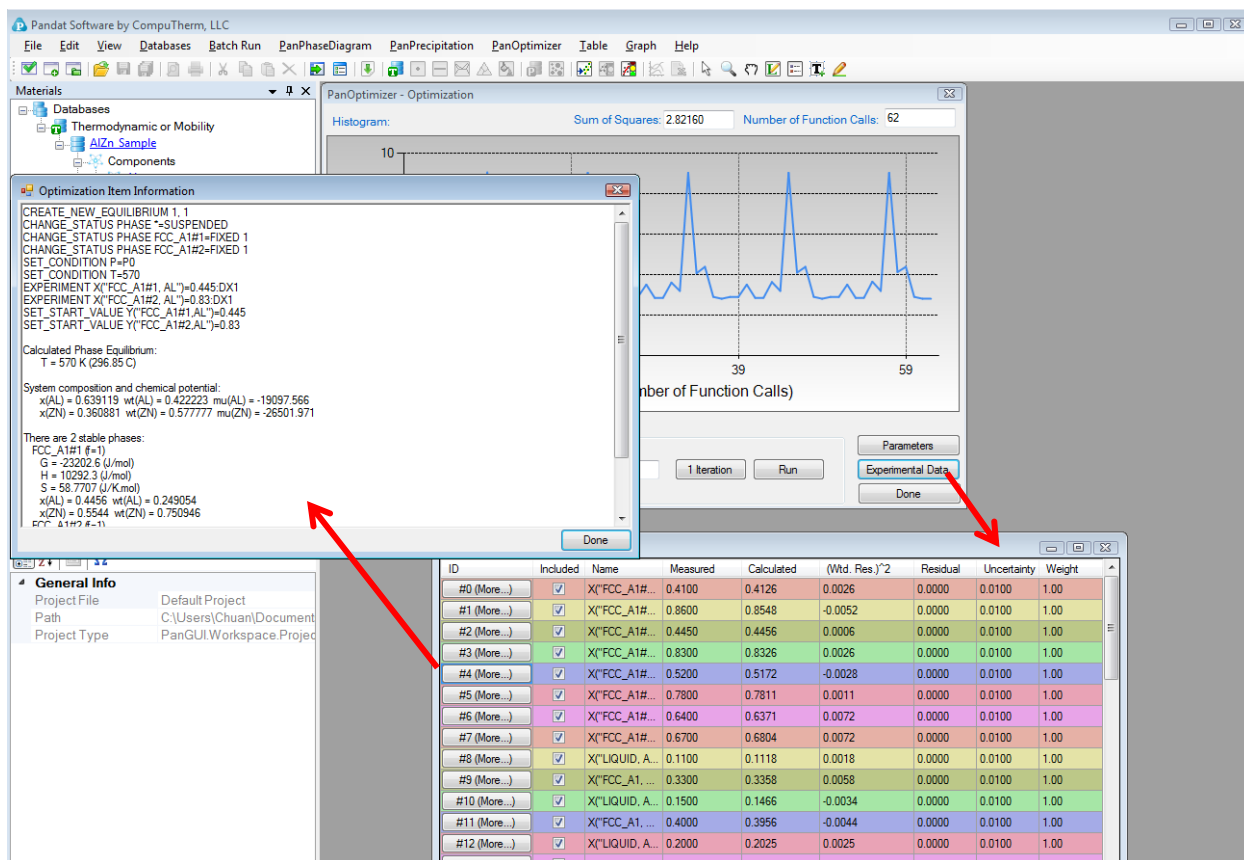


Figure 4.11 Dialog windows of Experimental Data and Optimization Item Information

4.3.3 Step 3: Save/Open Optimization Results

During optimization, the user may save and load optimization file through **Save Optimization Results** and **Open Optimization Results** (see Figure 4.12). The optimization results file has the extension name of *POR* that can only be read by PanOptimizer. Intermediate optimization results can be saved and restored through these two operations. These functions are very useful especially when a user is optimizing model parameters for a complicated system. The user can always go back to a certain middle stage and restart from there. This will save user's time by avoiding some repeated work.

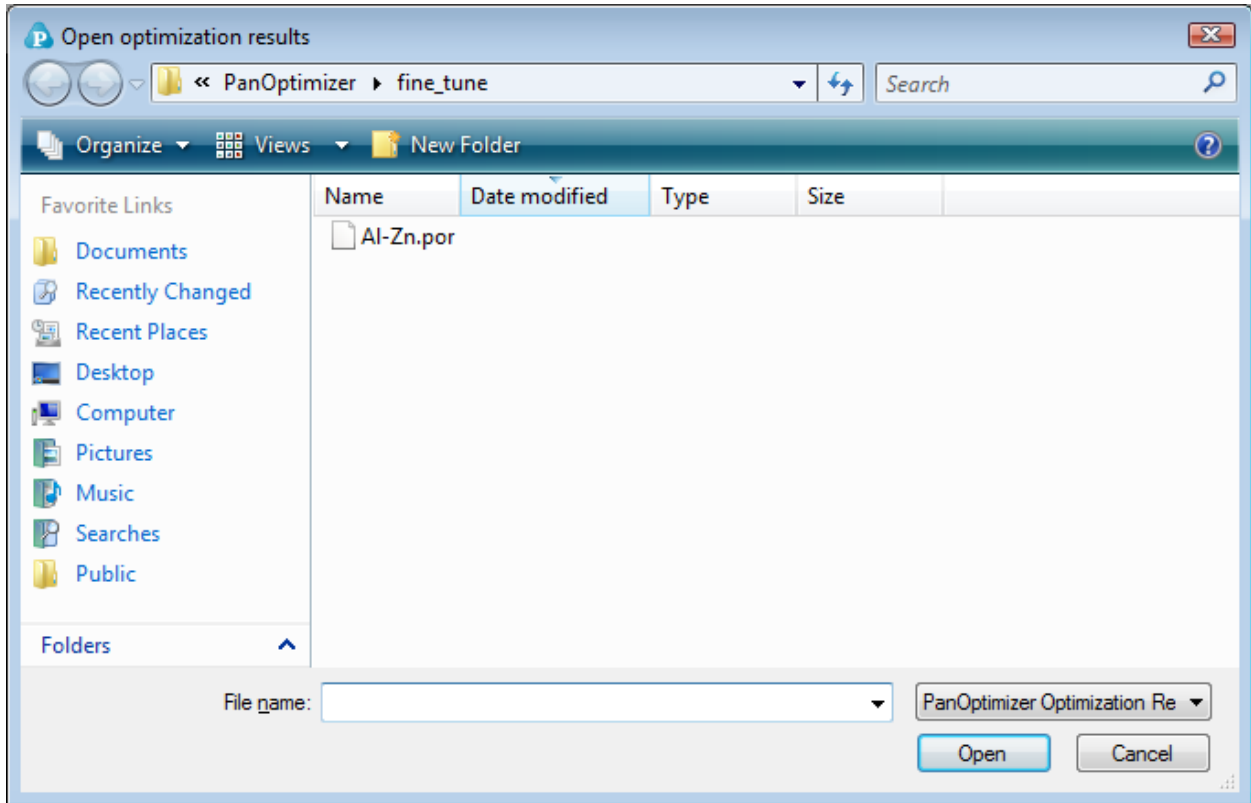


Figure 4.12 Dialog window of open the saved optimization results

4.4 Rough Search

To perform the rough search, user should follow the steps as described in the previous section. Some special points are described below.

