Pandat 2025

Example book



CompuTherm LLC Copyright® 2000 -2025



Contents

1	PanPhaseDiagram Examples 1
	Example 1.1 Al-Mg Binary Phase Diagram
	Example 1.2 Phase Fraction as a Function of Composition
	Example 1.3 Phase Fraction as a Function of Temperature
	Example 1.4 Point Calculation at Fixed Temperature and Composition12
	Example 1.5 Isotherm of Al-Mg-Zn at 500°C15
	Example 1.6 Isopleth of Al-Mg-Zn at 15 at% Zn19
	Example 1.7 Liquidus Projection of Al-Mg-Zn22
	Example 1.8 Solidification Simulation by Scheil Model and Lever Rule25
	Example 1.9 Calculation of Gibbs Energy Curves
	Example 1.10 Calculation of Activity at Constant Temperature
	Example 1.11 Calculation of Activity at Constant Composition
	Example 1.12 Calculation of Molar Volume and Density at Fixed Temperature
	Example 1.13 Calculation of Molar Volume and Density at Fixed Composition
	Example 1.14 Density Contour Diagram

Example 1.15 Activity Contour Diagram57
Example 1.16 Pressure Contour Diagram54
Example 1.17 3D Diagram57
Example 1.18 Temperature-Pressure Diagram67
Example 1.19 Phase Fraction Contour Diagram for Ti6464
Example 1.20 Phase Forming Driving Force in High Entropy Alloys67
Example 1.21 User-defined Property7
Example 1.22 Run Pandat in Console Mode
Example 1.23 High Throughput Calculation (HTC): Pattern Compositions75
Example 1.24 High Throughput Calculation (HTC): Random Compositions 80
Example 1.25 Friction-stir welding between AA5454 AI alloy and AZ91 Mg alloy82
Example 1.26 Calculation of Open Circuit Voltage (OCV) under Equilibrium Condition
Example 1.27 Para-equilibrium Phase Diagram97
Example 1.28 Calculation of T0 curve95
Example 1.29 Material to Material Calculation: Friction-stir welding
between AA5454 AI alloy and AZ91 Mg alloy98
PanOptimizer Example 101

Example 2.1 Parameter Optimization for the Fe-Cr-Ni Ternary System102

2

3	PanEvolution/PanPrecipitation Examples106
	Example 3.1 Precipitation Simulation of Ni-14AI (at%) Alloy107
	Example 3.2 TTT diagram of Ni-14Al (at%) Alloy115
	Example 3.3 Co-precipitation of γ' and γ'' in Ni-Al-Nb Ternary
	Example 3.4 Simulation of Hardness of Aluminum Alloy 6005124
	Example 3.5 Simulation of Softening of Aluminum Alloy 6005
	Example 3.6 Simulation of Yield Strength of Aluminum Alloy 356134
	Example 3.7 CCT diagram of Ni-14AI (at%) Alloy138
4	PanDiffusion Examples
	Example 4.1 Diffusion within a Single Phase: Uniform Initial Compositions
	Example 4.2 Diffusion within a Single Phase: Linear Initial Compositions .146
	Example 4.3 Diffusion between Two Phases: Uniform Initial Compositions
	Example 4.4 Diffusion between Two Phases at Varied Temperatures152
	Example 4.5 Diffusion among Multiple Regions155
	Example 4.6 Carburization with Fixed Composition at Boundary158
	Example 4.7 Carburization with Input Flux160
	Example 4.8 Carburization of a Tube with Fixed Environmental Activity163
	Example 4.9 Dissolution of γ' Particle in γ Matrix

	mple 4.10) Transformation from γ to α	169
Exa	mple 4.11	Fe-Si-C Uphill Diffusion	.172
Exa	mple 4.12	2 Dissolution of a Single θ-Al2Cu Particle in FCC Matrix	175
Exa	mple 4.13	Dissolution of Multiple Particles	178
Exa	mple 4.14	Decarburization of Fe-C Matrix	. 181
PanS	olidificat	tion Examples	184
		-	
Exa Coo	mple 5.1 ling Rate	Solidification Simulation of a Mg-Al alloy under a Giver	ו 185.
Exa Coc Exa Allo	mple 5.1 Iling Rate mple 5.2 y	Solidification Simulation of a Mg-Al alloy under a Given Prediction of Hot Cracking Susceptibility of an Al-Cu-Mg	. 185 . 185 . 189

5

1 PanPhaseDiagram Examples

Example 1.1 : AI-Mg Binary Phase Diagram

- Example 1.2 : Phase Fraction as a Function of Composition
- Example 1.3 : Phase Fraction as a Function of Temperature
- Example 1.4 : Point Calculation at Fixed Temperature and Composition
- Example 1.5 : Isotherm of AI-Mg-Zn at 500°C
- Example 1.6 : Isopleth of AI-Mg-Zn at 15 at% Zn
- Example 1.7 : Liquidus Projection of Al-Mg-Zn
- Example 1.8 : Solidification Simulation by Scheil Model and Lever Rule
- Example 1.9 : Calculation of Gibbs Energy Curves
- Example 1.10 : Calculation of Activity at Constant Temperature
- Example 1.11 : Calculation of Activity at Constant Composition
- Example 1.12 : Calculation of Molar Volume and Density at Fixed Temperature
- Example 1.13 : Calculation of Molar Volume and Density at Fixed Composition
- Example 1.14 : Density Contour Diagram
- Example 1.15 : Activity Contour Diagram
- Example 1.16 : Pressure Contour Diagram
- Example 1.17 : 3D Diagram
- Example 1.18 : Temperature-Pressure Diagram
- Example 1.19 : Phase Fraction Contour Diagram for Ti64
- Example 1.20 : Phase Forming Driving Force in High Entropy Alloys
- Example 1.21 : User-defined Property
- Example 1.22 : Run Pandat in Console Mode

Example 1.23 : High Throughput Calculation (HTC): Pattern Compositions

Example 1.24 : High Throughput Calculation (HTC): Random Compositions

Example 1.25 : Friction-stir welding between AA5454 AI alloy and AZ91 Mg alloy

Example 1.26 : Calculation of Open Circuit Voltage (OCV) under Equilibrium Condition

Example 1.27 : Para-equilibrium Phase Diagram

Example 1.28 : Calculation of T0 curve

Example 1.1 Al-Mg Binary Phase Diagram

Purpose: Learn to calculate and use a binary phase diagram

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.1.pbfx

Calculation Procedures:

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Perform section (2D) calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.1.1;

Y-Axis Point ✓ T(C) 800 x(Al) 1 x(Mg) 0 Total: 1 Origin Point ✓ Value ✓ Y ✓ Value ✓ Y ✓ Value ✓ Y ✓ X-Axis Point ✓ X-Axis Point ✓ X(Al) 1 x(Mg) 0 x(Mg) 0 x(Mg) 1 x(Mg) 1 xouth 1	· · · · · · · · · · · · · · · · · · ·		
Value Value ✓ T(C) 800 x(A) 1 x(Mg) 0 Total: 1 Origin Point ✓ Value ✓ Value ✓ Y ✓ Origin Point ✓ Value ✓ Y ✓ Value ✓ Y ✓ X-Axis Point ✓ X-Axis Point ✓ ✓ ✓<			
✓ T(C) 800 x(A) 1 x(Mg) 0 Total: 1 Origin X Scanline Density: 0 X-Axis Point X-Axis Point Value ▼ T(C) 0 x(A) 1 x(A) x(Mg) 0 x(A) Total: 1 Total:	ОК		
x(A) 1 x(Mg) 0 Total: 1 Origin Point Image: Scanline Density: Value X-Axis Point T(C) 0 x(Al) 1 x(Mg) 0 x(Al) 1 x(Mg) 0 x(Mg) 1 Total: 1	Cancel		
x(Mg) 0 Total: 1 Origin Point Image: Scanline Density: Value X-Axis Point T(C) 0 x(Mg) 0 x(Mg) 0 x(Mg) 0 x(Mg) 1 x(Mg) 0 x(Mg) 1 Total: 1	Options		
Total: 1 Origin Point ✓ Value ✓ Yalue ✓ Y	Extra Outputs		
Volue Value T(C) 0 x(A) 1 x(Mg) 0 Total: 1	Load Condition		
Value X-Axis Point T(C) 0 x(A) 1 x(Mg) 0 x(Mg) 1 Total: 1	Save Condition		
Value X-Axis Point ▼ T(C) 0 x(A) 1 x(Mg) 0 x(Ai) 1 x(Mg) 0 Total: 1	Select Phases		
Value X-Axis Point T(C) 0 x(A) 1 x(Mg) 0 Totat: 1	Select Comps		
Value X-Axis Point ▶ T(C) 0 x(Ai) 1 x(Mg) 0 Total: 1	Contour Lines		
Value X-Axis Point T(C) 0 x(A) 1 x(Mg) 0 Total: 1	Mobile Comps.		
Value Value Value ▶ T(C) 0 ▶ T(C) 0 x(A) 1 x(A) 0 x(Mg) 0 x(Mg) 1			
T(C) 0 T(C) 0 x(A) 1 x(A) 0 x(Mg) 0 x(Mg) 1 Total: 1 Total: 1			
x(A) 1 x(A) 0 x(Mg) 0 x(Mg) 1 Table 1 Table 1			
x(Mg) 0 I Total: 1 Total: 1			
Total: 1 Total: 1			
Total.			

Figure 1.1.1: 2D calculation with composition from pure AI to pure Mg and temperature from

0°C to 800°C

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Zoom the interested area following the procedure in Pandat User's Guide 2.3.3;



Figure 1.1.2: Calculated AI-Mg binary phase diagram

- Phase stability as a function of composition and temperature;
- Congruent melting temperature and composition of a phase. For example the congruent melting temperature of the AlMg Gamma phase is at 463.3°C and x (Mg) =0.537;

• Invariant reaction temperatures and phase compositions. For example the three phase equilibrium: Liquid->AlMg_Gamma+Hcp is at 436.3°C, the composition, x (Mg), of each phase at equilibrium is indicated in Figure 1.1.2. Details on the invariant reactions can be found in the "invariant" table as shown in Figure 1.1.1, and composition of each phase involved in the invariant reaction can be found in the "invariant_tieline" tables as shown in Figure 1.1.4.

Pandat Software by CompuThem, LLC											
	- ×										
f(@Hcp)	f(@Liquid)										
mole/mole	mole/mole										
	1.000000										
	1.000000										
0.315043	1.000000										
	f(@Hcp) mole/mole 0.315043										

Figure 1.1.3: The invariant table showing all the three-phase equilibrium in the AI-Mg binary

A Pandat Software	by CompuTher	mIIC						_	
	D . I		D DI	D: D D					- X
	Databases	Batch Cald	<u>P</u> anPha	seDiagram PanP	recipitation PanOptimizer PanD	Intrusion Pan <u>Solidification P</u> rope	nty <u>l</u> able <u>G</u> rap	on Heip	
		6 10 10	× 🖻 🗉	3 🕑 🔂 🕒 🗄			87 V3 🔍 X7 🛙	. 🗉 🕮 🖊	
Workspace		Ψ×	🔀 2D_A	Al-Mg.graph	📰 invariant.table 🔛 inv	ariant_tieline.table ×			-
Pandat Work	space 'default'	***		Т	reaction	phase_name	x(Al)	x(Mg)	w(Al
<u>⊨</u> <u>default</u>		.		c ~			mole/mole ~	mole/mole >	ka/ka 🗸
	g priase diagram raph	"		450 4672	Liquid => Eco + AlMa, Poto	Liquid	0.627666	0.262224	0.661444
	2D_AI-Mg			450.4672	Liquid => Fee + AIMg_Beta	Equid	0.037000	0.165946	0.001444
👝 🕞 Ta	ble		2	450.4672	Liquid => Fcc + AlMg_Beta	AlMa Beta	0.611354	0.388646	0.635872
	Default		3	450.4672	Liquid => Fee + AlMg_Beta	Liquid	0.637666	0.362334	0.661444
	invariant		4	430.4072	Elquid -> 100 · AlMg_beta	Liquid	0.037000	0.002034	0.001444
	invariant_tieli	ne	6	449 5016	Liquid => AlMo, Beta + AlMo, Ga	Liquid	0 576044	0.423956	0.601337
	- I	_	7	449.5016	Liquid => AIMg_Beta + AIMg_Ga	AlMa Reta	0.611354	0.399646	0.625972
			· /	449.5016	Liquid => AIMg_Beta + AIMg_Ga	AlMa Gamma	0.519503	0.480497	0.545508
			ŝ	449 5016	Liquid => AIMg_Beta + AIMg_Ga	Liquid	0.576044	0.423956	0.601337
			10	443.3010	Elquid V Almg_beta V Almg_da	Eiquid	0.370044	0.423330	0.001337
			11	436 2780	Liquid => AlMg_Gamma + Hcp	Liquid	0 310102	0.689898	0 332888
Workspace Databas	ses		12	436 2780	Liquid => AIMg_Gamma + Hcp	AlMa Gamma	0.399399	0.600601	0.424707
Property			12	436,2780	Liquid => AIMg_Gamma + Hcp	Hen	0.115955	0.884045	0.127103
20 2↓ 🖾			14	436 2780	Liquid => AlMo, Gamma + Hop	Liquid	0.310102	0.689898	0.332888
✓ General Info			15	100.2700	Eldera trang_aanna hop		0.010102	0.000000	0.002000
Folder Name	Al-Mg phase	diagram\1	16	409.7759	AlMa Gamma + AlMa Beta => Al	AIMo, Gamma	0.505622	0 494378	0.531702
Path	C:\Users\fanz	h\Docume	17	409 7759	AlMa Gamma + AlMa Beta => Al	AlMo Beta	0.611354	0.388646	0.635872
	ns C	_	18	409,7759	AlMg Gamma + AlMg Beta => Al	AIMg Eps	0.566038	0.433962	0.591505
reaction	-		19	409.7759	AIMg Gamma + AIMg Beta => AI	AlMg Gamma	0.505622	0.494378	0.531702
phase_name			20						
x(AI)	mole/mole		21	250.0882	AIMg Eps => AIMg Gamma + AI	AlMg Gamma	0.463558	0.536442	0.489616
w(Al)	kg/kg		22	250.0882	AIMg Eps => AIMg Gamma + Al	AlMa Eps	0.566038	0.433962	0.591505
w(Mg)	kg/kg		23	250.0882	AIMg_Eps => AIMg_Gamma + Al	AlMg_Beta	0.611354	0.388646	0.635872
			24	250.0882	AIMg Eps => AIMg Gamma + AI	AlMg Gamma	0.463558	0.536442	0.489616
			<						>
		_							

system

Figure 1.1.4: The invariant_tieline table showing the composition of each phase involved in the invariant reaction in the AI-Mg binary system

Example 1.2 Phase Fraction as a Function of Composition

Purpose: Learn to calculate and use a phase fractions vs. composition plot

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.2.pbfx

Figure 1.2.1 is the Al-Mg binary phase diagram, which clearly shows the single phase region, two-phase region, three-phase equilibrium. However if you want to know the fraction of a stable phase in a two-phase field at a certain temperature, you need to draw a horizontal line at this temperature and calculate it by line (1D) calculation. In this example, we calculate the fraction of each phase as a function of composition, x (Mg), at 300°C (the red dash line).



Figure 1.2.1: AI-Mg binary phase diagram

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Perform 1D calculation following the procedure in Pandat User's Guide 3.3.2;
- Set Calculation Condition as shown in Figure 1.2.2;

Lin	e Ci	alculation	/	/			X
	Sta	art Point		_	End Point		
			Value]		Value	
		T(C)	300		🖉 T(C)	300	
	۲	x(Al)	1]	x(Al)	0	Options Extra Outputs
		x(Mg)	0		x(Mg)	1	Load Condition
		Total:	1	$\mathbf{\Sigma}$	Total:	1	Save Condition
							Select Phases Select Comps
	Nur	mber of step	s: 100		Individual Pl	nases	



- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

- The composition range that a phase is stable at the selected temperature;
- In a single phase field, the fraction of the stable phase is 1;
- In a two-phase field, the fraction of one phase decrease from 1 to 0, while the other increase from 0 to 1 as shown in Figure 1.2.3
- Details on the fraction of each phase as a function of composition can also be found in the Default table as shown in Figure 1.2.4;