4.4.1 Step 1: File preparation

- **Prepare the thermodynamic database file (.TDB)**

The thermodynamic database preparation is the same as described above for Normal Optimization

- **Prepare the experimental file (.POP)**

Keyword CREATE_ROUGH_EQUILIBRIUM is used to define phase equilibrium for rough search. When creating an equilibrium data set for rough search, the status of phases in equilibrium can only be FIXED. The keyword PHASE_POINT is used to define the state space of the phases in equilibrium including temperature, pressure and composition. No thermodynamic property is allowed to be optimized for multiple-phase equilibria. However, a special case is the single-phase equilibrium. The thermodynamic property data of the single-phase equilibrium can be used as experimental data to optimize the model parameters. Taking the binary Al-Zn system as an example, we will define a rough equilibrium between Fcc_A1 and Hcp_A3 at 500K. (A complete POP file for rough search can be found at the Pandat installation dictionary):

```
$ Tie-line between HCP_A3 and FCC_A1 at 500K
$ 10 is the weight factor of this equilibrium
CREATE_ROUGH_EQUILIBRIUM @@, 1, 10
CHANGE_STATUS PHASE FCC_A1, HCP_A3 = FIX 1
```

PHASE_POINT P = P0, T = 500

PHASE_POINT X(FCC_A1, AL) = 0.92, X(HCP_A3, AL) = 0.01

For a phase described by a sublattice model, the initial value of an element or species should be specified using SET_START_VALUE.

4.4.2 Step 2: Carry out optimization

- Load/compile experimental file

This step is the same as that in normal optimization. The “**Rough Search**” button in toolbar will be activated automatically if a POP file for rough search is loaded into the PanOptimizer.

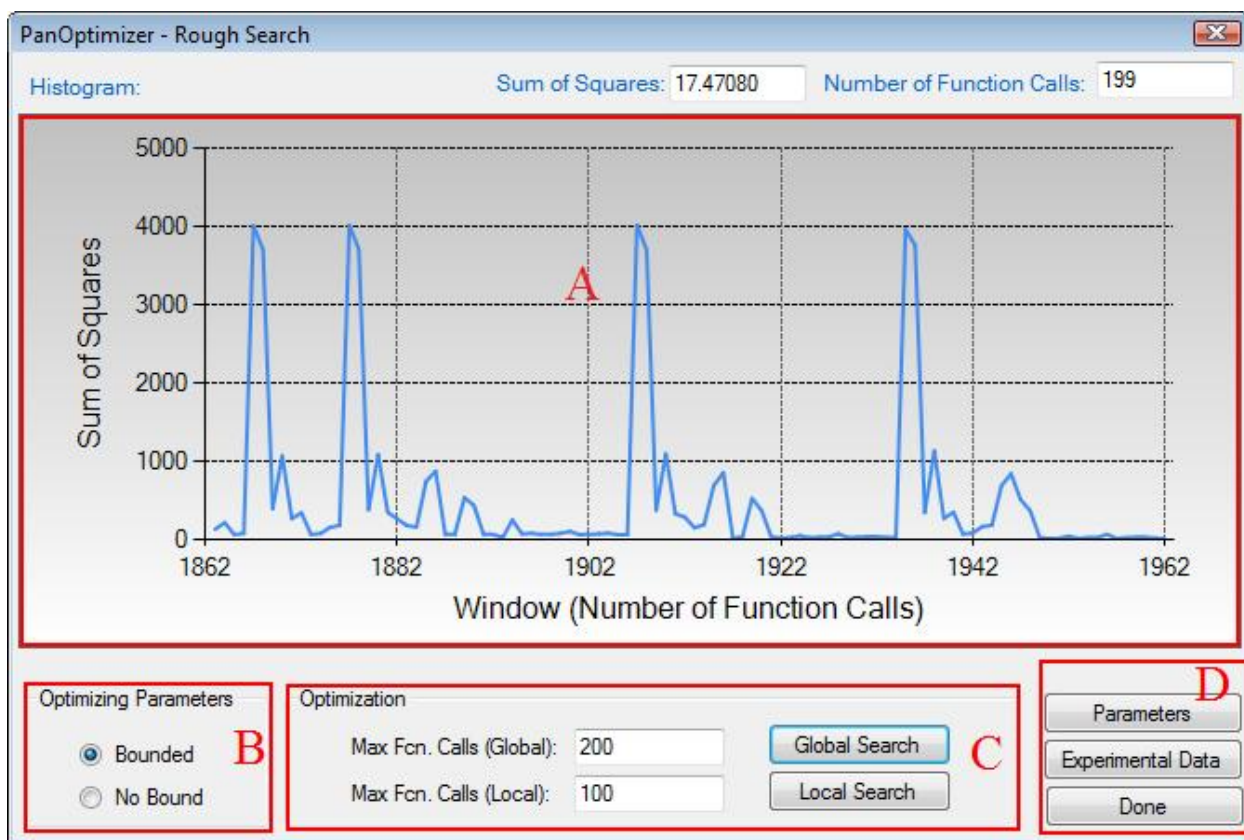


Figure 4.13 Control panel for rough search

- **Rough Search**

Again, there are four control areas in the control panel for rough search as shown in Figure 4.13 (only Area C and D are described below since the other two areas A and B are the same as the Normal Optimization control panel).

- **Optimization - Rough Search (C)**

There are two types of built-in optimization algorithms for **Rough Search** and they are **Global Search** and **Local Search**, as shown in area C. **Global Search** is to search a set of good initial values of the model parameters within the whole searching domain, while **Local Search** leads to a quick convergence to an optimal solution based on the given initial values of model parameters. The user can set the maximum number of function calls for both algorithms. Let's again take the binary Al-Zn system as an example. The phase boundary and invariant reaction information as shown in Figure 4.14 is used for the rough search and the result of rough search is shown in Figure 4.15.

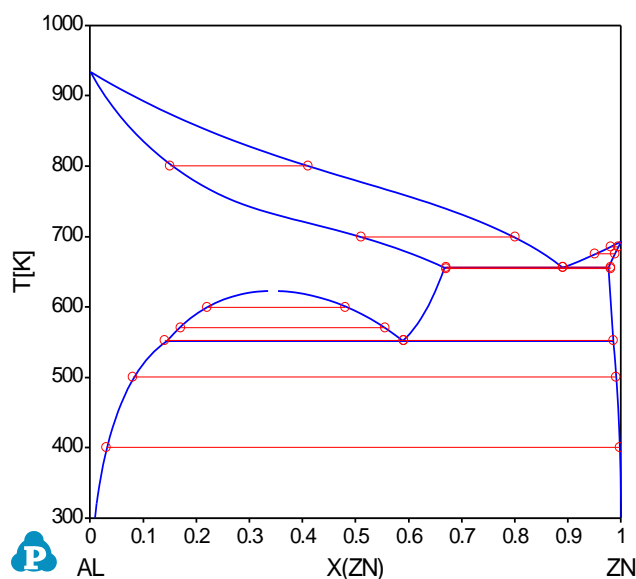


Figure 4.14 The phase boundary data used for rough search

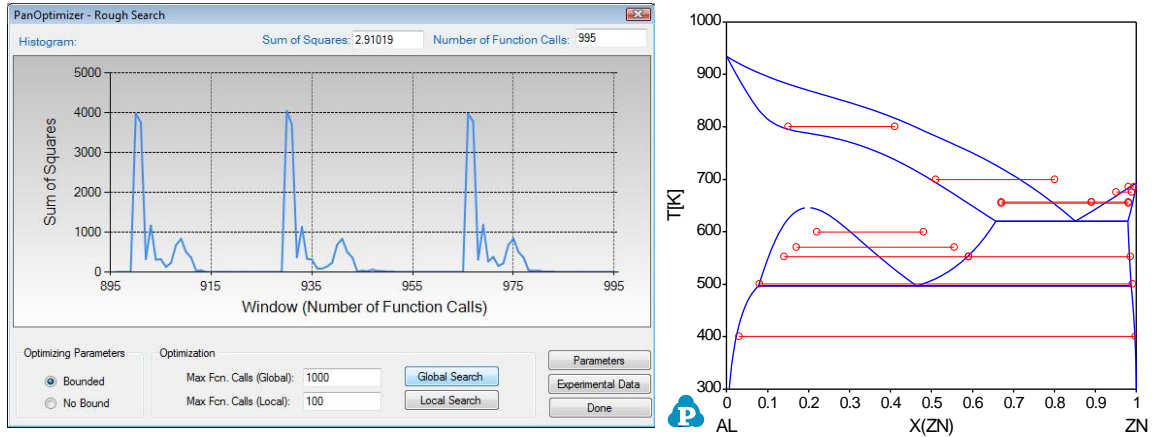


Figure 4.15 The calculated phase boundary compared with the experimental data after the rough search with Global Optimization