Figure 1.2.3: Phase fraction variation as a function of composition

Pandat Software by CompuTherm, LLC															
Ele Edit View Databases Batch	Calc P	anPhaseDiagram	PanPrecipitatio	in <u>PanOptimizer</u>	PenDiffusion Pa	anSolidification Property I	ible <u>G</u> raph <u>H</u> elp								
🔽 🖬 📂 🖬 🕼 📾 🗛 🗞 🖻 1	a×I	e 🗉 🖲 🚽	• 🗆 🗠 🖉	S 🗿 🖉 🖾 🖸		📴 🗵 🖄 📓 🛤 🗎 🔍	n 🗋 🗉 🕱 🧷								
Workspace # ×	/10 20	Al-Malarach	invariant table	invariant tiel	ne table	estable 2 Default graph	Default.table								
Pandat Workspace 'default' ***		T	P	v(AD	x(Ma)	obare name	KGAMa Beta)	(GAMo Enr.)	KOAMo Gamma)	ROFee)	(GHm)	G(GAMo Beta)	G(GAIMa Ear)	G(@AMa Gamma)	Q(@Ecc)
in See default				A(*)	2(118)	phase_name	(grang_bea)	(grang_cps)	(grang_country)	((0) 00)	(arrop)	o(grang_ocu)	o(grang_cps)	o(grang_oanna)	citer cc)
- Part Section_Densitie		C	* bar	* mole/mole	mole/mole		mole/mole	mole/mole	mole/mole	mole/mole	mole/mole	J/mole	J/mole	J/mole	J/mole J.
2D_AI-Mg	1	300.0000	1.000000	1.000000	0.000000	Fcc				1.000000					-18,756.90
🔒 🛅 Table	2	300.0000	1.000000	0.990000	0.010000	Fcc				1.000000					-18,978.90
- Default	3	300.0000	1.000000	0.980000	0.020000	Fcc				1.000000					-19,136.50
tiefine	4	300.0000	1.000000	0.970000	0.030000	Fcc				1.000000					-19,270.80
invariant tieline	5	300.0000	1.000000	0.960000	0.040000	Fcc				1.000000					-19,390.50
- inc_default	6	300.0000	1.000000	0.960000	0.050000	Fcc				1.000000					-19,499.70
Graph	7	300.0000	1.000000	0.940000	0.060000	Fcc				1.000000					-19,600.60
- 80 Default	8	300.0000	1.000000	0.930000	0.070000	Fcc				1.000000					-19,695.00
ia- Table	9	300.0000	1.000000	0.925000	0.075000	Fcc				1.000000					-19,740.10
Cam Device	10	300.0000	1.000000	0.924375	0.075625	Fcc				1.000000					-19.745.70
	11	300.0000	1.000000	0.924002	0.075999	Fcc				1.000000					-19,749.00
	12	300.0000	1.000000	0.924002	0.075999	Fcc+AIMg_Beta	0.000000			1.000000		-22,511.40			-19,749.00
	13	300.0000	1.000000	0.923750	0.076250	Fcc+AIMg_Beta	0.000805			0.999195		-22,511.40			-19,749.00
	14	300.0000	1.000000	0.922500	0.077500	Fcc+AIMg_Beta	0.004803			0.995197		-22,511.40			-19,749.00
	15	300.0000	1.000000	0.920000	0.050000	Fcc+AlMg_Beta	0.012799			0.987201		-22,511.40			-19,749.00
	16	300.0000	1.000000	0.910000	0.090000	Fcc+AIMg_Beta	0.044784			0.955216		-22,511.40			-19,749.00
	17	300.0000	1.000000	0.900000	0.100000	Fcc+AlMg Beta	0.076769			0.923231		-22,511.40			-19,749.00
🗱 Databases 🔄 Workspace	18	300.0000	1.000000	0.890000	0.110000	Fcc+AlMg_Beta	0.108753			0.891247		-22,511.40			-19,749.00
Property # ×	19	300.0000	1.000000	0.880000	0.120000	Fcc+AIMg_Beta	0.140738			0.859262		-22,511.40			-19,749.00
🗊 21 🔟 🖸	20	300.0000	1.000000	0.870000	0.130000	Fcc+AlMg_Beta	0.172723			0.827277		-22,511.40			-19,749.00
Appearance	21	300.0000	1.000000	0.860000	0.140000	Fcc+AlMg Beta	0.204708			0.795292		-22,511.40			-19,749.00
BackgroundC AppWorkspac	22	300.0000	1.000000	0.850000	0.150000	Fcc+AlMg_Beta	0.236693			0.763307		-22,511.40			-19,749.00
GridColor ControlDark	23	300.0000	1.000000	0.840000	0.160000	Fcc+AlMg Beta	0.268678			0.731322		-22.511.40			-19.749.00
CallBorderSh Single	24	300.0000	1.000000	0.830000	0.170000	Fcc+AlMg Beta	0.300663			0.699337		-22.511.40			-19,749.00
DefaultCellSh DataGridViewCellS	25	300,0000	1.000000	0.820000	0.180000	Ecc+AlMg Beta	0.332648			0.667352		-22.511.40			-19.749.00
✓ Layout	26	300.0000	1.000000	0.810000	0.190000	Fcc+AlMg Beta	0.364632			0.635368		-22.511.40			-19.749.00
AutoSizeColu None	27	300.0000	1.000000	0.800000	0.200000	Fcc+AlMg Beta	0.396617			0.603383		-22.511.40			-19,749.00
	28	300,0000	1 000000	0 790000	0.210000	Ecc+AlMa Beta	0.428602			0.571398		-22 511 40			-19 749 00
	29	300,0000	1.000000	0.780000	0.220000	Ecc+AlMg Beta	0.460587			0.539413		-22.511.40			-19.749.00
	30	300,0000	1 000000	0 770000	0.230000	Fcc+AlMg Beta	0.492572			0.507428		-22.511.40			-19 749 00
	31	300,0000	1 000000	0 760000	0.240000	Ecc+AlMg Beta	0.524557			0.475443		-22.511.40			-19 749 00
	32	300,0000	1,000000	0.750000	0.250000	Ecc+AlMg Beta	0.556542			0.443458		-22.511.40			-19.749.00
	33	300,0000	1 000000	0 740000	0.260000	Fcc+AlMa Beta	0.588527			0.411473		-22 511 40			-19 749 00
	34	300,0000	1 000000	0 730000	0.270000	Ecc+AlMo Beta	0.620511			0.379489		-22.511.40			-19 749 00
	35	300 0000	1 000000	0 720000	0.280000	Ecc+AlMg Beta	0.652496			0.347504		-22.511.40			-19 749 00
	36	300.0000	1,000000	0.710000	0.290000	Fee+AlMo Beta	0.684481			0.315519		-22 511 40			-19 749 00
	37	300.0000	1,000000	0.700000	0 300000	Fcc+AlMa Beta	0.716466			0.283534		-22 511 40			-19 749 00
	39	300,0000	1 000000	0.690000	0.310000	EccaAlMa Bata	0.748451			0.251549		2251140			19 749 00
		200.0000	1.000000	0.000000	0.010000	Contraing_0000	0.70001			0.0300004		00.011.40			10.740.00

Figure 1.2.4: Default table showing phase fraction variation as a function of composition

Example 1.3 Phase Fraction as a Function of Temperature

Purpose: Learn to calculate and use a phase fractions vs. temperature plot

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.3.pbfx

In Example 1.2 : Phase Fraction as a Function of Composition, we have calculated the fraction of each phase as a function of composition. In most cases, people would like to know phase transformation when temperature varies. In this example, we calculate the fraction of phases as a function of temperature for an AIMg binary alloy with composition of x(Mg)=0.3 (the red dash line in Figure 1.3.1). Such a calculation is especially valuable for a multi-component alloy.



Figure 1.3.1: AI-Mg binary phase diagram

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Perform 1D calculation following the procedure in Pandat User's Guide 3.3.2;
- Set Calculation Condition as shown in Figure 1.3.2;

Line Calcu	ulation	/	/			Part Calculate	×
Start F	Point			End Point			
		Value			Value		
►т	(C)	700		► T(C)	0	Canc	
×	(AI)	0.7		x(Al)	0.7	Optio Extra Ou	ns
×	(Mg)	0.3		x(Mg)	0.3		ndition
т	otal:	1	$\mathbf{\Sigma}$	Total:	1	Save Cor	ndition
						Select P	hases
Numb	er of steps	s: 100 💌		Individual P	hases		



- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

- Liquid is the only stable phase at high temperature until 496.1 °C, which is the liquidus temperature;
- Below liquidus, Fcc phase forms and its fraction increases while that of the Liquid phase decreases until the eutectic temperature 450.47 °C;
- At eutectic temperature 450.47 °C, Liquid is disappeared (drops to 0% from 68.3%), fraction of the AlMg_Beta phase jumps from 0% to 60.21% and that of the Fcc phase jumps from 31.7% to 39.79%;
- Details on the fraction of each phase as a function of temperature can also be found in the Default table as shown in Figure 1.3.4;



Figure 1.3.3: Phase fraction variation as a function of composition

Pandat Software by CompuTherm, LLC																- 0 ×
Eile Edit View Databases Bato	h Calc <u>P</u>	anPhaseDiagram	PanPrecipitation	n <u>PanOptimizer</u>	PanDiffusion Pa	nSolidification Property]	Eable Graph Help									
i 🖬 🗃 🗃 🖬 🕼 🗿 🖶 X 🗞	6×I			🛐 🗿 🛱 🕅		📴 🗵 🖻 📓 🐘 🗛 🔍	0 E E 🕱 🧷									
Workspace # ×	/ 10 20	Al-Malarach	invariant table	invariant tiel	ine table	etable 1 Default graph	Default.table	aultoraph 2001	Default.table							•)
Pandat Workspace 'default' ***	/	T	P	×(Al)	x(Ma)	obare name	K@AMg Bets)	#@Ecc)	fi@Liquid)	G(GAIMa Bata)	G(@Erc)	G(@Liquid)	G	w(AD	w(Ma)	n ka
a 😡 default		· · ·		A(N)	A(mg)	phase_name	(@vinig_beta)	(wree)	(Gridua)	G(@voing_bea)	G(err cc)	G(eyciquo)	9	w(ru)	w(mg)	1049
- Section_default		c	* bar	 mole/mole 	 mole/mole 		mole/mole	mole/mole	mole/mole	J/mole	J/mole	J/mole	J/mole	kg/kg	▼ kg/kg	* kg
2D_AI-Mg	22	553.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-36,813.40	-36,813.40	0.721474	0.278526	0.026179
🛛 🔚 Table	23	546.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-36,312.00	-36,312.00	0.721474	0.278526	0.026179
	24	539.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-35.812.40	-35.812.40	0.721474	0.278526	0.026179
tieline	25	532.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-35,314.70	-35,314.70	0.721474	0.278526	0.026179
invariant traffice	26	525.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-34,818.80	-34,818.80	0.721474	0.278526	0.026179
ine default	27	518.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-34,324.80	-34,324.80	0.721474	0.278526	0.026179
Graph	28	511.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-33,832.60	-33,832.60	0.721474	0.278526	0.026179
Default	29	504.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-33,342.40	-33,342.40	0.721474	0.278526	0.026179
🚊 🥘 Table	30	497.0000	1.000000	0.700000	0.300000	Liquid			1.000000			-32,854.00	-32.854.00	0.721474	0.278526	0.026179
Default	31	496,1250	1.000000	0.700000	0.300000	Liquid			1.000000			-32,793.10	-32,793.10	0.721474	0.278526	0.026179
- Etample_vs	32	496,1060	1.000000	0.700000	0.300000	Liquid			1.000000			-32,791,80	-32,791,80	0.721474	0.278526	0.026179
30 Default	33	496 1060	1.000000	0 700000	0.300000	Liquid+For		0.000000	1.000000		-30.637.00	-32 791 80	-32 791 80	0 721474	0.278526	0.026179
a Table	24	495 6820	1,000000	0.700000	0.300000	LiquidaEcc		0.003327	0.996673		-30.617.30	32 769 80	.32 762 70	0 721474	0.278526	0.026179
Default	36	495 2500	1,000000	0.700000	0.300000	LiquidaEcc		0.005789	0.993211		30,595,60	32 746 90	32 732 30	0.721474	0.278526	0.026179
	26	493 5000	1,000000	0.700000	0.300000	LiquideEco		0.020514	0.979496		-30 514 30	-32 664 90	-32,610,90	0.721474	0.279526	0.026179
	30	400.0000	1.000000	0.700000	0.300000	Liquid Fee		0.047405	0.053505		30,340,20	32,460,70	22,260,10	0.721474	0.079506	0.020170
	37	493,0000	1.000000	0.700000	0.300000	Liquid+Fee		0.090192	0.902995		-30,349.30	-32,905.70	-32,303.10	0.721474	0.278526	0.026179
Catabases Workspace		403.0000	1.000000	0.700000	0.300000	Liquid+Fee		0.033133	0.000007		-30.013.00	32,030,10	-01.000.20	0.721474	0.270020	0.020179
Property B Y	- 39	476.0000	1.000000	0.700000	0.300000	Liquid+Pec		0.140732	0.051200		23,630.00	-31,710.40	-31,416.60	0.721474	0.270526	0.026179
Endlin o	40	469.0000	1.000000	0.700000	0.300000	Liquid+Pcc		0.196474	0.803526		-29,362.40	-31,336.90	-30,949.00	0.721474	0.278526	0.026179
	41	462.0000	1.000000	0.700000	0.300000	Liquio+rcc		0.242035	0.757165		-29,034.60	-30,952.00	-30,466.40	0.721474	0.276526	0.026179
 Appearance BackgroundC AppWorkspace 	42	455.0000	1.000000	0.700000	0.300000	Liquid+Fcc		0.288208	0.711792		-28.707.40	-30,564.00	-30.028.90	0.721474	0.278526	0.026179
GridColor ControlDark	43	451.5000	1.000000	0.700000	0.300000	Liquid+Fcc		0.310643	0.689357		-28,544.20	-30,368 90	-29,802.00	0.721474	0.278526	0.026179
BorderStyle FixedSingle	44	450.6250	1.000000	0.700000	0.300000	Liquid+Pcc		0.316234	0.683766		-28,503.40	-30,320.00	-29,745.50	0./214/4	0.278526	0.026179
CellBorderSty Single	45	450.4670	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.602127	0.397873		-30.554.30	-28.496.00		-29.735.30	0.721474	0.278526	0.026179
DefaultCellSh DataGridViewCellS	46	450.4670	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.602127	0.397873		-30,554.30	-28,495.00		-29,735.30	0.721474	0.278526	0.026179
AutoSizeColy Mana	47	450.4670	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.602127	0.397873		-30,554.30	-28,496.00		-29,735.30	0.721474	0.278526	0.026179
Autosizecolu None	48	450.4670	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.602127	0.397873		-30,554.30	-28.496.00		-29,735.30	0.721474	0.278526	0.026179
	49	450.1870	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.602499	0.397501		-30.538.40	-28.478.10		-29.719.40	0.721474	0.278526	0.026179
	50	449.7500	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.603078	0.396922		-30,513.60	-28,450.20		-29,694.60	0.721474	0.278526	0.026179
	51	448.0000	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.605371	0.394629		-30,414.50	-28,338.50		-29,595.20	0.721474	0.278526	0.026179
	52	441.0000	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.614167	0.385833		-30.019.30	-27.894.20		-29.199.40	0.721474	0.278526	0.026179
	53	434.0000	1.000000	0.700000	0.300000	Fcc+AJMg_Beta	0.622407	0.377593		-29,626.20	-27,453.60		-28,805.80	0.721474	0.278526	0.026179
	54	427.0000	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.630142	0.369858		-29,235.10	-27,016.70		-28,414.60	0.721474	0.278526	0.026179
	55	420.0000	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.637416	0.362584		-28,846.00	-26,583.60		-28,025.70	0.721474	0.278526	0.026179
	56	413.0000	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.644268	0.355732		-28,459.00	-26.154.30		-27.639.20	0.721474	0.278526	0.026179
	57	406.0000	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.650732	0.349268		-28,074.10	-25,728.70		-27,254.90	0.721474	0.278526	0.026179
	58	399.0000	1.000000	0.700000	0.300000	Fcc+AIMg_Beta	0.656840	0.343160		-27,691.30	-25,306.80		-26,873.00	0.721474	0.278526	0.026179
	59	392.0000	1.000000	0.700000	0.300000	Fcc+AlMg_Beta	0.662617	0.337383		-27.310.60	-24,888.80		-26,493.50	0.721474	0.278526	0.026179
		201 0000	1 000000	0.300000	0.000000	P	0.000000	0.000011		00.000.00	04.474.50		00.110.00	0 701 474	0.070500	0.0001300

Figure 1.3.4: Default table showing phase fraction variation as a function of temperature

Example 1.4 Point Calculation at Fixed Temperature and Composition

Purpose: Learn to calculate and get detailed phase stability information at a given temperature and composition

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.4.pbfx

From the Al-Mg phase diagram shown in Figure 1.4.1, we know that two phases, $AlMg_Beta+Fcc$, are stable at the point indicated by Φ (the cross of the two dash lines). Other than that, no detail information about this point can be read directly from this phase diagram. In this example, we perform a Point Calculation to obtain the detail information at the selected point.



Figure 1.4.1: AI-Mg binary phase diagram

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Perform 0D calculation following the procedure in Pandat User's Guide 3.3.1;
- Set Calculation Condition as shown in Figure 1.4.2;

Poi	nt Calculation		×
	Point		
		Value	
	T(C)	300	Cancel
	x(Al)	0.3	Options
	▶ x(Ma)	0.7	Extra Outputs
	- X(Mg)		Load Condition
	Total:	1	Save Condition
			Select Phases
			Select Comps
			Load Chemistry
			Save Chemistry
			-

Figure 1.4.2: Point Calculation for an alloy with 30 at% AI and 70 at% of Mg at 300°C

Calculation Method 2 from labeling:

• After the AI-Mg phase diagram is calculated, click **[**] on the Labeling mode, then put the cursor at the selected point and press Ctrl button, click the mouse.

- Two phases, AlMg_Gamma and Hcp, are stable at the given condition (temperature and composition);
- The G, H, S, and Cp of the system at the given composition and temperature are 22744.9 J/mol, 6539.3 J/mol, 51.0935 J/K·mol, and 30.2876 J/K·mol, respectively;
- The equilibrium composition of AlMg Gamma is x(AI) = 0.409686, x(Mg) = 0.590314;
- The mole fraction of AlMg Gamma is 0.687999 (weight fraction is 0.696044);
- The G, H, Cp, G^{ex}, and H^{ex} of AlMg_Gamma at equilibrium composition are -23186.3 J/mol, 5976.71 J/mol, 31.3752 J/K·mol, 135.828 J/mol, and 146.6 J/mol, respectively;
- The site fraction of AlMg_Gamma are: $y_{Mg}^{I} = 1$, $y_{Al}^{II} = 0.0291951$, $y_{Mg}^{II} = 0.970805$, $y_{Al}^{III} = 0.96088$, $y_{Mg}^{III} = 0.0391201$;

- The equilibrium composition of Hcp is x(AI) = 0.058129, x(Mg) = 0.941871;
- The mole fraction of Hcp phase is 0.312001 (weight fraction is 0.303956);
- The G, H, Cp, G^{ex}, and H^{ex} of Hcp at equilibrium composition are -21771.6 J/mol, 7779.87 J/mol, 27.8893 J/K·mol, 179.735 J/mol, and 184.813 J/mol, respectively;
- The site fraction of Hcp is the same as its composition since it is essentially one sublattice model, the second sublattice is occupied by vacancy.



Figure 1.4.3: Calculated results for an alloy with 30 at% Al and 70 at% of Mg at 300°C

Example 1.5 Isotherm of AI-Mg-Zn at 500°C

Purpose: Learn to calculate and use an isothermal section in a ternary system

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example #1.5.pbfx

A complete phase diagram of a ternary system should be described by a triangular prism in a 3D space with each edge of the triangle base representing the composition axis of each component and the vertical axis the temperature. Due to the complexity of many ternary systems, phase stability of a ternary system is usually described by Isothermal sections parallel to the triangle base (constant temperature) and isoplethal sections vertical to the triangle base plane. In this example, we will calculate an isothermal section of Al-Mg-Zn at 500°C.