By setting the maximum number of function evaluations to be 1000 and clicking **Global Search**, the program finally stops at the sum of squares of 2.91. Figure 4.16 shows the calculated phase boundaries after a global search with 1000 function evaluations. It can be seen that the optimized parameters give a very similar topology with the known Al-Zn phase diagram. By clicking **Local Search**, the sum of squares decreases from 2.91 to 0.059, which reproduces the phase diagram in better agreement with the experimental one as can be seen in Figure 4.16.

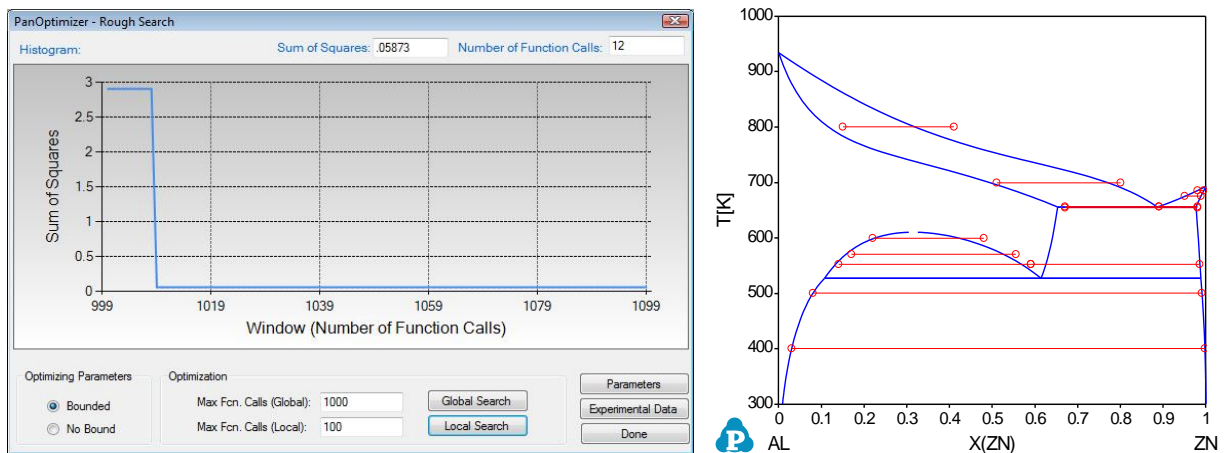


Figure 4.16 The calculated phase boundary compared with the experimental data after the rough search with Local Optimization

- **Optimization Results (D)**

Again during rough search, user can check model parameters through **Parameters**. In addition, chemical potential differences between any two phases in equilibrium can be accessed by **Experimental Data**. They are reflected by the values in column “(Wtd. Residual)²” as shown in the dialog window in Figure 4.17. Similarly, the weight factor of the equilibrium can be adjusted as needed during optimization procedure. The chemical potential values of each phase in equilibrium can be accessed by clicking the buttons in the first column.

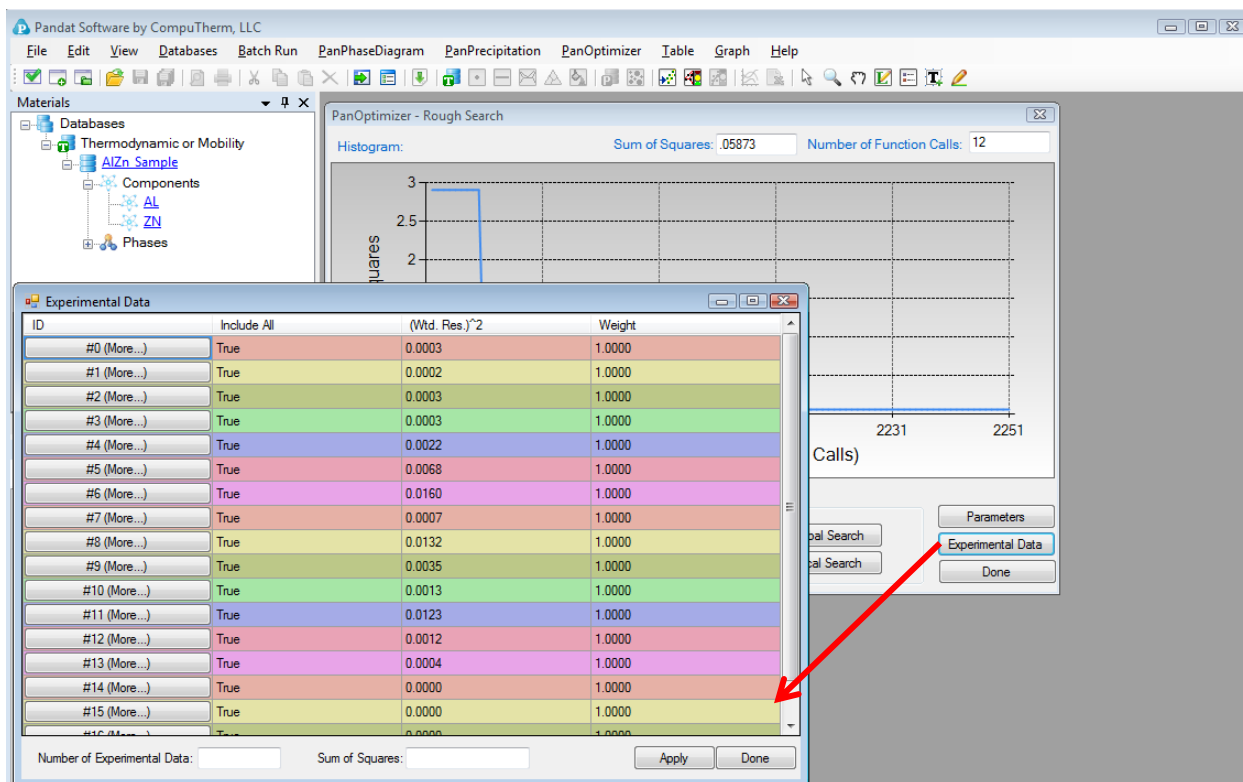


Figure 4.17 Dialog window for Rough Equilibrium Information

5. PanPrecipitation

A module of Pandat™ software, which is seamlessly integrated with the thermodynamic calculation engine–PanEngine for the necessary thermodynamic input and mobility data, is designed for the simulation of precipitation kinetics during heat treatment process. It is built as a shared library and integrated into Pandat as a specific module that extends the capability of Pandat for kinetic simulations, while taking full advantage of the automatic thermodynamic calculation engine (PanEngine) and the user-friendly Pandat Graphical User Interface (PanGUI). For this reason, precipitation simulations for highly complex alloys under arbitrary heat treatment conditions can be accomplished with only a few operations. Figure 5.1 shows the three-layered architecture of this modeling tool.