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform 2D calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.5.1;



Figure 1.5.1: 2D calculation of an isotherm of Al-Mg-Zn at 500°C

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add tie-lines following the procedure in Pandat User's Guide 2.3.1;



Figure 1.5.2: Calculated isotherm of Al-Mg-Zn at 500 °C

- Phase stability in different composition areas, single phase, two-phase, and three-phase regions, can be viewed clearly at this temperature;
- Equilibrium between two phases is connected by tie-lines, and the equilibrium compositions of the two phases can be read at the end points of the tie-line; Details on the tie-lines can be found in Table->tieline as shown in Figure 1.5.3. In this table, the compositions of the two phases connected by each tieline are listed for all the calculated tielines;
- Three-phase equilibrium is shown by the tie-triangle. The composition of each phase in the three-phase equilibrium is listed in invariant_tieline table, as shown in Figure 1.5.4.

🚯 Pandat Software by CompuTherm, LLC								- 0	×
<u>Eile Edit View Databases Batch Calc</u>	<u>P</u> anPhaseDiag	ram <u>P</u> anPrecipit	ation <u>P</u> anOptimizer <u>P</u> anDiffusion	n Pan <u>S</u> olidificati	on <u>P</u> roperty]	able <u>G</u> raph <u>H</u>	lelp		
🗔 🖬 🔗 🖩 🎒 🖗 🛎 🗴 🛍 🏷	🛃 🔚 🖲	🛃 🖸 🗖 🖂) 📴 🐹 🎆 👰	🖉 🎯 🛃 🔍	୍ 🔍 ମ 🔳 📰	I. 🖉		
Workspace 🕂 🛪	2D_AI-I	Mg.graph 🔲	invariant.table 📰 invaria	ant_tieline.table	😥 2D_AI-M	g-Zn.graph*	ieline.table	×	
Graph ^		т	phase_name	x(Al)	x(Mg)	x(Zn)	w(Al)	w(Mg)	^
2D_AI-Mg		c v		mole/mole ~	mole/mole ~	mole/mole ~	kg/kg ~	kg/kg ~	
Default		500.0000	Fee	0 790910	1.010358E-008	0 209090	0.600502	7.013663E-009	
🥅 tieline	2	500.0000	Liquid	0.472177	1.460986E-007	0.527823	0.269609	7.514453E-008	
	3								
Isotherm of Al-Mo-Zn at 500C	4	500.0000	Fcc	0.790913	1.704691E-007	0.209086	0.609507	1.183360E-007	1
Graph	5	500.0000	Liquid	0.472176	2.464966E-006	0.527822	0.269609	1.267835E-006	
2D_AI-Mg-Zn	6								1
Workspace Databases	7	500.0000	Fcc	0.790967	2.737593E-006	0.209030	0.609587	1.900497E-006	
Property I X	8	500.0000	Liquid	0.472164	3.957717E-005	0.527796	0.269608	2.035666E-005	
	9								
	10	500.0000	Fcc	0.791075	7.877858E-006	0.208917	0.609746	5.469663E-006	
 Appearance BackgroundColor AppWorkspace 	11	500.0000	Liquid	0.472141	0.000114	0.527745	0.269608	5.855805E-005	
GridColor ControlDark	12								
BorderStyle FixedSingle	13	500.0000	Fcc	0.791291	1.818285E-005	0.208691	0.610064	1.262764E-005	
DefaultCellStyle DataGridViewCellStyle { E	14	500.0000	Liquid	0.472095	0.000263	0.527642	0.269606	0.000135	1
✓ Layout	15								
AutoSizeColumns/ None	16	500.0000	Foc	0.793016	0.000102	0.206882	0.612614	7.084500E-005	
	17	500.0000	Liquid	0.471731	0.001460	0.526809	0.269599	0.000752	
	<							>	

Figure 1.5.3: The tieline table showing the detailed information of calculated tieline

🚯 Pandat Software by CompuTherm, LLC							- 0	×
<u>E</u> ile <u>E</u> dit <u>V</u> iew <u>D</u> atabases <u>B</u> atch Calc	PanPhaseE	Diagram <u>P</u> anPreci	pitation <u>P</u> anOptimizer <u>P</u> anDiffe	usion PanSolidification Property	<u>T</u> able <u>G</u> raph	Help		
🕞 🖬 🚰 🖬 🚰 🖄 🛎 🗶 🛍 🏷		1 🕑 📑 💽 🖂 1		🗏 😼 🔣 📲 🗑 🖭 强 🕅	। 🗟 🔍 🗗 📘 [😑 🕮 🖉		
Workspace $+ \times$	🔲 inv	ariant_tieline.table	2D_AI-Mg-Zn.graph*	📰 tieline.table 📰 inv	ariant.table	invariant_tiel	ine.table ×	Ŧ
🥅 invariant 🔹 🔨		т	reaction	phase_name	x(Al)	x(Mg)	x(Zn)	
Isotherm of Al-Mg-Zn at 500C		c ~			mole/mole ~	mole/mole ~	mole/mole	~ k ~
😑 🎇 Graph	1	500.0000		Liquid	0.108822	0.506845	0.384333	0.072
2D_AI-Mg-Zn	2	500.0000		C14	0.053458	0.336829	0.609713	0.029
Default	3	500.0000		T_AIMgZn	0.143574	0.387826	0.468600	0.088
tieline 🗸	4	500.0000		Liquid	0.108822	0.506845	0.384333	0.072
Workspace Databases								
Property 4 ×								
21 E								
Y Appearance								
BackgroundColor AppWorkspace								
GridColor ControlDark BorderStyle EixedSingle								
CellBorderStyle Single								
DefaultCellStyle DataGridViewCellStyle { E								
Y Layout								
AutoSizeColumns/ None	<							>
								_

Figure 1.5.4: The invariant_tieline table showing the composition of each phase in the invariant

reaction

Example 1.6 Isopleth of Al-Mg-Zn at 15 at% Zn

Purpose: Learn to calculate and use an isoplethal section in a ternary system

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.6.pbfx

As mentioned in Example 1.5 : Isotherm of AI-Mg-Zn at 500°C, isopleths are sections vertical to the triangle base plane of the triangular prism. An isopleth is important in understanding phase relationship in a ternary system when temperature is a variable. In this example, we will calculate an isoplethal section in the AI-Mg-Zn ternary parallel to AI-Mg binary with 15 at% of Zn.

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform 2D calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.6.1;



Figure 1.6.1: 2D calculation of an isopleth parallel to Al-Mg binary with 15 at% Zn

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;



Figure 1.6.2: Calculated isopleth parallel to AI-Mg binary with 15 at% Zn

- Phase stability as a function of composition of Mg and temperature. Single phase, twophase, and three-phase regions, can be viewed clearly at different composition and temperature;
- Tie-lines cannot be viewed on an isopleth since they are usually not on the same isoplethal plane except for a pseudo-binary. The tieline information is listed in tieline Table as shown in Figure 1.6.3.

• The invariant reactions and the phase composition for every phase in the invariant reaction are listed in invariant_tieline table as shown in Figure 1.6.4.

n Pandat Software by CompuTherm, LLC								- 0	×			
<u>File Edit View Databases Batch Calc</u>	PanPhaseDiag	ram <u>P</u> anPrecipit	ation <u>P</u> anOptimizer <u>P</u> anDiffusion	n Pan <u>S</u> olidificati	on <u>P</u> roperty <u>I</u>	able <u>G</u> raph <u>H</u>	elp					
▝▖▖▌▓▝▖▌▓▝▋▎▓▝▌▝▝▋▋▋▌▋▋₩₽₽₩₩₽₽₩₩₽₽₩₩₽₽₩₽₽₽₩₽₽₽₽₽₽₽₽₽₽												
Workspace 🕂 🛪	tieline.	table 🧰 i	nvariant.table 📰 invariant_t	ieline.table	😵 2D_Al-Mg-Zn	.graph 📃	tieline.table \times		Ŧ			
Table ^		т	phase_name	x(Al)	x(Mg)	x(Zn)	w(AI)	w(Mg)	^			
tieline		c ~		mole/mole ~	mole/mole ~	mole/mole ~	kg/kg ~	kg/kg	~			
invariant	1	469.7362	Liquid	0.578720	0.271280	0.150000	0.487711	0.205936				
Invariant_tieline Isopleth of Al-Mg-Zn at 15. Zn	2	469.7362	Fcc	0.898239	0.074690	0.027071	0.871125	0.065249				
Graph	3								_ 1			
🗌 🐼 2D_Al-Mg-Zn 🗸 🗸	4	469.7370	Liquid	0.578722	0.271278	0.150000	0.487712	0.205935				
Workspace Databases	5	469.7370	Fcc	0.898239	0.074689	0.027071	0.871126	0.065248				
Property 🖡 🗙	6								- 1			
1 21 m	7	469.7549	Liquid	0.578749	0.271251	0.150000	0.487734	0.205914	_			
Appearance	8	469.7549	Fcc	0.898248	0.074679	0.027073	0.871130	0.065239				
BackgroundColor AppWorkspace	9	460 7006	1 factor	0.570000	0.071107	0.150000	0 407777	0.005070				
GridColor ControlDark	10	469.7906	Eco	0.909264	0.271197	0.027079	0.487777	0.205672	-			
CellBorderStyle Single	12	400.1000		0.0002.04	0.074000	0.027070	0.071140	0.000220				
DefaultCellStyle DataGridViewCellStyle { E	13	470.0767	Liquid	0.579239	0.270761	0.150000	0.488127	0.205533				
AutoSizeColumns/ None	<	470.0707	-	0.000000	0.074400	0.007110	0.071014	0.005000	> ~			
				_	_	_			<u> </u>			

Figure 1.6.3: The tieline table showing the detailed information of calculated tieline

<u>File Edit View Databases Batch Ca</u>	c <u>P</u> anPhas	eDiagram <u>P</u> anPre	cipitation PanOptimizer PanDif	usion PanSolidification Property	<u>T</u> able <u>G</u> raph	<u>H</u> elp	
🗔 🖻 🔗 🗟 🎒 🖸 🖶 🕷 🗅	× I 🛃 🖻	🛃 💽 🖻	🖻 🛆 🔕 📦 🐯 🔞 🐼 🕿	📖 🐷 🕍 🔚 😹 🔎 💽 🚿	। 🖓 🔍 🕅 📘	🗉 🏨 🖉	
Workspace 🛛 🕹 🕹	😿 2D_AI	-Mg-Zn.graph	🔲 tieline.table 🔲 inva	iant.table 🧰 invariant_tieli	ne.table ×		
Pandat Workspace 'default' ***		т	reaction	phase_name	x(Al)	x(Mg)	
<u>default</u> <u>default</u> <u>inversion</u> isopleth of Al-Mg-Zn at 15_		c ~			mole/mole ~	mole/mole ~	mc 🗸
Graph	1	475.4617	T_AIMgZn + Liquid => Fcc + C14	T_AIMgZn	0.196070	0.329807	0.474
C 2D Al-Mg-Zn	2	475.4617	T_AIMgZn + Liquid => Fcc + C14	Liquid	0.468124	0.184109	0.347
Workspace Databases	3	475.4617	T_AIMgZn + Liquid => Fcc + C14	Fcc	0.902262	0.029388	0.068
	4	475.4617	T_AIMgZn + Liquid => Fcc + C14	C14	0.076135	0.332468	0.591
roperty 4 A	5	475.4617	T_AIMgZn + Liquid => Fcc + C14	Liquid	0.468124	0.184109	0.347
21	6	475.4617	T_AIMgZn + Liquid => Fcc + C14	Foc	0.902262	0.029388	0.068
Appearance	7	475.4617	T_AIMgZn + Liquid => Fcc + C14	T_AIMgZn	0.196070	0.329807	0.474
GridColor ControlDark	8	475.4617	T_AIMgZn + Liquid => Fcc + C14	C14	0.076135	0.332468	0.591
BorderStyle FixedSingle	9						
CellBorderStyle Single DefaultCellStyle DataGridViewCellSt	<						>

Figure 1.6.4: The invariant_tieline table showing composition of each phase involved in the

invariant reaction

Example 1.7 Liquidus Projection of Al-Mg-Zn

Purpose: Learn to calculate and use a liquidus projection in a ternary system

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.7.pbfx

As mentioned in Example 1.5 : Isotherm of AI-Mg-Zn at 500°C and Example 1.6 : Isopleth of <u>AI-Mg-Zn at 15 at% Zn</u>, isotherms and isopleths are two types of phase diagrams used to view the phase relationship in a ternary system. Another type of phase diagrams commonly used to understand a ternary system is the liquidus projection which is the projection of the liquid surface onto the base triangle plane. In this example, we will calculate the liquidus projection of AI-Mg-Zn ternary system.

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform phase projection following the procedure in Pandat User's Guide 3.3.6;
- Set Calculation Condition as shown in Figure 1.7.1;

Isotherms		ОК
Calculat	e Isotherms: 🔽	Cancel
Temperature	Interval [C]: 50	Options
		Extra Outputs
Default Axis Name	S	Land Canditia
X Axis:	x(Zn) 👻	Load Conditio
Y Axis:	x(AI) -	Save Conditio
		Select Phases
Select Target Pha	se	Select Comps
Target Phase:	Liquid 🗸	
She	ow Results for Subsystems: 📝	
	Shaw 2D Diagram	

Figure 1.7.1: Phase projection calculation setting dialog

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the isothermal lines by put the cursor on each line and then press F2;





- The phase name labeled in each region indicates the primary solidified phase from liquid when the given alloy composition falls in that region;
- The univariant liquid projection lines (blue lines) trace the composition of the liquid phase for the three-phase equilibrium among the liquid and the other two phases separated by the liquid projection line;

- The isothermal lines (from red to green with temperature descending) represent the liquidus temperatures. The liquidus temperature for all the compositions along each line is identical;
- Each triple point at the intersection of three projection lines represents a invariant reaction (four phases in a ternary system) involving the liquid phase. All the invariant reactions are listed in invariant table as shown in Figure 1.7.3. The composition of each phase involved in the invariant reaction is listed in invariant_tieline table as shown in Figure 1.7.4.

Pandat Software by CompuTherm, LLC														9-01	6 X
Fie Edit Youw Databases Batch Calc	BenPh	eseDiegrem gen	Precipitation <u>PerrOptimizer</u> <u>PanE</u>	iffusion PanGolidification Brop	erty <u>I</u> able <u>G</u> r	aph <u>H</u> elp									
🗆 🖬 🖆 🖬 💕 🖄 🖶 I X 🖻 🖻 I	× 🖻 🛛	3 I I I I I I I I	🖃 🖂 🔊 i 🖉 🖾 🖂 🖻	i 🖬 i 🗄 i 📴 🖄 🖄 🐘 i 🕷 i	4 9, 0 🔲	E 🕱 🖉									
Workspace 3 ×	/ 🗆 in	ariant.table	inverient_tieline.table 111 isotherm	table 📶 Default table 📶 tieli	netable 📶 inv	oriant table 🔚	invariant_ticline.tab	He 10 20 Al-M	lg-Zngraph"	Default table	ticline.table	inverient.table	inverient_tieline.table	Default.table	= = ×
Pandat Workspace 'default' ***		Т	reaction	phase_name	#phases	x(Al)	x(Mg)	x(Zn)	w(Al)	w(Mg)	w(Zn)	(@AMg_Beta)	t@AMg_Gamma)	t(@C14)	165
a P section_default		c .	1			mole/mole	 mole/mole 	* mole/mole	* kg/kg	* kaka	 kalka 	 mole/mole 	mole/mole	molelmole	mole/
- A projection_default		660 2200	Linuidan Ess	LinuidaEco	2	1.000000	0.000000	0.000000	1000000	0.000000	0.000000				100000
G - Cooph	2	649.8500	Liquid as Hop	LiquidaHen	2	0.000000	1000000	0.000000	0.000000	1 000000	0.000000				
PP Al-Mg-Zn	3	419 5280	Liquid +2 Hop	Liquid+Hcp	2	0.000000	0.000000	1 000000	0.000000	0.000000	1 000000				
- Table	4				-										
- E Default	5	450.4670	Liquid => Fcc + AlMo Beta	Liquid+Fcc+AMg Beta	3	0.637666	0.362334	0.000000	0.661444	0.338556	0.000000	0.881903			0.118097
Tourist Valina	6	449 5020	Liquid => AMg Beta + AMg	Liquid+AlMa Beta+AlMa Ga.	3	0.576044	0.423956	0.000000	0.601337	0.398663	0.000000	0.615573	0.384427		
iotherm	7	435,2780	Liquid +> AMg Gamma + Hop	Liquid+AlMg Gamma+Hcp	3	0.310102	0.689698	0.000000	0.332888	0.667112	0.000000		0.684957		
section_default_1	8	415.8000	Liquid = C14 => Mg2Zn3	Liquid+Mg2Zn3+C14	3	0.000000	0.643610	0.356390	0.000000	0.401644	0.598356			0.798670	
	9	382.0300	Liquid => Hop = Foc	Liquid+Hep+Fee	3	0.110828	0.000000	0.889172	0.048915	0.000000	0.951085				0.279455
	10	381,2400	Liquid - C14 -> Mg2Zn11	Liquid+C14+Mg2Zn11	3	0.000000	0.036611	0.913389	0.0000000	0.034045	0.965955			0.277179	
	11	366.9990	Liquid => Mg2Zn11 = Hcp	Liquid+Mg2Zn11+Hcp	3	0.000000	0.070105	0.929895	0.000000	0.027258	0.972742				
	12	346.9990	Liquid = Mg2Zn3 => MgZn	Liquid+MgZn+Mg2Zn3	3	0.000000	0.703980	0.296020	0.000000	0.469198	0.530802				
	13	339.6200	Liquid = Hcp => Mg7Zn3	Liquid+Hcp+Mg7Zn3	3	0.000000	0.711960	0.288050	0.0000000	0.478809	0.521191				
	14	339.5810	Liquid +> Mg7Zn3 + MgZn	Liquid+Mg7Zn3+MgZn	3	0.000000	0.710911	0.289069	0.0000000	0.477547	0.522453				
	15														
	16	475 4620	Liquid = T => Fee = C14	Liquid+Fcc+C14+T	4	0.468124	0.184109	0.347766	0.316993	0.112301	0.570706			0.558158	0.441842
	17	448.1530	Liquid +> T + AlMg_Gamma +	Liquid+T+AIMg_Gamma+AIM.	4	0.519888	0.431124	0.048968	0.506240	0.378156	0.115603	0.377657	0.455567		
B Databases Workspace	18	446.5130	Liquid +> T + AIMg_Beta + Fcc	Liquid+T+AIMg_Beta+Fcc	4	0.601735	0.342158	0.056107	0.575316	0.294679	0.130004	0.592632			0.191158
Property # X	19	434.1590	Liquid = C14 + T => Mg2Zn3	Liquid+C14+T+Mg2Zn3	4	0.055053	0.606534	0.338413	0.038728	0.384341	0.576931			0.663860	
10 24 m Ω	20	357.5090	Liquid - C14 -> Mg2Zn11 + Fcc	Liquid+Mg2Zn11+Fcc+C14	4	0.104908	0.076680	0.818412	0.048628	0.032017	0.919356			0.230089	0.126698
 Appearance 	21	353.5250	Liquid + T + Mg2Zn3 => MgZn	Liquid+T+Mg2Zn3+MgZn	4	0.045923	0.686388	0.267689	0.034977	0.470916	0.494106				
BackgroundCr AppWorkspace	22	351.8760	T + Hop +> Liquid + AlMg_Ga	Liquid+T+Hcp+AlMg_Gamma	4	0.116067	0.695813	0.188119	0.096824	0.522961	0.380315		0.223573		
BorderStyle FixedSingle	23	345.0100	Liquid => Mg2Zn11 = Hcp + Fcc	Liquid+Mg2Zn11+Hcp+Fcc	4	0.081867	0.060094	0.858038	0.036953	0.024434	0.938613				0.177936
CellBorderStyl Single	24	338.9090	Liquid = Mg7Zn3 => MgZn + Hcp	Liquid+MgZn+Hcp+Mg7Zn3	4	0.001340	0.711283	0.287377	0.001001	0.478679	0.520320				
DefaultCellStyl DataGridWewCellStyle	25	336.9220	Liquid +> T + MgZn + Hcp	Liquid+T+MgZn+Hcp	4	0.051188	0.700938	0.247874	0.039888	0.492010	0.468102				
Aud/SizeColum Nome	5														

Figure 1.7.3: Invariant table showing all the invariant reactions involving liquid phase

ile Edit View Databases Batch Calc	PanPhase	Diagram PanPres	ipitation PanOptimizer PanDiff	usion PanSolidification Property	Table Graph	Help	
	- 🗈 🖻		A A B B R R P	IIII I 🛛 🖄 III 🖓 📖 🕅	b ⊂ c ⊓ L	Ξτ. 🧷	
/orkspace $rac{1}{2} imes 4$	😵 PP_AI-	Mg-Zn.graph	PP_AI-Mg-Zn.graphx	invariant.table invari	ant_tieline.table	×	
Activity in Al-Mg at 300C		т	reaction	phase name	x(Al)	x(Mg)	x
section_default		с ×			mole/mole ×	mole/mole ×	mole V
i → M section_default_1		C F			molemole	molemole	mole -
section_default_2	1	660.3201	Liquid => Fcc	Liquid	1.000000	0.000000	0.00000
section default 4	2	660.3201	Liquid => Fcc	Fcc	1.000000	0.000000	0.0000
Liquidus projection of Al-Mg	3						
🚊 😿 Graph	4	649.8497	Liquid => Hcp	Liquid	0.000000	1.000000	0.0000
PP_AI-Mg-Zn	5	649.8497	Liquid => Hcp	Нср	0.000000	1.000000	0.0000
PP_AI-Mg-Zn 🗸	6						
>	7	419.5276	Liquid => Hcp	Liquid	0.000000	0.000000	1.0000
/orkspace Databases	8	419.5276	Liquid => Hcp	Нср	0.000000	0.000000	1.0000
roperty 🛛 🕹 🗙	9						
1 2 I 🔤	10	450.4672	Liquid => Fcc + AIMg_Beta	Liquid	0.637666	0.362334	0.0000
Appearance	11	450.4672	Liquid => Fcc + AIMg_Beta	Fcc	0.834154	0.165846	0.0000
BackgroundColo AppWorkspace	12	450.4672	Liquid => Fcc + AIMg_Beta	AIMg_Beta	0.611354	0.388646	0.0000
GridColor ControlDark	13	450.4672	Liquid => Fcc + AIMg_Beta	Liquid	0.637666	0.362334	0.0000
CellBorderStyle Single	14						
DefaultCellStyle DataGridViewCellStyle {	15	449.5016	Liquid => AIMg Beta + AIMg Ga	Liquid	0.576044	0.423956	0.0000
' Layout	16	449.5016	Liquid => AIMg Beta + AIMg Ga	AlMa Beta	0.611354	0.388646	0.0000
AutoSizeColumn: None	17	449.5016	Liquid => AlMg Beta + AlMg Ga	AlMo Gamma	0.519503	0.480497	0.0000
	18	449.5016	Liquid => AIMg Beta + AIMg Ga	Liquid	0.576044	0.423956	0.0000

Figure 1.7.4: Invariant_tieline table showing composition of each phase involved in the

invariant reaction

Example 1.8 Solidification Simulation by Scheil Model and Lever Rule

Purpose: Learn to perform solidification simulation for a given alloy composition

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example #1.8.pbfx

Pandat has two models for solidification simulation, one based on Lever rule and the other Scheil model. Lever rule assumes infinite slow cooling so that equilibrium is reached at every step of solidification. Scheil model assumes fast cooling and fast diffusion in the liquid so that liquid maintains uniform composition, no diffusion in the solid and local equilibrium is reached between liquid and solid at the interface. In this example we will perform two solidification simulations using the two models for an alloy with 40 at% of AI, 50 at% of Mg and 10 at% of Zn. We will then compare the simulation results by plotting them on the same plot.

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform solidification simulation following the procedure in Pandat User's Guide 3.3.7;
- Set Calculation Condition as shown in Figure 1.8.1, check "Scheil" for the first calculation and "Lever" for the second calculation

Lic	uid Compos	sition	OK
		Value	Cancel
►	T(C)	1000	
	x(Al)	0.4	Options Extra Outputs
	x(Mg)	0.5	
-	x(Zn)	0.1	Load Condition
	Total:	1	
			Select Phases
			Select Comps
			Load Chemistry
			Load Chemistry Save Chemistry
- So	lidification Mo	del	Load Chemistry Save Chemistry
So	lidification Mo	del um (Scheil) 🔘 Equilibrium (Lever)	Load Chemistry Save Chemistry
So	lidification Mo Non-equilibri Start si	del um (Scheil) 💿 Equilibrium (Lever) imulation from liquidus surface 📝	Load Chemistry Save Chemistry
So	lidification Mo Non-equilibri Start si	del um (Scheil)	Load Chemistry Save Chemistry
So	lidification Mod Non-equilibri Start si	del um (Scheil) Equilibrium (Lever) imulation from liquidus surface End when no more liquid T_End [C]: 0	Load Chemistry Save Chemistry

Figure 1.8.1: Input the alloy composition for solidification simulation

- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

- Figure 1.8.2 shows the fraction of solid as a function of temperature from Scheil simulation. Solidification starts at 457°C and ends at 336.9°C, the freezing range is 120.1°C;
- The primary solidified phase is T_AIMgZn phase, AIMg_Gamma starts to solidify at 447.5°C and Hcp starts to solidify at 351.8°C. Put the cursor on the line segment, a tool tip will pop out showing the phase(s) solidified in that composition and temperature range (Figure 1.8.2). Press 'F2' to label it;

- Detail information for the simulation, such as solidification start temperature for a certain phase, the total fraction of each solid at different temperatures, latent heat, and total heat evolved can be found in the Default Table as shown in Figure 1.8.3;
- Certain properties can be selected from the Default table and plotted. Figure 1.8.4 shows the fraction of each solid phase as a function of temperature, and Figure 1.8.5 shows the Latent heat and total heat evolution as a function of temperature;
- Figure 1.8.6 shows the lever rule simulation which follows equilibrium calculation. It therefore shows a very narrow solidification range, starting from 457°C and ending at 437°C;
- Only two phases solidified from lever rule simulation, i.e., T_AIMgZn phase and AIMg_ Gamma phase;
- Details on the fraction of solid phase, heat evolution, and so on can also be found in the Default table;
- Figure 1.8.7 shows the overlapped plots from Scheil simulation and Lever rule simulation. To merge two plots together, we first open the plot from Lever rule simulation as shown in Figure 1.8.6, right click the mouse and choose "Copy Data", then open the plot from Scheil simulation as shown in Figure 1.8.2, right click the mouse and choose "Paste Data". The two plots from Lever rule simulation and Scheil simulation are merged in the same diagram as shown in Figure 1.8.7;



Figure 1.8.2: Fraction of solid as a function of temperature from Scheil simulation

n Pandat Software by CompuTherm, LLC						- 🗆 ×
<u>File Edit View Databases Batch Calc</u>	PanPha	seDiagram <u>P</u> anPi	recipitation Pan	Optimizer <u>P</u> anD	iffusion PanSolidification Property Table G	raph <u>H</u> elp
🛯 🖬 📂 🖬 🎒 🎮 🔺 🖕 🖄	× 🗈 🛙	- I I I I I I I I I I I I I I I I I I I	- 🎮 🛦 🗛 👔		T 🛛 🖄 🗑 🗠 🕨 🖕 🖓 🖓 🖓	L 🗉 T. 🧷
Workspace I X	🔯 Defa	ault.graph 🕺	Default.graph	🕺 Defaul	it.graph 🕺 Default.graph 🔲 Defau	ilt.table X 📼
Lever rule		т	fl	fs	phase name	0 ^
Graph						-
		c ~	mole/mole	mole/mole		J/mole
⊟-le Table	1	457.0180	1.000000	0.000000	Liquid+T_AIMgZn	0.000000
solidification default	2	457.0077	0.999765	0.000235	Liquid+T_AIMgZn	-2.378610
Graph	3	456.9877	0.999295	0.000705	Liquid+T_AIMgZn	-7.133830
Default	4	456.9477	0.998356	0.001644	Liquid+T_AIMgZn	-16.636270
a Table	5	456.8677	0.996481	0.003519	Liquid+T_AlMgZn	-35.609190
Default	6	456.7077	0.992744	0.007256	Liquid+T_AIMgZn	-73.427550
Granh	7	456.3877	0.985318	0.014682	Liquid+T_AIMgZn	-148.5569
Default	8	455.7477	0.970666	0.029334	Liquid+T_AIMgZn	-296.8059
🔄 🔚 Table 🗸 🗸	9	454.4677	0.942138	0.057862	Liquid+T_AIMgZn	-585.4226
< >	10	451.9077	0.888102	0.111898	Liquid+T_AIMgZn	-1,132.3518
Workspace Databases	11	449.3477	0.838732	0.161268	Liquid+T_AIMgZn	-1,634.9201
Property 4 ×	12	448.0677	0.815918	0.184082	Liquid+T_AIMgZn	-1,869.0440
21 41 m	13	447.7477	0.810415	0.189585	Liquid+T_AIMgZn	-1,925.7681
× Appendiate	14	447.5877	0.807690	0.192310	Liquid+T_AIMgZn	-1,953.8942
BackgroundColo AppWorkspace	15	447.5477	0.807012	0.192988	Liquid+T_AIMgZn	-1,960.8989
GridColor ControlDark	16	447.5277	0.806673	0.193327	Liquid+T_AIMgZn	-1,964.3976
BorderStyle FixedSingle	17	447.5177	0.806504	0.193496	Liquid+T_AIMgZn	-1,966.1461
DefaultCellStyle DataGridViewCellStyle (18	447.5085	0.806349	0.193651	Liquid+T_AIMgZn+AIMg_Gamma	-1,967.7469
✓ Layout	19	447.5077	0.806156	0.193844	Liquid+T_AIMgZn+AIMg_Gamma	-1,969.2127
AutoSizeColumn None	20	447.4877	0.801606	0.198394	Liquid+T_AIMgZn+AIMg_Gamma	-2,003.8815
	21	447.4477	0.792655	0.207345	Liquid+T_AIMgZn+AIMg_Gamma	-2.072.0911
	22	447.3677	0.775333	0.224667	Liquid+T_AIMgZn+AIMg_Gamma	-2,204.1675
	23	447.2077	0.742838	0.257162	Liquid+T_AIMgZn+AIMg_Gamma	-2,452.2105
	24	446.8877	0.685288	0.314712	Liquid+T_AIMgZn+AIMg_Gamma	-2,892.4821
	25	446.2477	0.593059	0.406941	Liquid+T_AIMgZn+AIMg_Gamma	-3.601.5332 ¥
	<					>

Figure 1.8.3: Detailed solidification information listed in the Default table



Figure 1.8.4: Fraction of each solid phase as a function of temperature



Figure 1.8.5: Heat evolution as a function of temperature



Figure 1.8.6: Fraction of solid as a function of temperature by Lever rule simulation



Figure 1.8.7: Merge the Scheil and Lever simulation results together

Example 1.9 Calculation of Gibbs Energy Curves

Purpose: Learn to calculate the Gibbs energy of a system or individual phase

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.9.pbfx

Figure 1.9.1 is the Al-Mg binary phase diagram. In this example, we learn to calculate the Gibbs energy of the system and the Gibbs energy of each phase as a function of composition, x (Mg), at 300°C (the red dash line).



Figure 1.9.1: Al-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "Property" on the menu bar and select "Thermodynamic Property";
- Set Calculation Condition as shown in Figure 1.9.2. The property selected is G, and the reference states are set as Fcc for Al and Hcp for Mg, the Gibbs energy of the system (stable phases in each composition range) will be calculated as shown by Figure 1.9.4;
- If the "Individual Phases" is checked, and G (@*) is selected instead of G, the Gibbs energy curve of every phase as a function of composition will be calculated as shown by Figure 1.9.5;

Start Point			End Point			
	Value				Value	
T(C)	300		▶ T(C)		300	Cancer
x(Al)	1	1	x(Al)		0	Options
×(Ma)	0		×(Ma)		1	Extra Outputs
X(Mg)			X(Mg)		·	Load Condition
Total:	1		Total:		1	Save Condition
						Select Phases
						Select Comps
						Sciect compa
Number of ste	ps: 100 ≑	Indivi	dual Phases		Point Calculation	
Choose Targe	t Properties for Plot:	Refere	nce State ('De	fau	ult' as defined in tdb):	_
G H	S(@")		Component	_	Ref. Phase	
S S	mu(*@*)	•	Al	•	Fcc	
Ср	🔲 a(*@*)		Mg	•	Нср 🔻	·
				-		
mu(*)		-				
= mu(*) = a(*) = G(@*)		-	ll		·	

Figure 1.9.2: Calculation of the Gibbs energy for individual phases or the system from

"Property" calculation

Lin	e Calculation	-				×
	Start Point			End Point		
		Value			Value	
	T(C)	300		• T(C)	300	Cancer
	x(Al)	1		x(Al)	0	Options Extra Outputs
	x(Mg)	0		x(Mg)	1	Load Condition
	Total:	1	$\mathbf{\Sigma}$	Total:	1	Save Condition
						Select Phases Select Comps
	Number of step	s: 100		Individual Pl	hases	

Figure 1.9.3: Calculation of the Gibbs energy for individual phases by Line calculation

Calculation Method 2, from Line calculation function in PanPhaseDiagram module:

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "PanPhaseDiagram" on the menu bar and select "Line Calculation";
- Set Calculation Condition as shown in Figure 1.9.3, check the "Individual Phases";

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;

- Figure 1.9.4 shows the Gibbs energy of the system as a function of x (Mg), i.e., the Gibbs energy at each composition represents the Gibbs energy of the stable phase(s) at that composition;
- Figure 1.9.5 shows the Gibbs energy curve of every individual phase as a function of x(Mg)
- Detail Gibbs energy values can be found in the "thermodynamic property" table



Figure 1.9.4: Calculated Gibbs energy of the system



Figure 1.9.5: Calculated Gibbs energy of each individual phase by Line calculation

Example 1.10 Calculation of Activity at Constant Temperature

Purpose: Learn to calculate activities of components in a system

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example #1.10.pbfx

Figure 1.10.1 is the Al-Mg binary phase diagram. In this example, we learn to calculate the activity of Al and Mg as a function of composition, x (Mg), at 300°C (the red dash line).



Figure 1.10.1: AI-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "Property" on the menu bar and select "Thermodynamic Property";

 Set Calculation Condition as shown in Figure 1.10.2. The property selected is a (*), and the reference states are set as Fcc for Al and Hcp for Mg; (*) means the activity of every component (both Al and Mg in this case);

Thermodynamic Pr	roperty Calculation						×
Start Point			End Point				
	Value]			Value		
► T(C)	300		► T(C)		300		Cancel
x(Al)	1	1	x(Al)		0		Options Extra Outputs
x(Mg)	0		x(Mg)		1		
Total:	1		Total:		1		Save Condition
Number of ste	os: 100 🔃		Jual Phases		Point Calculation	n	Select Phases Select Comps
Choose Target	Properties for Plot:	Referer	nce State ('De	efau	ult' as defined in tdb):		
G	S(@*)		Component		Ref. Phase		
S	mu(*@*)	•	A	-	Fcc	•	
Cp	📄 a(*@*)		Mg	-	Нср	•	
 ✓ a(") □ G(@") □ H(@") 		*	<u></u>	•		•	
				_		-	



Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "PanPhaseDiagram" on the menu bar and select "Line Calculation";
- Add the new table following the procedure in Pandat User's Guide 2.4.1;;

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;

Information obtained from this calculation:

• Figure 1.10.3 shows the activities of Al and Mg as a function of x (Mg) using Fcc Al and Hcp Mg as reference states;

- Activity of Al is 1 at x (Al) =1 (x (Mg) =0) since it is pure Fcc Al at this temperature and Fcc is used as the reference state; Activity of Al decreases with the increase x (Mg) and becomes zero at x (Mg) =1;
- Activity of Mg is 0 at x (Al) =1 (x (Mg) =0) and increases with the increase x (Mg) and becomes 1 at x (Mg) =1;
- Activity of either component is constant in a two-phase field.