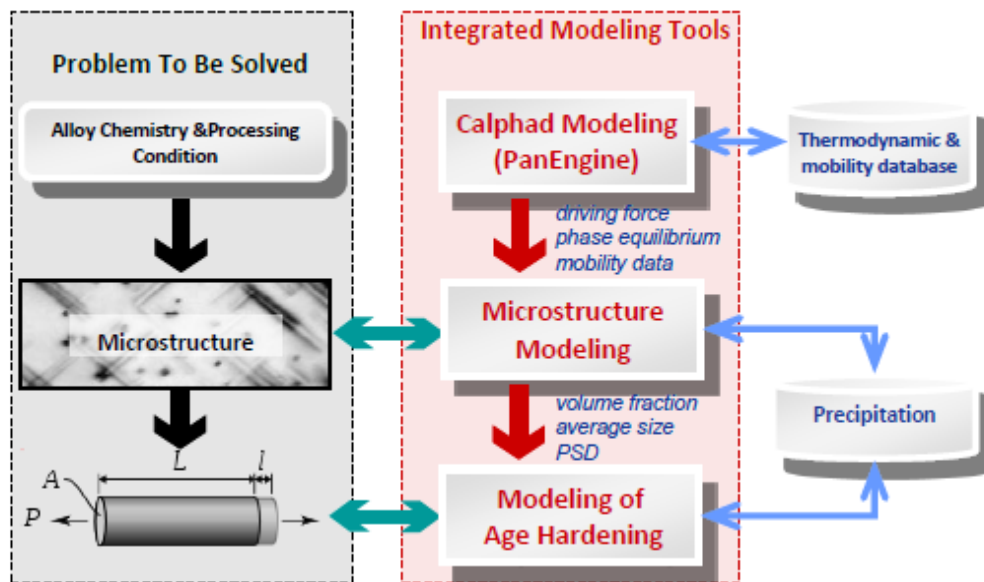


Figure 5.1 The three-layered architecture of the integrated modeling tool

5.1 Features of PanPrecipitation

5.1.1 Overall Design

- Concurrent nucleation, growth/dissolution, and coarsening of precipitates
- Temporal evolution of average particle size and number density
- Temporal evolution of particle size distribution
- Temporal evolution of volume fraction and composition of precipitates

5.1.2 Data Structure

PanPrecipitation is a purely object-oriented module written in C++ with generic data structures like PanEngine, balancing performance, maintainability and scalability. The basic data structure for storing precipitation information in the system of interest is schematically shown in Figure 5.2.

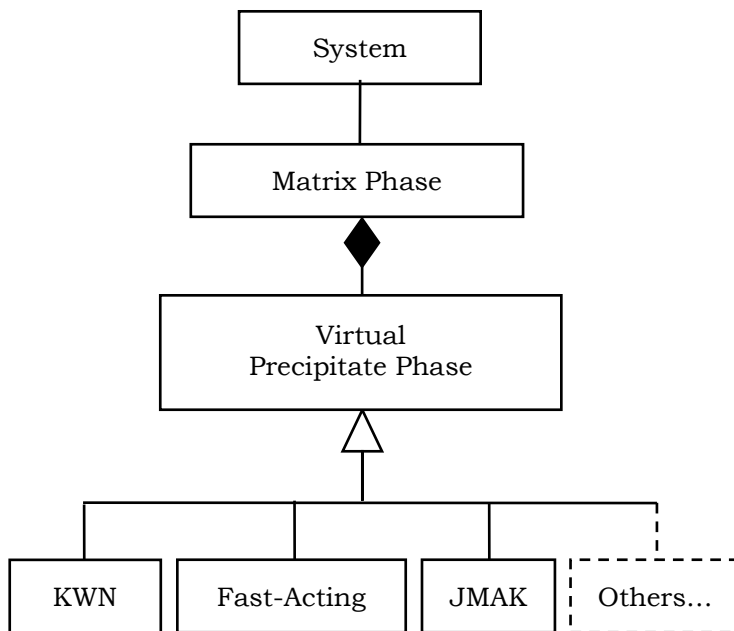


Figure 5.2 Date structure of system information in PanPrecipitation.

In general, a system contains a matrix phase and a number of precipitate phases. Different precipitate phase may behave differently, which should be described by different kinetic models. On the other hand, the calculation speed is directly related to the complexity of the model. It therefore requires multi-level models for different purposes. The current PanPrecipitation module includes two built-in models: the Kampmann/Wagner Numerical (KWN) model and the Fast-Acting model. One unique advantage is that this generic data structure allows easy integration of other precipitation models with the PanPrecipitation module as shown in Figure . This gives users great flexibility in choosing the proper kinetic models, including their own user-defined models, for custom applications.

Based on the above data structure, input parameters for the matrix and its precipitate phases are organized in “Extensible Markup Language” (XML) format, which is a standard markup language and well-known for its extendibility. In accordance with the XML syntax, a set of well-formed tags are specially designed to define the kinetic model for each precipitate phase and its corresponding model parameters such as interfacial energy, molar volume, nucleation type, and morphology type. In PanPrecipitation, two kinetic models known as the KWN and Fast-Acting were implemented and available for user's choice. Both models can be used to simulate the co-precipitation of phases with various morphologies (sphere and lens), with concurrent processes of nucleation, growth and coarsening. With the selection of the KWN model, the particle size distributions (PSD) of various precipitate phases can be obtained in addition to the temporal evolution of the average size and volume fraction as obtained from the Fast-Acting model.

5.1.3 Kinetic Models

In PanPrecipitation, KWN model is based on the Kampmann and Wagner's work as implemented in a numerical framework, and extended to handle both homogeneous and heterogeneous nucleation, dealing with various morphologies for the simulation of precipitation kinetics of multi-component alloys under arbitrary heat treatment conditions. The following is a brief introduction to the KWN model along with its sub-models for nucleation, growth and coarsening.

Specifically, in the KWN model the continuous PSD is divided into a large number of size classes. The program takes a simulation step at every sample time hit. To maintain both accuracy and efficiency between two adjacent simulation steps, a fifth-order Runge-Kutta scheme is used to generate an adaptive step size based on the continuity equation.

At each simulation step, the number of new particles is first calculated using classical nucleation theory and then these new particles are allocated to an appropriate size class. The transient nucleation rate is given by,

$$J = N_v Z \beta^* \exp\left(-\frac{\Delta G^*}{kT}\right) \exp\left(\frac{-\tau}{t}\right) \quad (5.1)$$

where $\Delta G^* = \frac{4\pi}{3}(R^*)^2 \sigma$. R^* is the radius of the critical nucleus and $R^* = \frac{-2\sigma}{\Delta G_v}$.

ΔG_v is the chemical driving force for nucleation and σ is the interfacial energy of the matrix/particle interface. The pre-exponential terms in equation (5.1) are: N_v , the nucleation site density, Z , the Zeldovich factor and β^* , the atomic attachment rate. t is the time, τ the incubation time for nucleation, k the Boltzmann constant and T the temperature. The multi-component version of the parameters has been proposed by Kozeschnik et al. [2007Koz] and

implemented in PanPrecipitation. The nucleation site density and nucleation driving force are modified to deal with heterogeneous nucleation.

Next, the growth of existing particles for each size class is computed by assuming diffusion-controlled growth, where the Gibbs-Thomson size effect is also taken into account. The growth model for multi-component alloys proposed by Morral and Purdy [1994Mor] is adopted in PanPrecipitation and modified to handle the growth/dissolution of various precipitate phases with different morphologies. The motion rate of the curved interface, e.g., the interface of a spherical or lens-like precipitate is given by,

$$v = \frac{dR}{dt} = \frac{K}{R} \left(\frac{1}{R^*} - \frac{1}{R} \right) \quad (5.2)$$

with

$$K = \frac{2\sigma V_m}{(\Delta C^{\alpha\beta}) [M]^{-1} [\Delta C^{\alpha\beta}]} \quad (5.3)$$

where R is the radius of the interface, R^* is the radius of the critical nucleus and σ being the interfacial energy between matrix (α) and precipitate phase (β), V_m being the molar volume of the precipitate phase, $(\Delta C^{\alpha\beta})$ and $[\Delta C^{\alpha\beta}]$ being the row and column vector of the solute concentration difference between α and β , and $[M]$ being the chemical mobility matrix.

Finally, the PSD and the volume fraction of the particles are updated and the matrix composition is recalculated based on the mass conservation equation (5.4) in the end of each simulation step. The updated values are then used in the next time step.

$$C_i^* = \left(1 - \sum_P \phi_P \right) C_i^\alpha + \sum_P \phi_P C_i^P \quad (5.4)$$

where C_i^* is the initial mole fraction of component i , ϕ_p is the mole fraction of precipitate phase P , n_p is the number of precipitate phases, C_i^α is the mole fraction of component i in the matrix phase α , and C_i^P is the mole fraction of component i in precipitate phase P .

It should be noted that coarsening in the KWN model arises naturally and becomes dominant when the supersaturation is sufficiently low. In the Fast-Acting model, however, the coarsening is considered explicitly. Accordingly, a coarsening model based on the LSW theory [1961Lif, 1961Wag] is employed, which characterizes the curvature-driven particle growth. The multi-component version can be written as,

$$\bar{R}^3 - \bar{R}_0^3 = \frac{4}{9} Kt \quad (5.5)$$

Where \bar{R} is the average particle radius at time t , \bar{R}_0 is the average particle radius at the onset of coarsening and K is the kinetic parameter defined in equation (5.3). Its accuracy and efficiency are ensured by controlling the adaptive step size with a fifth-order Runge-Kutta scheme. At each simulation step, the same nucleation and growth models, as given in equations (5.1) and (5.2), are used for the estimation of the average size changes. It is worth pointing out that the thermodynamic equilibrium information, the driving force and the diffusivity data needed for both KWN and Fast Acting simulations are obtained by directly coupling with the automatic thermodynamic calculation engine – PanEngine. Therefore, no initial values are required for the thermodynamic calculation at each simulation step. This makes PanPrecipitation very reliable and user-friendly in the simulation of precipitation kinetics, especially for multi-component alloys.

5.2 PanPrecipitation Functions

The current version of **PanPrecipitation** menu includes the following major functions: **Load Precipitation Database**, **Select Alloy Parameter**, and **Precipitation Simulation**

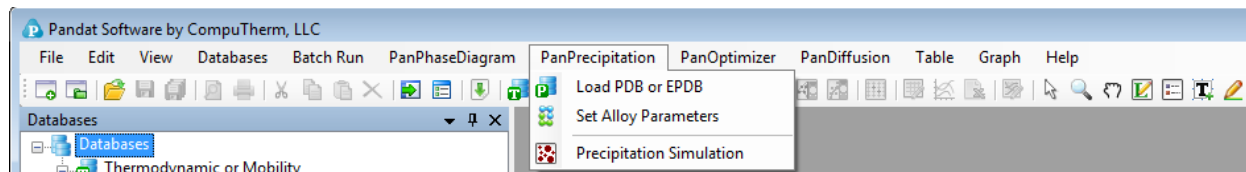


Figure 5.3 Menu functions of PanPrecipitation

The shortcut of the two commonly used functions **Load Precipitation Database** and **Precipitation Simulation** are also displayed in the Toolbar as shown in Figure 5.4.

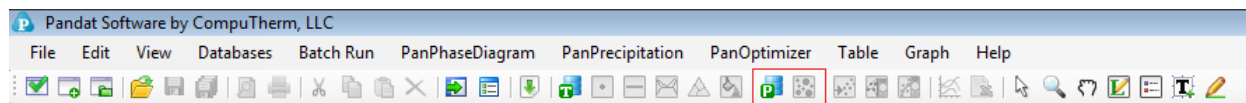



Figure 5.4 Toolbar buttons of PanPrecipitation

- **Load Precipitation Database**: Load a precipitation database into PanPrecipitation module for simulation.
- **Select Alloy Parameter**: Select an alloy parameter available in precipitation database for simulation.
- **Select Precipitate Phases**: Select one or more precipitate phases available in precipitation database for simulation.
- **Precipitation Simulation**: Perform the precipitation simulation.

5.3 Tutorial

In this tutorial, the Ni -14 at% Al alloy is taken as an example to demonstrate the functionalities provided by PanPrecipitation. The four files mentioned in this section (“NiAl.tdb”, “Ni-14Al_Precipitation.kdb”, “Ni-14Al_Exp.dat” and “Ni-14Al_Precipitation.pbf”) can be found in the installation folder of Pandat. In general, user should follow four steps to carry out a precipitation simulation:

5.3.1 Step 1: Create a Workspace

Let's start this tutorial by “creating a workspace”. By clicking the  button at the toolbar, the “**Create a New Workspace**” popup window will be open. User can choose the “**PanPrecipitation**” icon and define the location (project name, directory and/or workspace name), then click the “**Create**” button to create a precipitation workspace. User can also create a default precipitation workspace by double-click the “**PanPrecipitation**” icon.

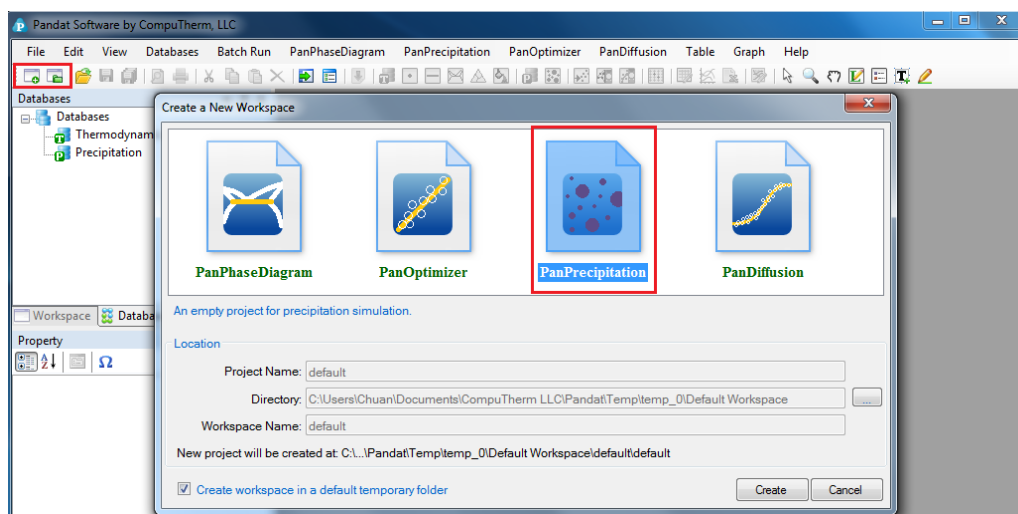


Figure 5.5 Dialog window for creating a workspace

5.3.2 Step 2: Load Thermodynamic and Mobility Database

The next step is to load the database, which is `NiAl.tdb` in this example. Different from the normal thermodynamic database, this database also contains mobility data for the matrix phase (FCC_A1) in addition to the thermodynamic model parameters. Both are needed for carrying out precipitation simulation.