Figure 1.10.3: Activities of AI and Mg in AI-Mg binary at 300°C

Example 1.11 Calculation of Activity at Constant Composition

Purpose: Learn to calculate activities of components as a function of temperature

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.11.pbfx

Figure 1.11.1 is the Al-Mg binary phase diagram. In this example, we learn to calculate the activity of Al and Mg as a function of temperature at a fixed composition (the red dash line).





Calculation Method 1, From menu bar "Property":

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "Property" on the menu bar and select "Thermodynamic Property";
- Set Calculation Condition as shown in Figure 1.11.2. The property selected is a (*), and the reference states are set as Liquid for both Al and Mg;

ermo	odynamic Pr	operty Calculation				X
Star	rt Point			End Point		OK
		Value]		Value	
►	T(C)	800		► T(C)	0	Cancel
	x(AI)	0.7		x(Al)	0.7	Options
-	x(Ma)	03		x(Ma)	0.3	Extra Outputs
	X(Mg)			X(Mg)		Load Condition
	Total:	1		Total:	1	Save Condition
						Select Phases
						Select Comps
Nur	mber of step	s: 80 🚖	🔲 Individ	dual Phases	Point Calcula	tion
Che	one Target	Proportion for Plat	Poforo	noo State ('De	foult' on defined in th	(b)·
	G G	S(@*)	Neiere	Component	Ref Phase	
	H	Cp(@*)	•	A		-
H	S Cp	mu("@") a("@")		Ma	✓ Liquid	-
	mu(*)		*		▼	-
	3(") G(@*)					
	H(@*)					



Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "PanPhaseDiagram" on the menu bar and select "Line Calculation";
- Add the new table following the procedure in Pandat User's Guide 2.4.1;;

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;

- Figure 1.11.3 shows the activities of Al and Mg as a function of temperature using Liquid Al and Liquid Mg as reference states;
- In the Liquid phase field at high temperature, activities of both Al and Mg decrease as temperature decreases;

- In the Fcc+Liquid two-phase field, the activity of Al decreases as temperature decreases, but the activity of Mg increases as temperature decreases. This is because in this two-phase field the activity of each component follows its activity along the liquidus line. The composition of Mg increases along the liquidus line with decreasing temperature, which makes its activity increase;
- In the AlMg_Beta+Fcc two-phase field, activities of both Al and Mg decrease with the decrease of temperature refer to the Liquid Al and Mg reference states;



Figure 1.11.3: Activities of AI and Mg at 70% at% AI and 30 at% Mg as a function of temperature

Example 1.12 Calculation of Molar Volume and Density at Fixed Temperature

Purpose: Learn to calculate physical properties in a system

Module: PanPhaseDiagram

Thermodynamic and molar volume Database: AlMg MV.tdb

Batch file: Example_#1.12.pbfx

Figure 1.12.1 is the Al-Mg binary phase diagram. In this example, we learn to calculate the molar volume and density of the system as a function of x (Mg) at 300°C (the red dash line).



Figure 1.12.1: AI-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load AlMg_MV.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "Property" on the menu bar and select "Physical Property";
- Set Calculation Condition as shown in Figure 1.12.2. The property selected is Vm (molar volume) and density;

Ph	ysical Property	Calculation				×
	Start Point			End Point		
		Value			Value	Capoel
	T(C)	300		T(C)	300	Cancer
	▶ x(Al)	1		▶ x(Al)	0	Options Extra Outputs
	x(Mg)	0		x(Mg)	1	
	Total:	1		Total:	1	Save Condition
						Select Phases Select Comps
	Number of ste	ps: 100 🛓	Individe	dual Phases	Point Calculation	
	Choose Targe	t Physical Properties fo	or Plot:			
	 Vm alpha_Vm density Vm(@*) density(@*) 					

Figure 1.12.2: Setup calculation of molar volume and density from pure AI to pure Mg at 300 °C

Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load AlMg_MV.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "PanPhaseDiagram" on the menu bar and select "Line Calculation";
- Add the new table following the procedure in Pandat User's Guide 2.4.1, and select Table Type as "Physical_Property"

- Figure 1.12.3 shows the calculated molar volume which increases with the increase of Mg content;
- Figure 1.12.4 is the calculated density which shows the opposite trend as that of the molar volume;
- Details information can be found in the physical_property Table as shown in Figure 1.12.5;



Figure 1.12.3: Calculated molar volume of the system from pure AI to pure Mg in AI-Mg binary at 300 °C



Figure 1.12.4: Calculated density from pure AI to pure Mg in AI-Mg binary at 300 °C

Elle Edit View Databases Batch Calc	PanPhase	Diagram PanF	recipitation PanOptimizer PanD	iffusion PanSolid	ification Propert	y Iable Grap	h Help			
		I 🖲 📑 🖻 E	- 🖂 🗛 🖓 🖉 🖾 🖂 -	1 🗷 H 📴 🖢	s 🗠 🕞 🐻 🕯		T. 2			
Workspace 🛛 🖗 🗙	/ 10 Vm	.oraph 10 der	isity.graph* 10 Default.graph	generated table	10 graph g.graph	2 physical pr	operty.table			
Pandat Workspace 'default' ***		T	phase name	x(A)	x(Mg)	w(Al)	w(Ma)	Vm	density	
		0		malafanala	m mala/mala	a hata	- halta	a and a main		
Graph		le.	•	Indepitione	• [mole/mole	- Juging	- N9/N9	• Cur ajmor	• gen o •	
N Vm	49	300.0000	AMg_Beta+AMg_Eps	0.611354	0.388646	0.635872	0.364128	11.596600	2.238920	
density	50	300.0000	AMg_Beta+AMg_tps	0.610677	0.389323	0.635213	0.364787	11.589900	2.238150	
E-TE TADIE	51	300.0000	AMg_Beta+AMg_Eps	0.610000	0.390000	0.634553	0.365447	11.593200	2.23/3/0	
ine default 1	52	300.0000	AlMg_Beta+AlMg_Eps	0.600000	0.400000	0.624795	0.375205	11.641800	2.225890	
Graph	53	300.0000	AMg_Beta+AMg_Eps	0.590000	0.410000	0.615018	0.364982	11.690400	2.214410	
- B Default	54	300.0000	AlMg_Beta+AlMg_Eps	0.580000	0.420000	0.605219	0.394781	11.738900	2.202930	
graph_g	55	300.0000	AMg_Beta+AMg_Eps	0.570000	0.430000	0.595401	0.404599	11.787500	2.191450	
Default	56	300.0000	AlMg_Beta+AlMg_Eps	0.566038	0.433962	0.591505	0.408495	11.806800	2.186910	
generated	57	300.0000	AlMg_Gamma+AlMg_Eps	0.566038	0.433962	0.591506	0.408495	11.806800	2.186910	
	58	300.0000	AMg_Eps	0.566038	0.433962	0.591505	0.408495	11.806800	2.186910	
	59	300.0000	AlMg_Gamma+AlMg_Eps	0.566038	0.433962	0.591505	0.408495	11.806800	2.186910	
	60	300.0000	AlMg_Gamma+AlMg_Eps	0.565283	0.434717	0.590763	0.409237	11.809800	2.186190	
	61	300.0000	AlMg_Gamma+AlMg_Eps	0.564528	0.435472	0.590020	0.409980	11.812900	2.185480	
	62	300.0000	AlMg_Gamma+AlMg_Eps	0.563019	0.436981	0.588535	0.411465	11.818900	2.184060	
	63	300.0000	AlMg_Gamma+AlMg_Eps	0.560000	0.440000	0.585562	0.414438	11.831100	2.181210	
	64	300.0000	AlMg_Gamma+AlMg_Eps	0.550000	0.450000	0.575703	0.424297	11.871400	2.171770	
Madagas	65	300.0000	AlMg_Gamma+AlMg_Eps	0.540000	0.460000	0.565823	0.434177	11.911800	2.162330	
managere monopace	66	300.0000	AlMg_Gamma+AlMg_Eps	0.530000	0.470000	0.555923	0.444077	11.952100	2.152890	
terty \$X	67	300.0000	AlMg_Gamma+AlMg_Eps	0.520000	0.480000	0.546002	0.453998	11.992400	2.143450	
24 🔤 🔽	68	300.0000	AlMg_Gamma+AlMg_Eps	0.510000	0.490000	0.536061	0.463939	12.032700	2.134010	
Appearance	69	300.0000	AlMg_Gamma+AlMg_Eps	0.500000	0.500000	0.526098	0.473902	12.073000	2.124570	
GridColor ControlDark	70	300.0000	AlMg_Gamma+AlMg_Eps	0.490000	0.510000	0.516115	0.483885	12.113400	2.115130	
BorderStyle FixedSingle	71	300.0000	AlMg_Gamma+AlMg_Eps	0.480000	0.520000	0.506111	0.493889	12.153700	2.105690	
CellBorderStyle Single	72	300.0000	AlMg_Gamma+AlMg_Eps	0.474221	0.525779	0.500320	0.499680	12.177000	2.100230	
DefaultCellStyle DataGridViewCellStyle	73	300.0000	AlMg_Gamma	0.474221	0.525779	0.500320	0.499680	12.177000	2.100230	
Layout	74	300.0000	AlMg_Gamma	0.470000	0.530000	0.496086	0.503914	12.177000	2.099310	
A00326000000 14006	75	300.0000	AlMg_Gamma	0.460000	0.540000	0.486040	0.513960	12.177000	2.097110	
	76	300.0000	AlMg_Gamma	0.450000	0.550000	0.475973	0.524027	12.177000	2.094910	
	77	300.0000	AlMg_Gamma	0.440000	0.560000	0.465885	0.534115	12.177000	2.092710	
	78	300.0000	AMg_Gamma	0.430000	0.570000	0.455775	0.544225	12.177000	2.090510	
	79	300.0000	AlMg_Gamma	0.420000	0.580000	0.445644	0.554356	12.177000	2.088310	
	80	300.0000	AlMg_Gamma	0.410000	0.590000	0.435492	0.564508	12,177000	2.086110	
	81	300.0000	AlMg_Gamma	0.409686	0.590314	0.435173	0.564827	12.177000	2.086050	
	82	300.0000	AlMg_Gamma+Hcp	0.409686	0.590314	0.435173	0.564827	12.177000	2.086050	
	83	300.0000	AlMg_Gamma+Hcp	0.409375	0.590625	0.434857	0.565143	12.178400	2.085770	
	84	300.0000	AlMg_Gamma+Hcp	0.408750	0.591250	0.434222	0.565778	12.181200	2.085220	
	85	300.0000	AlMg_Gamma+Hcp	0.407500	0.592500	0.432951	0.567049	12.186900	2.084110	
	86	300.0000	AlMg_Gamma+Hcp	0.405000	0.595000	0.430408	0.569592	12.198400	2.081900	
	87	300.0000	AlMg_Gamma+Hcp	0.400000	0.600000	0.425319	0.574681	12.221200	2.077480	

Figure 1.12.5: The physical_property table showing the stable phases varying with the composition and the calculated molar volume and density

Example 1.13 Calculation of Molar Volume and Density at Fixed Composition

Purpose: Learn to calculate physical properties in a system

Module: PanPhaseDiagram

Thermodynamic and molar volume Database AlMg MV.tdb

Batch file: Example_#1.13.pbfx

Figure 1.13.1 is the Al-Mg binary phase diagram. In this example, we learn to calculate the molar volume and density of the system as a function of temperature at a fixed composition (the red dash line).



Figure 1.13.1: AI-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load AlMg_MV.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "Property" on the menu bar and select "Physical Property";

• Set Calculation Condition as shown in Figure 1.13.2. The property selected is Vm (molar volume) and density;

Physica	al Property C	alculation	-	-	- 1740	×
Sta	art Point		4	End Point		OK
		Value			Value	Capoel
	T(C)	0		T(C)	800	Cancer
►	x(Al)	0.7		▶ x(Al)	0.7	Options Extra Outputs
	x(Mg)	0.3		x(Mg)	0.3	
	Total:	1		Total:	1	Save Condition
						Select Phases Select Comps
Nu	mber of step	es: 80 🚖	Individ Plot:	dual Phases	Point Calculation	
	Vm alpha_Vm density Vm(@*) density(@*)					

Figure 1.13.2: Setup calculation of molar volume and density from 0 to 800 °C at a fixed composition

Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load AlMg_MV.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- Click "PanPhaseDiagram" on the menu bar and select "Line Calculation";
- Add the new table following the procedure in Pandat User's Guide 2.4.1, and select Table Type as "Physical_Property"

- Figure 1.13.3 Calculated molar volume of the system in Al-Mg binary from 0 to 800°C at a fixed composition
- Figure 1.13.4 is the calculated density which shows the opposite trend as that of the molar volume;
- Details information can be found in the physical_property Table.



Figure 1.13.3: Calculated molar volume of the system in Al-Mg binary from 0 to 800°C at a fixed composition



Figure 1.13.4: Calculated density of the system in Al-Mg binary from 0 to 800°C at a fixed composition

Example 1.14 Density Contour Diagram

Purpose: Learn to calculate density contour diagram. In this example, the density contour lines will be plotted in the AI-Mg binary phase diagram so that density at different temperatures and compositions can be viewed together with phase stability.

Module: PanPhaseDiagram

Thermodynamic and molar volume Database AlMg MV.tdb

Batch file: Example_#1.14.pbfx

Calculation Procedures:

- Load AlMg_MV.tdb following the procedure in Pandat User's Guide 3.2.1, and select Al and Mg two components;
- First set up the calculation condition as shown in Figure 1.14.1 in the same way as we did to calculate AI-Mg binary phase diagram (see <u>Example 1.1 : AI-Mg Binary Phase</u> <u>Diagram</u>), then click "Contour Lines" to open the contour line dialog as shown in Figure 1.14.2;



Figure 1.14.1: Setup calculation for the AI-Mg binary phase diagram, then press "Contour

 Choose "Density" and click Add. the contour type of density will be added as shown in Figure 1.14.2, then press OK;

Set Contour Lines			×
Pre-Defined Contour Types:	Properties:		
Vm(@*) density(@*) Vm density User Custom Type Tc T0 G S V	Contour Type Start Stop Step Constraints	density 0.1 Contour Constraints	OK Cancel
Add Hemove Contour Curves: Name Contour density			
	Contour Type Contour Type.		

Figure 1.14.2: Add "density" contour lines in the "set contour lines" window

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

- Figure 1.14.3 shows the density contour diagram, i.e., plotting density contour lines on top of the Al-Mg binary phase diagram. The density on the same red line is constant;
- Density contour diagram is very useful in alloy design. Given the requirements on stable phases and alloy density, the alloy compositions can be identified from this one diagram;



Figure 1.14.3: Density contour diagram for the Al-Mg binary system

Example 1.15 Activity Contour Diagram

Purpose: Learn to calculate activity contour diagram. In this example, the activity contour lines of Mg will be calculated and plotted on the isothermal section of the Al-Mg-Zn ternary system at 500 °C.

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.15.pbfx

Calculation Procedures:

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- First set up the calculation condition as shown in Figure 1.15.1 in the same way as we did to calculate Al-Mg-Zn isotherm (see <u>Example 1.5</u>: <u>Isotherm of Al-Mg-Zn at 500°C</u>), then click "Contour Lines" to open the contour line dialog as shown in Figure 1.15.2;

	n (2D) Calcu	Ilation					
Y-A	xis Point						
		Value	1	Y			ОК
►	T(C)	500					Cancel
	x(Al)	1					Options
-	x(Mg)	0		Ori	igin	x	Extra Outputs
-	x(Zn)	0					Load Condition
	Total	1					Save Condition
	roun.	·					Select Phases
							Select Comps
					F	seudo	Contour Lines
			5	Scanl	ine Densit	<u>y</u> : 0 ≑	Mobile Comps.
Ori	gin Point		5	Scanl X-A	line Densiț xis Point	y: 0 🜩	Mobile Comps.
Ori	gin Point	Value	5	X-A	ine Densit xis Point	v: 0 🔹	Mobile Comps.
Ori	gin Point T(C)	Value 500		X-A	ine Densiț xis Point T(C)	7: 0 🔹 Value 500	Mobile Comps.
Ori	gin Point T(C) x(Al)	Value 500 0	S	X-A	tine Densit xis Point T(C) x(Al)	v 0 ♀ Value 500 0	Mobile Comps.
Ori	gin Point T(C) x(Al) x(Mg)	Value 500 0 1	S	X-A	xis Point T(C) x(Al) x(Mg)	y: 0 ♀ Value 500 0 0	Mobile Comps.
Ori	gin Point T(C) x(Al) x(Mg) x(Zn)	Value 500 0 1 0		X-A	T(C) x(Al) x(Mg) x(Zn)	y: 0	Mobile Comps.
Ori	gin Point T(C) x(Al) x(Mg) x(Zn) Total:	Value 500 0 1 0 1	S	X-A	T(C) x(Al) x(Mg) x(Zn) Total:	 value 500 0 0 1 	Mobile Comps.
Ori	gin Point T(C) x(Al) x(Mg) x(Zn) Total:	Value 500 0 1 0 1	s () () () () () () () () () () () () ()	X-A	xis Point T(C) x(Al) x(Mg) x(Zn) Total:	 r. 0	Mobile Comps.
Ori	gin Point T(C) x(Al) x(Mg) x(Zn) Total:	Value 500 0 1 0 1		X-A	xis Point T(C) x(Al) x(Mg) x(Zn) Total:	r 0 € Value 500 0 0 1 1	Mobile Comps.
Ori	gin Point T(C) x(Al) x(Mg) x(Zn) Total:	Value 500 0 1 0 1		X-A	T(C) x(AI) x(AI) x(Mg) x(Zn) Total:	 	Mobile Comps.