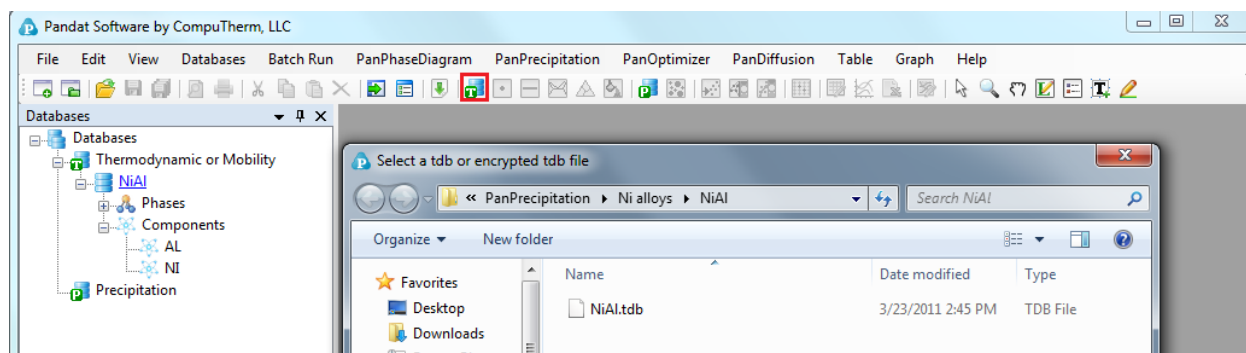



Figure 5.6 Dialog window for loading thermodynamic and mobility database


5.3.3 Step 3: Load Precipitation Database

A precipitation database is required for precipitation simulation, which contains kinetic parameters which are alloy dependent. Each alloy is composed of one matrix phase and a number of precipitate phases. To organize these parameters in a more intuitive way, the standard XML format is adopted and a set of well-formed tags are deliberately designed to define the kinetic model (KWN or Fast_Acting) for each precipitate phase and its corresponding model parameters such as interfacial energy, molar volume, nucleation type, and morphology type.


In this example, the `Ni-14Al_Precipitation.kdb` is prepared. This file can be opened by click  button in the toolbar and be viewed in the Pandat workspace or through third-party external editors, such as *NotePad*, *WordPad*

etc. In this example, the matrix phase for this alloy is “FCC_A1”, which has one precipitate phase “L12_FCC”. The “KWN” model with “Sphere” morphology and “Modified Homogeneous” nucleation type are selected for precipitation simulation. There are five model parameters: *Molar_Volume*, *Interfacial_Energy*, *Atomc_Spacing*, *Nucleation_Site_Parameter*, and *Driving_Force_Factor*. These parameters have been developed for the Ni-14Al alloy in this particular example; these parameters need to be optimized for different alloys in terms of experimental data.

Please note that, two sets of model parameters are given in the Ni-14Al_Precipitation.kdb file for two models: KWN or Fast_Acting models. User may select either one for the simulation as is shown in Figure 5.7.

To load a precipitation database, user should navigate the command through menu **PanPrecipitation** → **Load Precipitation Database**, or click icon  from the toolbar. After Ni-14Al_Precipitation.kdb is chosen, a dialog box pops out automatically for user to select the model, i.e., NI-14Al_FAST or NI-14Al_KWN, for the simulation. As shown in Figure 5.7, the “NI-14Al_KWN” is chosen in this example. The **Matrix Phase** window allows user to select the matrix phase and the **Precipitates** window allows user to choose one or more precipitate phases of interest for simulation. To select several phases at one time, press and hold the <Ctrl> key.

5.3.4 Step 4: Precipitation Simulation

After successfully loading both thermodynamic/mobility and precipitation databases, the function for precipitation simulation is then being activated. To perform a precipitation simulation, choose from Pandat GUI menu **PanPrecipitation** → **Precipitation Simulation**, or click icon  from the

toolbar. A dialog box entitled “PanPrecipitation – Precipitation Simulation”, as shown in Figure 5.8, pops out for user’s inputs to set up the simulation conditions: alloy composition and thermal history.

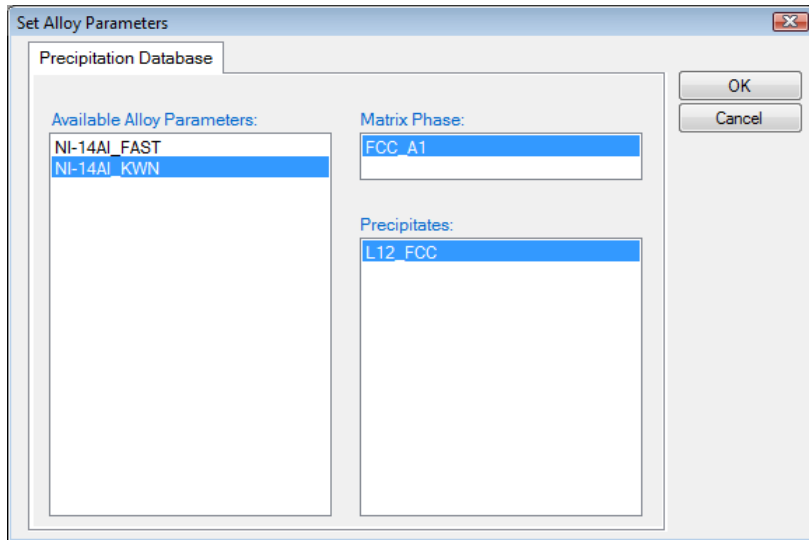


Figure 5.7 Dialog box for selecting alloy parameter

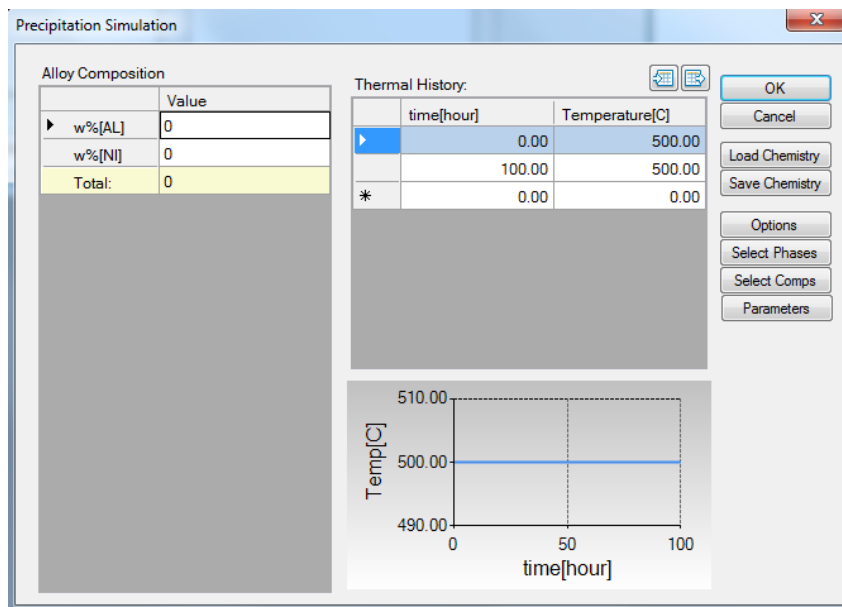


Figure 5.8 Dialog box for setting precipitation simulation conditions

Alloy Composition: User can set alloy composition by typing in or use the **Load Chemistry** function. User can also save the alloy composition through

Save Chemistry. This is especially useful when working on a multi-component system, so that user does not need to type in the chemistry every time.

Thermal History: Arbitrary heat treatment schedule can be inputted, with a linear *Time-Temperature* relationship (i.e., constant cooling or heating rate) at each two consecutive rows. *Time* at the first row must be zero representing the initial time. The thermal history set up in the figure 5.8 represents an isothermal heat treatment for 100 hours at 500°C. If the temperatures in the two rows are different, it represents constant cooling or heating. Multi-stages of heat treatment can be set by adding more rows in the Thermal History column.

User can access the **Options** window by clicking **Options**. The **Calculation Options** window allows user to change the units for pressure, temperature, time and composition required in the simulation (as shown in Figure 5.9). User can also define the output **Table** and **Graph** within the **Output Options** window (as shown in Figure 5.10).

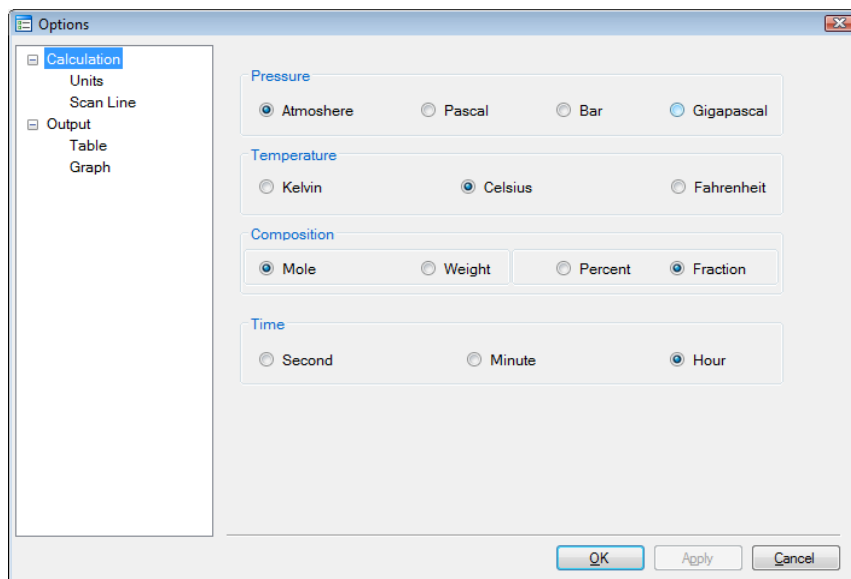


Figure 5.9 Dialog box for setting simulation units

In **Precipitation Simulation** window (as shown in Figure 5.8), click **OK** to run the simulation. After the simulation is completed, its results are displayed in two types of formats in the Pandat Explorer window: Graph and Table. By default, a graph plotting average size changes is displayed in the Pandat main window as shown in Figure 5.11. To view detailed simulation results, user can switch from Graph view to Table View by clicking tabs in the Pandat Explorer window.

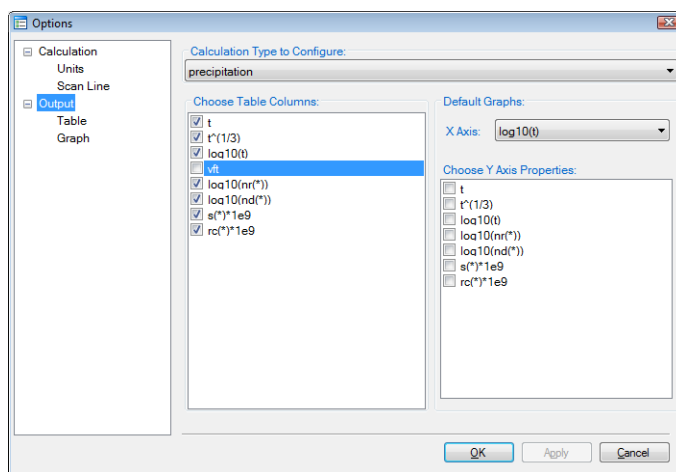


Figure 5.10 Dialog box for setting simulation outputs

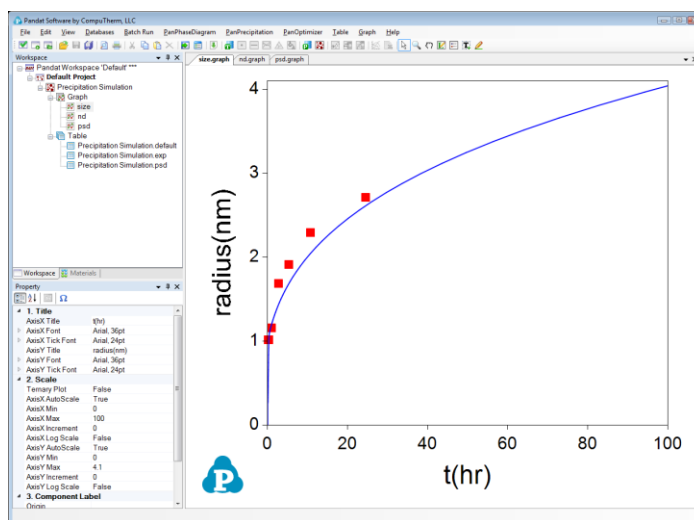



Figure 5.11 Default graph plotting average size changes

5.3.5 Step 5: Customize Simulation Results

As all other calculations available in Pandat, upon the completion of the precipitation simulation, a default table with related kinetic properties (such as time, total transformed volume fraction, average size of each precipitate phase, number density of each precipitate phase and nucleation rate of each precipitate phase) is automatically generated and a default graph for average size changes is displayed (Figure 5.11).

However, it should be emphasized that, in addition to the default tables, variety of properties, such as temperature, volume fraction of each individual precipitate phase, instant composition of matrix phase and also size distribution related information if the KWN model is used for simulation, can be retrieved through “**Add a new table**”.

5.3.6 Add a new table

Add a new table function can be activated by selecting the proper table within the workspace explore window and then click the  button or choose from the “Table” menu (as shown in Figure 5.12). This function allows user to create a new table at their own choices.