Figure 1.15.1: Setup calculation for an isotherm in the Al-Mg-Zn ternary at 500°C, then press "Contour Lines"

• Choose "User Custom Type" and click AddType in "a (Mg:Hcp)" for the Contour Type in the "Properties" window as shown in Figure 1.15.2, then press OK;

Defined Contour Types: F sr Custom Type	Contour Type Start Stop Step Constraints	a(Mg:Hcp) 0.1 Contour Constraints	OK Cancel
r Custom Type ') N(@*) Add Remove tour Curves:	Contour Type Start Stop Step Constraints	a(Mg:Hcp) 0.1 Contour Constraints	Cancel
) N@) Add Remove	Start Stop Step Constraints	0.1 Contour Constraints	Cancel
) N(@) Add Remove	Stop Step Constraints	0.1 Contour Constraints	
) N(@) Add Remove	Step Constraints	0.1 Contour Constraints	
) N@) Add Remove	Constraints	Contour Constraints	
Add Remove			
ame			
ame			
ame			
teur (Mailler)			
liour_a(Mg.Hcp)			
	Contour Type]
	Contour Type.		

Figure 1.15.2: Type in "a(Mg:Hcp)" for the Contour Type in the "Properties" window, it is to calculate the activity of Mg contour lines using Hcp Mg as reference state

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

- Figure 1.15.3 shows the activity contour diagram of Mg at 500 °C. The variation of Mg activity in the composition triangle is clearly seen at this temperature;
- Activity contour lines can also be plotted only in the selected phase field, such as in the Liquid phase field, in the Liquid+Fcc phase field. An example is given in Pandat User's Guide 3.3.5.1;



Figure 1.15.3: Activity contour diagram of Mg in the Al-Mg-Zn ternary at 500 °C

Example 1.16 Pressure Contour Diagram

Purpose: Learn to calculate pressure contour diagram. In this example, the pressure contour lines of total pressure and partial pressure of N2 in the Ti-N system will be calculated and plotted on the Ti-N binary phase diagram.

Module: PanPhaseDiagram

Thermodynamic Database: TiN_Gas_Pressure.tdb

Batch file: Example_#1.16.pbfx

Calculation Procedures:

- Load TiN_Gas_Pressure.tdb following the procedure in Pandat User's Guide 3.2.1, and select both Ti, Ni components;
- First set up the calculation condition as shown in Figure 1.16.1 for calculating Ti-N binary phase diagram, then click "Contour Lines" to open the contour line dialog as shown in Figure 1.16.2;



Figure 1.16.1: Setup calculation for Ti-N binary phase diagram, then click "Contour

Lines"

• Choose "User Custom Type" and click AddType in "log(P(@gas))" for the Contour Type in the "Properties" window as shown in Figure 1.16.2, then press OK;

Set Contour Lines			×
Pre-Defined Contour Types:	Properties:		
User Custom Type Tc T0 G S f(@*) HSN(@*) Add	Contour Type Start Stop Step Constraints	log(P(@gas)) -30 10 2 Contour Constraints	OK Cancel
Contour Curves: Name Contour_log(P(@gas))	Contour Type Contour Type.		

Figure 1.16.2: Type in " $\log(P(@gas))$ " for the Contour Type in the "Properties" window, it is to calculate the total pressure contour lines from $\log P = -30$ to 10 with step 2

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

- Figure 1.16.3 shows the contour diagram of total pressure in Ti-N system;
- If we type in "log(P(N2@gas))" as the Contour Type in the "Properties" window in Figure 1.16.2, we will obtained the contour diagram for partial pressure logP(N2) as shown in Figure 1.16.4;



Figure 1.16.3: Calculated contour diagram of total pressure in the Ti-N system



Figure 1.16.4: Calculated contour diagram of partial pressure of N₂ in the Ti-N system

Example 1.17 3D Diagram

Purpose: Learn to calculate a 3D diagram. In this example, 3D diagram is calculated for a hypothetical ternary system

Module: PanPhaseDiagram

Thermodynamic Database: ABC.tdb

Batch file: Example_#1.17.pbfx

Calculation Procedures:

- Load ABC.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform phase projection following the procedure in Pandat User's Guide 3.3.6;
- Set calculation condition as shown in Figure 1.17.1. From this setting, * is selected as Target Phase which means all the phases in the system are selected in the calculation.

50	Cancel Options
50	Options
	Extra Outputs
_	Load Condition
	Save Condition
•	
	Select Phases
_	Select Comps
•	
	•

Figure 1.17.1: Setup calculation for a 3D diagram

Post Calculation Operation:

• In the Property window, under "4: Invariant Tieline Property", choose "True" for the "Show Invariant Tieline", the invariant reaction lines in the three binaries as well as in the ternary will be shown (Figure 1.17.2);

- Rotate the 3D diagram to a position you like;
- Add a new Table as shown in Figure 1.17.3 to get the phase boundary data just for the BCC phase. Select x (C) as x-axis by selecting this column first, then press Ctrl and select x (A) as y-axis, then press Ctrl and select T as z-axis, plot 3D diagram as shown in Figure 1.17.4;
- Add a new Table as shown in Figure 1.17.5 to get the isothermal lines just for the BCC phase, notice that the Table Type must be "isotherm";
- Double click to open the 3D diagram for BCC (Figure 1.17.4), single click the table name for the isothermal lines. From the Property window, drag in x (C) first, then press Ctrl and drag in x (A), then press Shift and drag in T, the isothermal lines for the BCC phase will be plotted on it as shown in Figure 1.17.6;



Figure 1.17.2: Calculated liquidus projection of the Al-Mg-Zn system

		_		
Т	_^î		Columns	Cancel
P			T	Class All
P(*)			x(*)	Original Strs
P(@gas)		1	r(@BUC)=1	- ongridi oto
log10(P)		1		
phase_name	=			
#phases				
×(")				
w(")				
G				
н				
S				
Ср				
mu(*)				
f(@*)				
fw(@*)		Dou	ble click to enter edit mode;	J
x(*@*)		In ea Mati	dit mode, press 'Ctrl'+'m' to show list of h functions	

Figure 1.17.3: Add a new Table to get the phase boundary data just for the BCC phase



Figure 1.17.4: Plot 3D diagram for BCC phase only



Figure 1.17.5: Add a new Table to get the isothermal lines just for the BCC phase



Figure 1.17.6: 3D diagram for the BCC phase with isothermal lines

Example 1.18 Temperature-Pressure Diagram

Purpose: Learn to calculate a Temperature-Pressure diagram. In this example, a Temperature-Pressure diagram is calculated for pure Fe component.

Module: PanPhaseDiagram

Thermodynamic Database: Fe Pressure.tdb

Batch file: Example_#1.18.pbfx

Calculation Procedures:

- Load Fe Pressure.tdb following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.18.1;



Figure 1.18.1: Setup calculation of T-P diagram for pure Fe, x-axis is P and y-axis is T

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the graph following the procedure in Pandat User's Guide 2.3.3;

- Figure 1.18.2 shows the default plot when calculation is finished, it is T-log10(P). It clearly demonstrates the stability of each phase at different temperature and pressure;
- Detailed information on the three-phase reactions, i.e., the temperatures and pressures at triple points can be found in the "invariant" table;
- From Default table, other plots, such as T-P diagram, can be plotted as shown in Figure 1.18.3;



Figure 1.18.2: Temperature-log (Pressure) diagram for pure Fe component



Figure 1.18.3: Temperature-Pressure diagram for pure Fe component

Example 1.19 Phase Fraction Contour Diagram for Ti64

Purpose: Learn to calculate and plot phase fraction contour diagram in a multi-component system. In this example, a contour diagram is calculated and plotted for an isopleth in the Ti-Al-V-N-O five components system.

Module: PanPhaseDiagram

Thermodynamic Database: PanTi.pdb(this database is a thermodynamic database for multicomponent titanium alloys which is only available to users who have licensed it.)

Calculation Procedures:

- Load PanTi.pdb following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.19.1;

		Value		1	Y			ОК
▶	T(C)	1200						Cancel
	w%(Al)	0					Options	
	w%(N)	0.02 Origin X				x	Extra Outputs	
	w%(O)	0.1		••				Load Condition
	w%(Ti)	95.88	_		Save Condition			
	0.00	4		Pseudo 🗌				Select Phases
	w%(V)	4	_					Select Comps
Or	Total:	100		S	Scanl	P ine Density Axis Point	Pseudo □ /: 0 🜩	Contour Lines
Or	Total: igin Point			S	Scanl X-/	P ine Density Axis Point	Pseudo □ /: 0 ♀	Contour Lines
Or	Total: igin Point T(C)	100		s	Scanl X-/	P ine Density Axis Point T(C)	Pseudo	Contour Lines
Or •	Total: igin Point T(C) w%(Al)	100		S	Scanl X-/	P ine Density Axis Point T(C) w%(Al)	Pseudo □	Contour Lines
Or	Total: igin Point T(C) w%(Al) w%(N)	100 Value 600 0 0.02		s	X-/	P ine Density Axis Point T(C) w%(Al) w%(N)	Value 600 10 0.02	Contour Lines
Or	Total: igin Point T(C) w%(Al) w%(N) w%(O)	100 Value 600 0 0.02 0.1		s	X-4	P ine Density Axis Point T(C) w%(Al) w%(N) w%(O)	Value 600 10 0.02 0.1	Contour Lines
Or	Total: rigin Point T(C) w%(Al) w%(N) w%(O) w%(Ti)	100 Value 600 0 0.02 0.1 95.88		s N N	X-/	P ine Density Axis Point T(C) w%(Al) w%(N) w%(O) w%(O) w%(Ti)	Value 600 10 0.02 0.1 85.88	Contour Lines
Or	Total: igin Point T(C) w%(Al) w%(N) w%(O) w%(V)	100 Value 600 0 0.02 0.1 95.88 4		s N	X-J-	P ine Density Axis Point T(C) w%(A)) w%(A) w%(A) w%(O) w%(Ti) w%(V)	Value 600 10 0.02 0.1 85.88 4	Contour Lines

Figure 1.19.1: Setup a calculation for an isopleth along Ti-Al side with fixed V, O, and N compositions

 Click "Contour Lines" in the dialog shown in Figure 1.19.1, then set the Contour Type as shown in Figure Figure 1.19.2;

Set Contour Lines			×
Pre-Defined Contour Types:	Properties:		
M("@") Vm(@") density(@") Vm density User Custom Type Tc Tc T0 G Add Remove	Contour Type Start Stop Step Constraints	f(@Bcc) 0.1 0.9 0.1 Contour Constraints	OK Cancel
Contour_f(@Bcc)			
	Stop Stop value of the co	ntour line.	

Figure 1.19.2: Setup contour lines as the fraction of $Bcc (\beta)$ phase

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the graph following the procedure in Pandat User's Guide 2.3.3;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

- Figure 1.19.3 shows the isopleth Ti-Al-4V-0.1O-0.02N (wt%) with contour lines of fractions of the β phase. It clearly shows how the fraction of the β phase varies with temperature and composition. This plot provides a guidance on the selection of alloy composition and heat treatment condition if certain fraction of β phase is needed in the microstructure;
- For Ti64 (6 wt% of AI as indicated by the black dash line), the fraction of β phase (and α phase) in the α+β two-phase structure can be read from the contour diagram directly given a heat treatment temperature;



Figure 1.19.3: Contour diagram of the β phase fraction on the isopleth of Ti-Al-4V-0.1O-0.02N (wt%)

Example 1.20 Phase Forming Driving Force in High Entropy Alloys

Purpose: Learn to calculate and plot driving force contour lines on a multi-component phase diagram. Figure 1.20.1 shows an isopleth of CoCrFeNi – AI_x CoCrFeNi which indicates that addition of AI promotes the formation of Bcc and B2. However, it does not tell which phase has higher thermodynamic driving force at different temperature and composition. In this example, the driving force contour lines for B2 and Bcc are plotted on the Liquid+Fcc diagram in the AI-Co-Cr-Fe-Ni system to view the driving force of forming B2 and Bcc in this system.

Module: PanPhaseDiagram

Thermodynamic Database: PanHEA.pdb(this database is a thermodynamic database for high entropy alloys which is only available to users who have licensed it.)



Figure 1.20.1: Calculated isopleth of the CoCrFeNi–Al_xCoCrFeNi with x=0~2

Calculation Procedures:

- Load PanHEA.pdb following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.20.2;
- Click "Select Phases" and set status of each phase as shown in Figure 1.20.3;
- Click "Contour Lines" and then set the Contour Type as shown in Figure 1.20.4 to calculate the driving force contour lines for B2 phase, click OK;
- Click "Contour Lines" and then set the Contour Type as shown in Figure 1.20.5 to calculate the driving force contour lines for Bcc phase, click OK;

Y-Ax	kis Point					
		Value	1	Y		ОК
1	T(C)	1600				Cancel
;	x%(Al)	0				Options
,	x%(Co)	25	Origin X			Extra Outputs
	x%(Cr)	25				Load Conditio
	A /0(OI)	25				Save Conditio
;	х%(ге)	25				Select Phase
	x%(Ni)	25				Select Comp
1						
; ► T	Total:	100		Pse	eudo 🗌	Contour Line
د ۲	Total:	100	s	Pse canline Density:	eudo 🗌 0 😫	Contour Line Mobile Comps
د ۲	Total: jin Point	100	s	Pse canline Density: X-Axis Point	eudo 🗌 0 ≑	Contour Line Mobile Comps
) Image: Norige State S	Total: jin Point	100	s	Pse icanline Density: X-Axis Point	eudo 🗌 0 🔹 Value	Contour Line Mobile Comps
) Orig	Total: jin Point	100 Value 500	s	Pse canline Density: X-Axis Point T(C)	Value	Contour Line
orig	Total: jin Point	100 Value 500 0	l s	Pse canline Density: [X-Axis Point T(C) x%(Al)	value 500 33.2	Contour Line Mobile Comps
Orig	Total: jin Point T(C) x%(AI) x%(Co)	100 Value 500 0 25	s	Pse canline Density: [X-Axis Point T(C) x%(Al) x%(Co)	Value 500 33.2 16.7	Contour Line Mobile Comps
Orig	Total: jin Point T(C) x%(AI) x%(Co) x%(Cr)	100 Value 500 0 25 25	s	Pse canline Density: [X-Axis Point T(C) x%(Al) x%(Co) x%(Cr)	value 500 33.2 16.7 16.7	Contour Line Mobile Comps
Orig	Total: jin Point T(C) x%(Al) x%(Co) x%(Cr) x%(Fe)	100 Value 500 0 25 25 25	s	Pse canline Density: [X-Axis Point T(C) x%(Al) x%(Co) x%(Cr) x%(Fe)	value 33.2 16.7 16.7	Contour Line Mobile Comps
Orig	Total: jin Point T(C) x%(AI) x%(Co) x%(Cr) x%(Fe) x%(Ni)	100 Value 500 0 25 25 25 25 25	s N N	Pse canline Density: X-Axis Point T(C) x%(Al) x%(Co) x%(Cr) x%(Fe) x%(Ni)	value 500 33.2 16.7 16.7 16.7	Contour Line Mobile Comps

Figure 1.20.2: Setup calculation for the isopleth CoCrFeNi–Al_xCoCrFeNi

Suspended Phases (42):	Dormant Phases (2):	Entered Phases (2):	
AL8CR5_L AL9CR4_H AL9CR4_L AL9CR4_L AL9CR4_L AL9CR4_L AL9CR4_L ALC7_EPSILON1 BCC_B2 CHLA12 CUB_A13 D0_19_TI3AI EPS GAMMABRASS H_SIGMA Hcp L10_TiAI L12_FCC Laves_C14 Laves_C15 Laves_C36 MnNi Beta	B2 Bcc	Fcc Liquid	OK Cancel Sus/Ent All

Figure 1.20.3: Fcc and Liquid are selected to enter the calculation, B2 and Bcc are dormant in the calculation, but their driving force to become stable phases can be calculated

Set Contour Lines			×
Pre-Defined Contour Types:	Properties:		
M(*@*)	Contour Type	DF(@!B2)	ОК
Vm(@*)	Start		Cancel
density(@*)	Stop		
density	Step	2000	
User Custom Type	Constraints	Contour Constraints	
To			
10			
6			
Add Remove			
Contour Curves:			
Name			
Contour DE(@IR2)			
	Step		
	Step value of the con	tour lines.	

Figure 1.20.4: Setup calculation of driving force contour lines for B2 phase

Mr(*p) Orkor Tpo DF(elBoc) OK Vmr(\$*) Stat Stat Contour Tpo DF(elBoc) OK Vmr(\$*) Mare Stap Stat Contour Constraints Contour Constraints Contour_OF(elB2) Contour_OF(elB2) Contour_OF(elB2) Stap Contour_OF(elB2) Contour_OF(elB2) Stap Stap Stap Stap

Figure 1.20.5: Setup calculation of driving force contour lines for Bcc phase

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the graph following the procedure in Pandat User's Guide 2.3.3;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

Information obtained from this calculation:

- After operation of Figure 1.20.4, a diagram with driving force contour lines of B2 will be plotted, and after operation of Figure 1.20.5, a diagram with driving force contour lines of Bcc will be plotted;
- To merge the two plots together by choose one of the diagram, say the one with Bcc contour lines, to be shown in the main display window, then single click Table->Contour_DF(@!B2) table, drag x% (Al) to the main display window, then press Ctrl and drag T to the main display window;
- The merged diagram is shown in Figure 1.20.6. From this figure it is seen that at low Al composition, neither B2 or Bcc has the driving force to form (negative driving force); with high Al composition, both phases have the driving force to form, and B2 has higher driving force than that of the Bcc phase;



Figure 1.20.6: Driving force contour diagram for both Bcc and B2 phases

Example 1.21 User-defined Property

Purpose: Learn to define any property in a database in a format similar to that of the Gibbs energy and plot the contour lines of the defined property on a multi-component phase diagram.

Module: PanPhaseDiagram

Thermodynamic and property Database: AlNi_U.tdb

```
Batch file: Example_#1.21.pbfx
```

The molar volume of Al-Ni binary system is taken as an example here. Instead of using the specific variable V_m for molar volume, we define a property of *U* to represent the molar volume. In the database file (.tdb), first define the property *U* with the keyword "USER PROPERTY" as

Type Definition a USER PROPERTY U 1 !

Then, define the property U as a function of x, the mole fraction, with the keyword "VARIABLE x":

Type_Definition b GES AMEND_PHASE_DESCRIPTION * VARIABLE_X U !

For any phase with such a property U, include "ab" in the phase definition such as in "Liquid" phase,

```
Phase Liquid %ab 1 1 !
```

The parameters for the property are defined in the format similar to that of the Gibbs energy. An example file "AlNi.tdb" is included in the Pandat example folder. A batch file "Example_#1.21.pbfx" is also included in the same folder, which produces an identical contour diagram as shown in Figure 1.21.1 except that the property name is *U* instead of *V*_m. It should emphasize again that *U* can be any property.

- Load AlNi_U.tdb following the procedure in Pandat User's Guide 3.2.1, and select both components;
- Pop out dialog for Section (2D) Calculation, then click "Contour Lines" to open the contour line dialog as shown in Figure 1.21.2;

- Choose "User Custom Type" and click AddType in "U" for the Contour Type in the "Properties" window as shown in Figure 1.21.2.
- Click OK and perform calculation. The obtain diagram with labeling is shown as Figure 1.21.1.



Figure 1.21.1: AI-Ni binary phase diagram with the calculated contour lines of molar



Figure 1.21.2: Setup contour lines for Property U from interface

Example 1.22 Run Pandat in Console Mode

Purpose: Learn to run Pandat in the console mode for the calculation of Al-Mg binary phase diagram.

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.22.pbfx

Calculation Procedures:

• Run through a windows (.bat) file, double click the Example #1.22.bat;

The content of an example (.bat) file is shown below:



Figure 1.22.1: Example of the (.bat) file for console mode

Note that above figure shows an example windows (.bat) file. There are a few things that user needs to make sure before running this example:

- The full path of "Pandat.exe". The default path for Pandat 2025 is: "C:\Program Files\CompuTherm LLC\Pandat 2025\bin\Pandat.exe
- If the batch file (.pbfx) is not in the same folder of the windows (.bat) file, the full path of the batch file (.pbfx) needs to be given.
- The working folder for the console mode must have been created before running the windows (.bat) file. Then a Pandat workspace will be created in this folder and all simulation results are saved under this workspace. This argument is optional and no

graph files are generated if the working folder is not given. This will save many computer resources. In general, the user may not pass this argument so that only data (.dat) files are generated after each simulation. In "Example_#1.22.pbfx":

- A table name "AlMg_PhaseDiagram.dat" is given with an extension ".dat" and then a data file (.dat) will be created in the same folder as the batch file. User may give a full path for the data file in order to save it into a specified folder.
- The last argument is to control the output level with "1" the default value. The value of "2" is for more outputs and "0" for less.

Example 1.23 High Throughput Calculation (HTC): Pattern Compositions

Purpose: Learn to run high throughput calculation by setting pattern composition range and steps.

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Calculation Procedures:

- Load AlMgZn.tdb following the procedure in Pandat User's Guide3.2.1, and select all three components;
- Choose the HTC function from the menu "Batch Calc → High Throughput Calculation (HTC)" (as shown in Example 1.23).

<u>B</u> at	ch Calc	<u>P</u> anPhaseDiagram	<u>P</u> anPrecipita				
₽	Batch Run						
	Run All Batch in Folder						
	Load Co	ondition					
	Save Co	ondition as a Batch Fil	e				
	Create	a New Batch					
	Edit a B	atch File					
	High Tł	nroughput Calculation	n (HTC)				
	Result A	Analysis					
	Join An	alysis Reports					

Figure 1.23.1: HTC function under the "Batch Calc" menu

• Choose the calculation type from the drop-down list of HTC pop-up window and select "Solidification".

High Throughput Calculation		×
Choose Calculation Type:		ОК
solidification	~	Cancel

Figure 1.23.2: Dialog to choose calculation type of HTC

· Define the compositional space for HTC simulation;

After choosing the calculation type, a window pops out as shown in Figure 1.23.3. In this setting, the compositions of both Mg and Zn vary from 1 to 30 wt.% in a double composition loops. The "Steps" is set to 29, which means the composition increases by 1 wt% at each step. The total number of calculations is 30x30=900 in this setting. The composition of Al is set as balance by typing "-1" for steps or right-click the row of Al. No "Start" or "End" values are required for the balance component, which is Al in this case. After setting the composition pattern, user can also export these HTC alloy composition to a file by clicking the small icon marked with red square in Figure 1.23.3 After setup the compositional space for HTC and choose the proper solidification model, user can click "Run HTC" button to perform HTC simulations, which is 900 calculations in this case.

Liquid Compos	Start	End	# Stans	Run HTC
T(C)	1000	1000	0	Cancel
w%(Al)	-1	-1	-1	Options
w%(Mg)	1	30	29	Extra Outputs
▶ w%(Zn)	1	30	29	
				01.10
				Import Alloy
Solidification Mod	el ium (Scheil)) Equili	brium (Lever)	Import Alloy
Solidification Mod Non-equilibits	el ium (Scheil) art simulatior) Equili	brium (Lever) us surface <table-cell></table-cell>	Import Alloy
Solidification Mod Non-equilibit	el ium (Scheil) art simulatior Enc	Equilities of the second se	brium (Lever) us surface 🔮 nore liquid <table-cell></table-cell>	Import Alloy
Solidification Mod Non-equilib St	el ium (Scheil) art simulatior End	O Equili n from liquid d when no n T_End [0	brium (Lever) us surface nore liquid j: 0	Import Alloy

Figure 1.23.3: Dialog to setup compositional space for HTC

 Save the current workspace after all calculations are finished. It is suggested that user saves the current workspace immediately after the HTC calculation. This allows all the calculated results saved in the workspace for future use. • Choose "Result Analysis" from the "Batch Calc" menu. User can use this commend to analyze the calculated results for a group of alloys and pick a certain property from each calculation for comparison.

Bat	ch Calc	<u>P</u> anPhaseDiagram	<u>P</u> anPrecipita				
₽	Batch Run						
	Run All	Run All Batch in Folder					
	Load C	ondition					
	Save Co	ondition as a Batch File	2				
	Create	a New Batch					
	Edit a Batch File						
	High Throughput Calculation (HTC)						
	Result A	Analysis					
	Join An	alysis Reports					

Figure 1.23.4: "Result Analysis" function under the "Batch Calc" menu

 Open the workspace saved previously for "Result Analysis". User can perform several HTC calculations and save all the workspaces. User can then analyze the results of the selected HTC calculation by opening the corresponding workspace as shown in Figure 1.23.5.

Result Analysis -> Ch	oose Workspace	×
Choose Target Workspace	D:\Demo\ExampleBook_HTC\ExampleBook_HTC.pndx	Continue Cancel
	There are 900 calculations for analysis.	



• Define the criteria of the properties as filters for result analysis

ult Analysis -> Set R	ules	
Target Workspace:	D:\Demo\ExampleBook_HTC\default	Analyze
		Cancel
Common Tables for	All Calculations: (only one table can be chosen for analysis at one time)	
D:\Demo\ExampleBoo	ok_HTC\default\Solidification Simulation\Table\Default.table v	
Common Columns	for the Target Table: (drag and drop to change the oder) Sel/Cir All	
T fs phase_name Q H_Latent H_tot f_tot(@Lquid) f_tot(@T_AIMgZn)	□ f_jtot(@AlWg_Beta) □ f(@Hcp) □ f_jtot(@Mg2Zn11) Ø w(Mg) □ f_jtot(@Mg2Zn11) Ø w(Mg) □ f[deluquid) G □ f(@CT_MlNgZn) x k(M) □ f(@CT_MlNgZn) x k(M) □ f(@CT_MlNgZn) x k(Mg) □ f(@CT_MlngZn) x k(Mg) </td <td></td>	
. Set an Expression fl=1.0	n to Select Rows: (choose a template text and insert) Insert Selected Column Name	
fl=1.0		
2. Get Min/Max Valu T=MIN(T)	ue from Selected Row (choose a template text and insert)	
Examples: 1. finding the rows 2. finding the row w	✓ Empty Row Between Results with values in a certain range: fl < 1.0 AND fl > 0.9; ith minimum T with T=MIN(T).	

Figure 1.23.6: "Result Analysis" popup dialog to define the criteria of the properties

In Figure 1.23.6, the "Target Workspace" shows the workspace selected by the user for results analysis. It should point out that there can be more than one table in each calculation, the "Common Tables for All Calculations" allows user to choose the table for analysis. In the "Common Columns for the Target Table" window, names for all the output properties available in the selected table are listed. User can choose the properties to be listed in the "Analysis Report". As shown in Figure 1.23.6, temperature and the alloy composition will be listed in the "Analysis Report" in this case. Since the purpose of HTC is to compare a special target property for the several hundred/thousands of calculations, the "Set an Expression to Select Rows" at the bottom of the window allows user define the criteria. In Figure Figure 1.23.6, this criterion is $f_1 = 1$, i.e. the fraction of liquid is 1. With this filter, only the row satisfies this criterion will be listed in the "Analysis Report". It should point out that several criteria can be set in the "Set an Expression to Select Rows". Click "Analyze" to create the "Analysis Report" as shown in Figure 1.23.7. In this table, each row lists the liquidus temperature for the corresponding alloy composition. The liquidus temperatures for 900 alloys are listed in the same report which allows a quick comparison of liquidus temperature for different alloy composition. User can also plot 3D colormap and surface diagrams using the data in this report as shown in Figure 1.23.8.

/ 🖉 TL.r	eport				
	CalculationName	AlloyChemistry	Т	w(MG@LIQUID)	w(ZN@LIQUID)
			С ~	% ~	% ~
1	solidification_default	98AL+1MG+1ZN in w%	653.5360	1.000000	1.000000
2					
3	solidification_default_1	97AL+1MG+2ZN in w%	651.6410	1.000000	2.000000
4					
5	solidification_default_2	96AL+1MG+3ZN in w%	649.7380	1.000000	3.000000
6					
7	solidification_default_3	95AL+1MG+4ZN in w%	647.8280	1.000000	4.000000
8					
9	solidification_default_4	94AL+1MG+5ZN in w%	645.9110	1.000000	5.000000
10					
11	solidification_default_5	93AL+1MG+6ZN in w%	643.9860	1.000000	6.000000
12					
13	solidification_default_6	92AL+1MG+7ZN in w%	642.0550	1.000000	7.000000
14					
15	solidification_default_7	91AL+1MG+8ZN in w%	640.1160	1.000000	8.000000
16					
17	solidification_default_8	90AL+1MG+9ZN in w%	638.1690	1.000000	9.000000
18					
19	solidification_default_9	89AL+1MG+10ZN in w%	636.2160	1.000000	10.000000
20					
21	solidification_default_10	97AL+2MG+1ZN in w%	648.4620	2.000000	1.000000
22					
23	solidification_default_11	96AL+2MG+2ZN in w%	646.5690	2.000000	2.000000
24					
25	solidification_default_12	95AL+2MG+3ZN in w%	644.6700	2.000000	3.000000
26					
27	solidification_default_13	94AL+2MG+4ZN in w%	642.7640	2.000000	4.000000
28					
29	solidification_default_14	93AL+2MG+5ZN in w%	640.8510	2.000000	5.000000
30					
31	solidification_default_15	92AL+2MG+6ZN in w%	638.9320	2.000000	6.000000

Figure 1.23.7: Analysis report file of TL



Figure 1.23.8: 3D diagrams of the liquidus temperatures: colormap (left) and 3D surface (right)

Example 1.24 High Throughput Calculation (HTC): Random Compositions

Purpose: Learn to run high throughput calculation by importing alloy Compositions.

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Start the HTC function from the menu "Batch Calc → High Throughput Calculation (HTC)" Then choose "solidification" as calculation type.
- Check the "Import Alloys" box at the solidification simulation popup window, and then click the "Import" button to import the pre-prepared alloy composition file (Example_ #1.24_alloys.txt).
- Click the "Run HTC" button perform HTC simulations
- Save the workspace of the HTC results for further analysis as mentioned in <u>Example 1.23</u>
 <u>: High Throughput Calculation (HTC): Pattern Compositions</u>

	and compos				Bun HTC		iquia compo		1		Bun HTC
		Start	End	# Steps				Start	End	# Steps	Runnic
	T(C)	1000	1000	0	Cancel	►	T(C)	1000	1000	0	Cancel
	w%(Al)	0	0.1	10	Options		w%(Al)	0	0.1	10	Options
	w%(Mg)	0	0.1	10	Extra Outputs		w%(Mg)	0	0.1	10	Extra Output
	w%(Zn)	0	0.1	10	-		w%(Zn)	0	0.1	10	
					Select Phases						Select Phase
Solid	dification Mod	el rium (Scheil)) Equ	ulibrium (Lever)	Select Phases	- Sc	lidification Mod	el rium (Scheil)) Equ	ilibrium (Lever)	Select Phase
Solid O	dification Mod Non-equilib St	el rium (Scheil) art simulatio) Equ	ulibrium (Lever) idus surface	Select Phases	Se	olidification Mod Non-equilib St	lel rium (Scheil) art simulati) Equ	ilibrium (Lever) idus surface	Select Phase

Figure 1.24.1: HTC solidification dialogs before (left) and after (right) import alloy composition

file

Please refer to the Pandat User's Guide 1.1 10.1 for detail information of preparing the alloy composition file.

Example 1.25 Friction-stir welding between AA5454 AI alloy and AZ91 Mg alloy

Purpose: Learn to perform complicated multi-component vertical section calculations and understand the application of zero phase fraction (ZPF) line of the liquid phase. Commercial Mg database is required to perform the calculation of this example.

Module: PanPhaseDiagram

Thermodynamic Database: PanMg.pdb(this database is a thermodynamic database for multicomponent magnesium alloys which is only available to users who have licensed it.)

Due to the formation of brittle intermetallic phases in the fusion zone, joining Mg alloys with Al alloys through fusion welding is not very suitable. Friction stir welding (FSW) provides a potential method for joining Mg alloys and Al alloys. In this example, an AZ91 cast Mg alloy and rolled AA5454 Al alloy are assumed to be jointed through FSW. A vertical section from the composition of AZ91 to AA5454 shows the possible intermetallic phases could be formed in the welding interface. In addition, the zero phase fraction (ZPF) line of the liquid phase indicates the maximum temperature that can be tolerated during the welding process to avoid the melting zone in the interface. In Pandat, The ZPF line the liquid phase can be output through function "f (@Liquid) = 0" in the table.

- Load PanMg.pdb following the procedure in Pandat User's Guide 3.2.1, and select components: AI, Fe, Mg, Mn, Zn;
- Perform 2D calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.25.1;

Post Calculation Operation:

- Add a new Table as shown in Figure 1.25.2 to get the ZPF line data of the liquid phase (f (@Liquid)=0);
- Plot the ZPF line data in the added table into the default graph following the procedure in Pandat User's Guide 2.4.3;
- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;



Figure 1.25.1: Set vertical section calculation conditions: Composition from AA5454: AI-3Mg-1Mn-0.3Fe-0.01Zn(wt.%) at left edge to AZ91: Mg-8.2AI-1Zn-0.2Mn-0.01Fe (wt.%) at right edge;

Temperature range from 300 °C to 500 °C

Table Editor		×
Table Type: Default ~	Table Name: generated	ОК
Т	Columns	Cancel
Р	w(Mg)	
P(*)	Т	Clear All
	f(@Liquid)=0	Original Strs
P(@gas)		
log10(P)		

Figure 1.25.2: Output the ZPF line data of the liquid phase

Information obtained from this calculation:

- The obtained phase diagram is shown in Figure 1.25.3. To prevent partial melting during the friction-stir welding process, the local temperatures in the welding zone must be maintained below the threshold indicated by the red line. In this case, the minimum temperature to avoid such melting is 435.7 °C.
- Different intermetallic phases may form in the joining zone: The Al₃Mg₂ phase with some Al₆Mn precipitate near the Al alloy side, and Mg₁₇Al₁₂ phase with minor precipitation of Al₄Mn near the Mg alloy side.
- A similar approach can also be applied to analyze interactions between other materials, such as coating/substrate reactions.



Figure 1.25.3: The vertical phase diagram from AA5454 to AZ91 with phase field labels (The phase fields including Liquid phase are labeled as red)

Example 1.26 Calculation of Open Circuit Voltage (OCV) under Equilibrium Condition

Purpose: Learn to perform equilibrium calculation, use extra output table and extra output graph to output chemical potential and voltage value to simulate the open circuit voltage curve of an alloy system for battery application.

Module: PanPhaseDiagram

Thermodynamic Database: LiSn.tdb

Batch file: Example_#1.26.pbfx

Background: Carbon based anode material is widely used in Li-ion batteries. But its low charge density motivates the search for next generation of anode materials. Sn based alloy is one of potential anode candidates. The calculation of open circuit voltage curve of the Li-Sn system sheds a light on the potential capacity of the alloy system. This example shows how to calculate the open circuit voltage curves directly from PanPhaseDiagram module and compare with experimental data. In an alloy system, the equilibrium open-circuit voltage E is associated with chemical potential through the Nernst equation: $\mu_{Li} - \mu_{Li}^{o,ref} = -nFE$. *F* is Faraday's constant, 94685 C/volt. In this example of Li-Sn system, n = 1, then $E = -(\mu_{Li} - \mu_{Li}^{o,ref})/F$. At 688 K, Li and Sn are in liquid state, so the reference state is liquid Li.