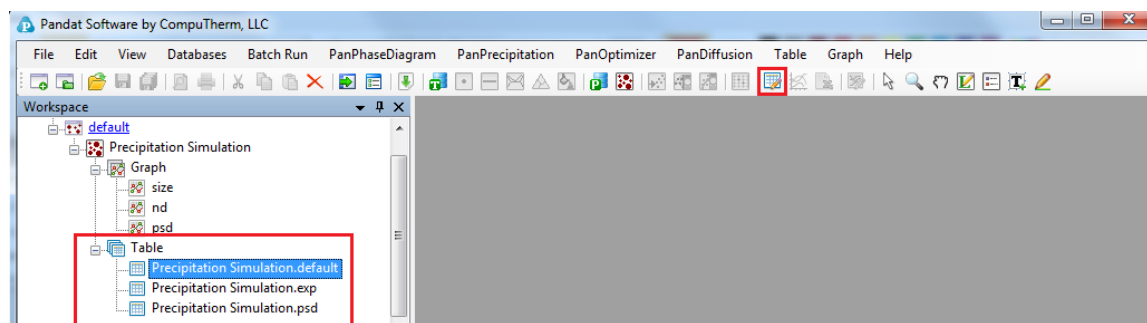


Figure 5.12 Dialog of add a new table

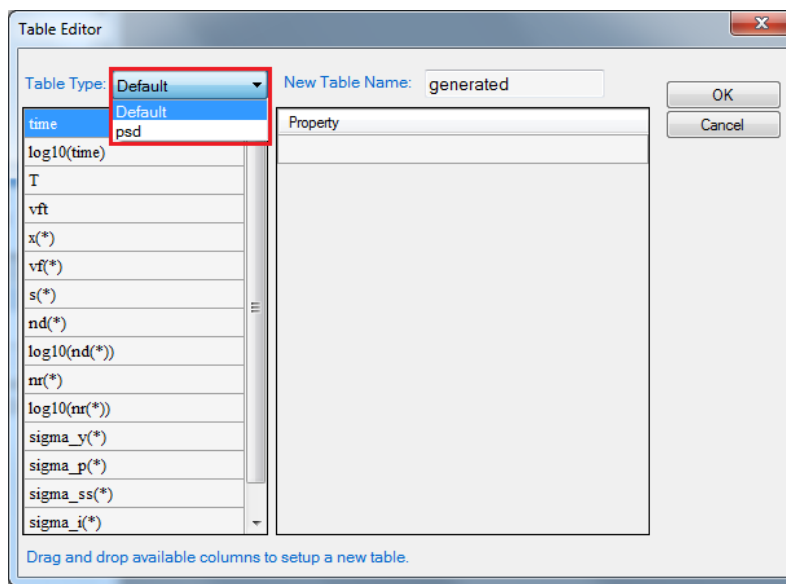


Figure 5.13 Dialog window of table editor

The basic layout of the window of **“Add a new table”** is shown in Figure 5.13. There are two major parts in this window. The left part is the available variables and contents. User can select available variables from the **“Table Type”** drop-down list as highlighted in Figure 5.13. The right part is the generated table field. User can drag the variables from the available table on the left side to the right side by clicking and holding the left mouse button.

5.3.7 Table Format Syntax

Moreover, mathematical calculation over these properties is allowed in PanPrecipitation. Accordingly, a variety of property diagrams can be generated based on the customized tables, which offers users an excellent flexibility for different applications (as shown in Figure 5.14). A detailed description of table format is given below. Figure 5.14 shows the Dialog window of table editor for customized new table. In Table 1 to 3, symbol “*” can be used to get quantities of the first available phase or component. As an example, s(*) retrieves the average size of phase L12_FCC, which is equivalent to s(L12_FCC). Table 1,

Table 2 and Table 3 list the syntaxes in the Table format for retrieving results of precipitation simulation. Table 4, Table 5 and Table 6 list the mathematical constants, operators and functions that can be used in a mathematical calculation over the quantities listed in Tables 1 to 3.

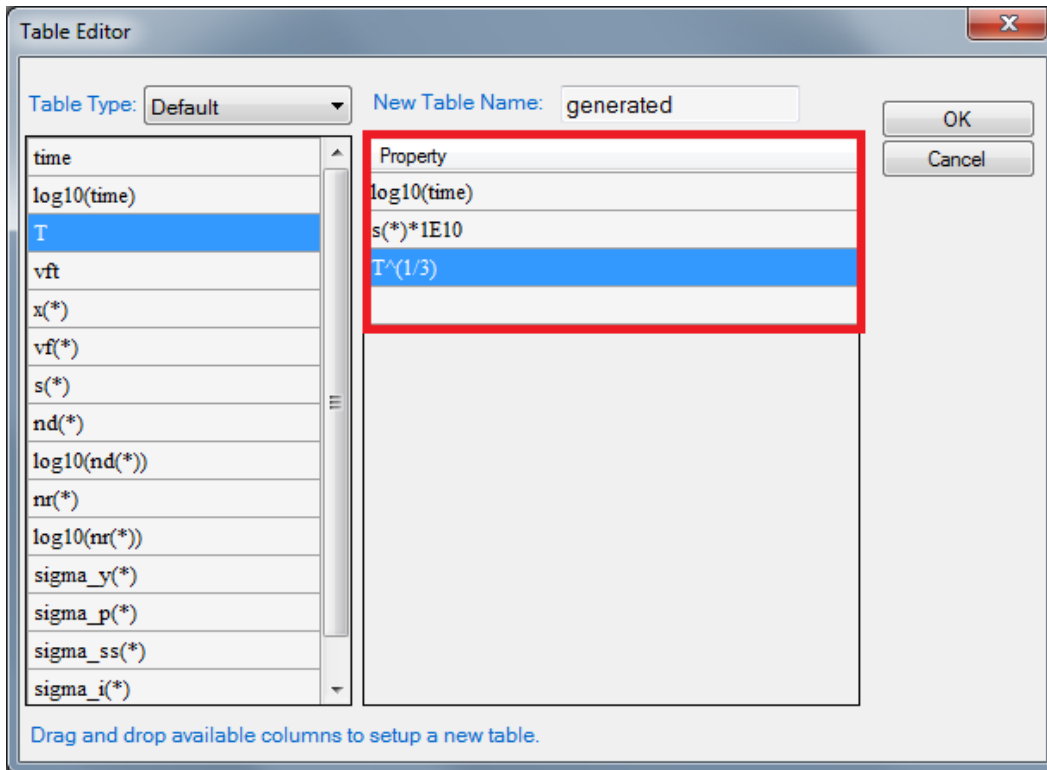


Figure 5.14 Dialog window of table editor for customized new table

In Tables 1 to 3, symbol “*” can be used to get quantities of the first available phase or component; As an example, $s(*)$ retrieves the average size of phase L12_FCC, which is equivalent to $s(L12_FCC)$.

Table 1. Table Format Syntax for Retrieving System Quantities

Name	Unit (SI)	Comments
t	sec	Time
T	K	Temperature
vft		Total Transformed Volume Fraction: $vft = \sum_p vf_p$ where vf_p is the transformed volume fraction of p phase
x0(comp)		Overall alloy composition
x(comp)		Instant composition of the matrix phase

Table 2. Table Format Syntax for Retrieving Precipitate phase quantities

Name	Unit (SI)	Comments
s(phase)	m	Average size
nd(phase)	m ⁻³	Number density
nr(phase)	m ⁻³ sec ⁻¹	Nucleation rate
vf(phase)		Volume fraction of specified phase

Table 3. Table Format Syntax for Retrieving Quantities of Particle Size Distribution (PSD)

Name	Unit (SI)	Comments
index = i		Ten PSDs are recorded over the total simulation time; Using index = i to get the last one ($t = t_{end}$)
psd_id		The PSD consists of a certain number of cells (size classes); psd_id gets the cell id.
psd_s(phase)	m	The characteristic size of a precipitate phase for each cell.
psd_nd(phase)	m ⁻³	The number density of a precipitate phase for each cell.
psd_gr(phase)	m/sec	The growth rate of a precipitate phase for each cell.
psd_ns(phase)		Normalized size of the cell $psd_ns(phase) = \frac{psd_s(phase)}{s(phase)}$
psd_nnd(phase)		Normalized number density of the cell $psd_nnd(phase) = \frac{psd_nd(phase)}{nd(phase)}$

Table 4. Mathematical Physical Constants

Name	Comments
_K	Boltzmann constant
_PI	Archimedes' constant.
_R	Molar gas constant.
_NA	Avogadro constant.
_E	Natural Logarithmic Base.

Table 5. Mathematical Operators

Name	Comments
+	Addition
-	Subtraction
*	Multiplication
/	Division
^	Exponentiation

Table 6. Mathematical Functions

Name	Comments
$\exp(x)$	Exponential
$\ln(x)$	Natural Logarithm of x
$\log_2(x)$	Base 2 Logarithm of x
$\log_{10}(x)$	Base 10 Logarithm of x
$\text{sqrt}(x)$	Square root of x
$\text{abs}(x)$	Absolute value of x
$\sin(x)$	Sine of x
$\cos(x)$	Cosine of x
$\tan(x)$	Tangent of x
$\text{asin}(x)$	Inverse sine of x
$\text{acos}(x)$	Inverse cosine of x
$\text{atan}(x)$	Inverse tangent of x

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