- Load LiSn.tdb following the procedure in Pandat User's Guide 3.2.1;
- Perform line (1D) calculation following the procedure in Pandat User's Guide 3.3.2;
- Set the calculation conditions as shown in Figure 1.26.1. The temperature is set as 688 K, as experimental data are available at 688 K for comparison. The composition range is from pure Sn, i.e. x (Sn) = 1, to pure Li, i.e. x (Li) = 1. The Number of steps is set to be 100;

Start Point		End Point		
	Value		Value	ОК
T(K)	688	► T(K)	688	Cancel
x(Li)	0	x(Li)	1	Options
x(Sn)	1	x(Sn)	0	Extra Outputs
Tatalı	1	Tatali	1	Load Condition
				Save Condition
				Select Phases
				Select Comps
				Mobile Comps

Figure 1.26.1: Line calculation conditions setting

• Set "Extra Outputs table": In order to output the open-circuit voltage value, some extra outputs are required. Click "Extra Outputs" in the interface shown in Figure 1.26.1, a new interface will appear as shown in Figure 1.26.2. Then click the blue "+" symbol to pop out the Table Editor as shown in Figure 1.26.3. From this Table Editor, one can select to output Extra properties which are not shown in the default table;

Set	Extra O	utputs				×
1	Tables Output	Graphs			× 🕂	OK
ſ		Table Name	Source	Columns	Edit	Carloci
	►	Default	Default	T;P;phase_name;x(*);f(@*);G(@*);G;w(*);n_kg	edit	

Figure 1.26.2: Dialog to set Extra Output

In this example, we output mu (Li:Liquid[Li]) as the chemical potential of Li in the system with reference to the liquid phase, i.e. . Then, we add another quantity -mu (Li:Liquid[Li])/96485 which is equivalent to in this system. The quantity x (Li)/x (Sn) represents the y in Li_ySn system. The settings are shown in Figure 1.26.3. After setting the table editor, click ox;

Tips: The properties can be dragged from the left column to the right column, or directly type in the right column. When click a property in the left column, the description of this property is shown as description in the bottom of the interface. For example, in Figure 1.26.3, a (*:Liquid [*]); Description: Activity of component in system with given reference state. Some simple calculations are also applied in the table setting, such as – mu(Li:Liquid[Li])/96485 and x(Li)/x(Sn) in this example.

Table Editor				×
Table Type: Default	Table	Name:	generated	ОК
G_id(@*)		Colur	nns	Cancel
H_id(@*)		Т		
S_id(@*)		x(LI)		Clear All
G_ex(@*)		x(SN)		Original Strs
H ex(@*)		x(LI)/x(SN)	
S ex(@*)		mu(LI:L	IQUID[LI])	
		-mu(LI:I	LIQUID[LI])/96485	
(tot)		phase_	name	
mu("@")	**			
a(*:Liquid[*])				
r(*:Liquid[*])				
G(:Liquid[*])				
mu(*@*:Liquid[*])				
H(*@*:Liquid[*])				
S(*@*:Liquid[*])				
tieline				
struct(@*)	Doub	le clic	to enter edit mode;	I
dGdy(*@*)	In ed Math	it mode functio	e, press 'Ctrl'+'m' to show list of ons	
Drag and drop available columns to se Description: Activity of component in sys Reference phase name must be given.	tup a nev stem with Example	w table. I n given re e: a(*:liq	Double click property cell to edit. eference state. uid[*])	

Figure 1.26.3: Define extra output table by drag properties from the left column to the right

column or directly type in in the right column

- Set "Extra Outputs graph": Click the icon "Graph" in "Set extra output" interface as shown in Figure 1.26.4, then click the blue "+" symbol to add extra Graph. An interface as shown in Figure 1.26.5 will appear. Select the "generated" table set in previous step in the "Table source". Drag x (Li) /x (Sn) from the left column to X axis in the right column; drag -mu (Li:Liquid[Li])/96485 from the left column to Y axis in the right column. Then click ox;
- When the interface goes back to Figure 1.26.1, click ox. Calculation starts.

Tables Graphs Extra Graphs: OK Graph Name Graph Type # of Plots Edit	Set Extra Outputs				×
Graph Name Graph Type # of Plots Edit	Tables Graphs				OK Cancel
	Graph Name	Graph Type	# of Plots	Edit	

Figure 1.26.4: Dialog to set Extra Graph Output

Graph Options					\times
Table Source: generated	V Graph	Name: graph	Is Triangle?	OK Cancel	
T	Y Avie	Y Avie	Source		
x(*) x(LI)/x(SNI)	x(LI)/x(SN)	-mu(LI:Liquid[LI])/9	generated		
mu(Ll:Liquid[L])) -mu(Ll:Liquid[L])/96485 phase_name					

Figure 1.26.5: Output Graphs options interface

Post Calculation Operation:

• Rescale the axis, and edit the axis title.

After the calculation, the calculated open circuit voltage curve of Li-Sn system is shown in Figure 1.26.6 with the default settings. Set the x-axis range from 0 to 6, and obtained as shown in Figure 1.26.7



Figure 1.26.6: Calculated open circuit voltage curve of Li-Sn system



Figure 1.26.7: Calculated open circuit voltage curve of Li-Sn system: Rescale x-axis of x(Li)/x (Sn) to 0-6

- Import experimental data. From the menu, click Table → Import Table From Files, choose LiSn.txt file to import the experimental data table into the Pandat workspace;
- Compare calculated results with experimental data. From the menu, click Graph → Edit Plots, or click the button is from the toolbar to open the setup Plot interface as shown in Figure 1.26.8. Select the imported LiSn table, choose LixSn as X axis, and E_Li(V) as Y axis. Then click ox;
- Then change "Plot Type" as "Point", "Marker Color" as "Transparent", "Marker Style" as "Circle"; Then experimental data are changed to red open symbol, added legend, change the Title of Y axis as (E vs E_{Li}) / V. The final produced figure is shown in Figure 1.26.9.



Figure 1.26.8: Setup Plot, add the experimental data into generated figure



Figure 1.26.9: The calculated OCV curve of Li-Sn system at 688 K in comparison with experimental data

Example 1.27 Para-equilibrium Phase Diagram

Purpose: Learn to perform phase diagram calculations in para-equilibrium condition with fast diffusion elements.

Module: PanPhaseDiagram

Thermodynamic Database: FeNiC.tdb

Batch file: Example_#1.27.pbfx

Background: In certain systems, some interstitial elements, such as C and N, diffuse much faster than others. Therefore, those elements can be treated as "mobile" components, while the others are treated as immobile components. The common case is the austenite to ferrite reaction in steels by a rapid carbon-diffusion controlled process.

- Load FeNiC.tdb following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.27.1;
- Click "Mobile Comps.", set "C" the mobile component as shown in Figure 1.27.2;
- After properly selected the C as mobile component, then click OK, it returns to the calculation condition window as shown in Figure 1.27.3. The mobile element highlighted with orange color.

(-A	xis Point						
		Value	t	Y			OK
	T(K)	1000					Cancel
▶	x(C)	0.05					Options
	x(Fe)	0.95		Ori	gin	x	Extra Outputs
	x(Ni)	0				_	Load Condition
	Total	1					Save Condition
	Total.						Select Phases
							Select Comps
						Pseudo	Contour Lines
			~		no Dono		1114 0
-			5	canlı	ne Dens	ity: U 🖵	Mobile Comps.
Dri	gin Point		5	Canlı X-Ax	kis Point	ity: U 💌	Mobile Comps.
Dri	gin Point	Value	5	X-A	kis Point	Value	Mobile Comps.
Dri	gin Point T(K)	Value 1000	5	X-Ax	rie Dens kis Point T(K)	Value 1000	Mobile Comps.
Dri	gin Point T(K) x(C)	Value 1000 0	5	X-Ax	rie Dens kis Point T(K) x(C)	Value 1000 0	Mobile Comps.
Dri	gin Point T(K) x(C) x(Fe)	Value 1000 0 1	5	X-Ax	T(K) x(C) x(Fe)	Value Value 0 0 0.95	Mobile Comps.
Drij	gin Point T(K) x(C) x(Fe) x(Ni)	Value 1000 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	>	X-As	rt(K) x(C) x(Fe) x(Ni)	Value 1000 0 0 0.95 0.05	Mobile Comps.
Dri	gin Point T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 1 0 1 0 1	>	X-Ax	T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 0.95 0.05 1	Mobile Comps.
Dri	T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 1 0 1	> >	X-Ax	r(K) x(C) x(C) x(Ni) Total:	Value 1000 0 0.95 0.05 1	Mobile Comps.
Dri	gin Point T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 1 0 1	2	X-Ax	T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 0.95 0.05 1	Mobile Comps.



Set Mobile Componer	nts	×						
Selected Components	s:							
Component	Mobile?	ОК						
С		Cancel						
Fe								
Ni								

Figure 1.27.2: Set mobile components

ecuc	on (2D) Calo	ulation					×
Y-A	xis Point						
		Value	1	Y			OK
	T(K)	1000			Cancel		
▶	x(C)	0.05					Options
	x(Fe)	0.95		Or	Extra Outputs		
-	x(Ni)	0					Load Condition
	Total	1					Save Condition
	Total.						Select Phases
							Select Comps
					P	seudo 🗌	Contour Lines
			s	can	line Densitv	0 1	Mahila Compo
						· • •	Mobile Comps.
Ori	gin Point			X-A	xis Point		wobie comps.
Ori	gin Point	Value		X-A	xis Point	Value	Mobile Comps.
Ori	gin Point T(K)	Value 1000		X-A	xis Point T(K)	Value 1000	
Ori	gin Point T(K) x(C)	Value 1000 0		X-A	T(K) x(C)	Value 1000 0	
Ori	gin Point T(K) x(C) x(Fe)	Value 1000 0 1		X-A	T(K) x(C) x(Fe)	Value 1000 0.95	
Ori	gin Point T(K) x(C) x(Fe) x(Ni)	Value 1000 0 1 0 0		X-A	T(K) x(C) x(Fe) x(Ni)	Value 1000 0.95 0.05	
Ori	gin Point T(K) x(C) x(Fe) x(Ni) Total:	Value Value 1000 0 1 0 1 1 0 1		X-A	T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0.95 0.05 1	
Ori	gin Point T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1		X-4	T(K) T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0.95 0.05 1	
Ori	gin Point T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 1 0 1 1 0 1		A-X	T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0.95 0.05 1	
Ori	gin Point T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0 1 0 1 1 0 1 0 1 0 1 0 0 0 0 0 0		A-X	xis Point T(K) x(C) x(Fe) x(Ni) Total:	Value 1000 0.95 0.05 1	



Post Calculation Operation:

- Add tie-lines and change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the graph following the procedure in Pandat User's Guide 2.3.3;
- The Para-equilibrium isothermal section is shown as Figure 1.27.4



Figure 1.27.4: Calculated para-equilibrium isothermal section of Fe-Ni-C at 1000 K

Example 1.28 Calculation of T₀ curve

Purpose: Learn to calculate the T₀ curve between two phases.

Module: PanPhaseDiagram

Thermodynamic Database: AlMgZn.tdb

Batch file: Example_#1.28.pbfx

Background: T_0 curve is the trace of a series of points in a two-phase field at which the Gibbs energy of the two phases are identical. It is the limit of partitionless phase transition, such as martensite transformation. In this example, we will learn how to calculate the T_0 curve between two solution phases. The T_0 curves between Hcp/Liquid and Fcc/Liquid are used as example in this case.

- Load AlMgZn.tdb following the procedure in Pandat User's Guide 3.2.1;
- Perform section (2D) calculation following the procedure in Pandat User's Guide 3.3.3;
- Set the calculation condition as shown in Figure 1.28.1; This is a normal setting for phase diagram calculation as shown in Example 1.1 : AI-Mg Binary Phase Diagram
- The Contour Lines function is used to calculate the T₀ curve, click the "Contour Lines" icon, the "Set Contour Lines" window pop up as shown in Figure 1.28.2. Add the T0 as the Contour Curves, select "Phase Name" as "Liquid", and the "Phase Name #2" as " * ", Pandat will calculate the T₀ curve between liquid and all solid solution phases. In this example, they are Fcc in Al side, and Hcp in Mg side.

-A)	xis Point						
		Value] 1	Y			ОК
I	T(C)	800					Cancel
	x(Al)	1					Options
_	x(Mg)	0		Ori	igin	x	Extra Outputs
	Total	1	•		_	-	Load Condition
	rotai.						Save Condition
							Select Phases
							Select Comps
					F	seudo 🗌	Contour Lines
			s	Scanl	F line Density	Pseudo □ /: 0 🜩	Contour Lines Mobile Comps
)rig	gin Point		s	Scanl X-A	F line Density xis Point	Pseudo □ r: 0 🜩	Contour Lines Mobile Comps
)rig	gin Point	Value	s	Scanl X-A	F line Density xis Point	Pseudo	Contour Lines Mobile Comps
)rig	gin Point T(C)	Value 0	s	Scanl X-A	F line Density xis Point T(C)	Pseudo r: 0 Value 0	Contour Lines Mobile Comps
)rig	gin Point T(C) x(Al)	Value 0 1	s	X-A	F line Density xis Point T(C) x(Al)	Pseudo	Contour Lines Mobile Comps
)rig	gin Point T(C) x(Al) x(Mg)	Value 0 1 0	s	X-A	F line Density xis Point T(C) x(Al) x(Mg)	vseudo vseudo vseudo Value Value 0 1	Contour Lines Mobile Comps
)rig	gin Point T(C) x(Al) x(Mg) Total:	Value 0 1 0 1 1 0 1	s	X-A	F line Density xis Point T(C) x(Al) x(Mg) Total:	Value 0 0 1	Contour Lines Mobile Comps
)rig	gin Point T(C) x(Al) x(Mg) Total:	Value 0 1 0 1 1 0 1	s	X-A	F line Density xis Point T(C) x(AI) x(Mg) Total:	Value 0 0 0 1	Contour Lines Mobile Comps
)rig	T(C) x(Al) x(Mg) Total:	Value 0 1 0 1 1	S	Scanl	F ine Density ixis Point T(C) x(Al) x(Mg) Total:	Pseudo	Contour Lines
)rig	gin Point T(C) x(Al) x(Mg) Total:	Value 0 1 0 1	s	Scanl	F ine Density ixis Point T(C) x(AI) x(Mg) Total:	Pseudo c 0 Value 0 1	Contour Lines Mobile Comps

Figure 1.28.1: 2D calculation with composition from pure AI to pure Mg and temperature from 0°C to 800°C

Set Contour Lines		×
Pre-Defined Contour Types:	Properties:	
ThRac(@') User Custom Type Te G G G (@') HSN(@')	Phase Name Liquid Phase Name #2 Step 0.1	Cancel
Contour Curves: Name		
Contour_10		

Figure 1.28.2: The Set Contour Lines window

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add Label to the graph following the procedure in Pandat User's Guide 2.3.3;



Figure 1.28.3: The calculated AI-Mg phase diagram together with T_0 curves of Fcc/Liquid and Hcp/Liquid

Information obtained from this calculation:

• The T0 curves in AI-Mg system between Fcc/Liquid and Hcp/liquid are obtained.

Example 1.29 Material to Material Calculation: Friction-stir welding between AA5454 AI alloy and AZ91 Mg alloy

Purpose: This example demonstrate the material to material function in Pandat software. The calculation conditions are the same as **Example 1.25**.

Module: PanPhaseDiagram

Thermodynamic Database: PanMg.pdb(this database is a thermodynamic database for multicomponent magnesium alloys which is only available to users who have licensed it.)

Calculation Procedures:

- Load PanMg.pdb following the procedure in Pandat User's Guide 3.2.1, and select components: AI, Fe, Mg, Mn, Zn;
- Perform Material to Material calculations through the menu bar "PanPhaseDiagram → Section Calculation: Material to Material";
- Set Calculation Condition as shown in Figure 1.29.1 The left edge material is defined as AA5454: AI-3Mg-1Mn-0.3Fe-0.01Zn(wt.%); the right edge material is AZ91: Mg-8.2AI-1Zn-0.2Mn-0.01Fe (wt.%). The temperature range is from 300 °C to 500 °C. Note that, instead of manually entering the composition, users can directly select the material from the Materials Chemistry Database (DB) if it has been saved, as described in Pandat User's Guide: Material-to-Material Calculation 3.3.6.

Post Calculation Operation:

- Add a new Table as shown in Figure 1.29.2 to get the ZPF line data of the liquid phase (f (@Liquid)=0);
- Plot the ZPF line data in the added table into the default graph following the procedure in Pandat User's Guide 2.4.3;
- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;





Table Editor			×
Table Type: Default	Table	Name: generated	ОК
т		Columns	Cancel
Р		w(AZ91)	
D/*)		т	Clear All
r()	1	f(@Liquid)=0	Original Strs
P(@gas)			
log10(P)			



Information obtained from this calculation:

The obtained phase diagram is shown in Figure 1.29.3. The weight percent of the material AZ91 is used as X-axis. This figure is similar to the Figure 1.25.3 in <u>Example 1.25</u> where the weight percent of element Mg is used as X-axis.

- To prevent partial melting during the friction-stir welding process, the local temperatures in the welding zone must be maintained below the threshold indicated by the red line. In this case, the minimum temperature to avoid such melting is 435.7 °C.
- Different intermetallic phases may form in the joining zone: The AI_3Mg_2 phase with some AI_6Mn precipitate near the AI alloy side, and $Mg_{17}AI_{12}$ phase with minor precipitation of AI_4Mn near the Mg alloy side.
- A similar approach can also be applied to analyze interactions between other materials, such as coating/substrate reactions.



Figure 1.29.3: The vertical phase diagram from AA5454 to AZ91 with phase field labels (The phase fields including Liquid phase are labeled as red)

2 PanOptimizer Example

Example 2.1 : Parameter Optimization for the Fe-Cr-Ni Ternary System

Example 2.1 Parameter Optimization for the Fe-Cr-Ni Ternary System

Purpose: Learn to optimize thermodynamic parameters for a ternary system.

Module: PanOptimizer

Database: Fe-Cr-Ni_OPT.tdb

pop file: Fe-Cr-Ni_OPT.pop

Figure 2.1.1 shows an experimentally determined isothermal section of the Fe-Cr-Ni ternary system at 900°C. Two solution phases, Bcc (α) and Fcc (γ), and one intermetallic compound (σ) are stable at this temperature. The experimental data includes tie-lines (equilibrium between two different phases) and tie-triangles (equilibrium of three different phases). This example shows how to optimize the thermodynamic parameters for this system using the given experimental data.





Prepare file:

 Prepare the database file and pop following the procedure in Pandat User's Guide: Step 1: Prepare Files 4.3.1; The binary thermodynamic parameters are selected from literature, which are proven to describe the corresponding binary systems precisely. And the ternary interaction parameters are set for optimization. User may go through the database file (Fe-Cr-Ni_OPT.tdb) for more details.

The experimental data are input into the pop file (Fe-Cr-Ni_OPT.pop). The tie-lines are stored in table format by giving an overall alloy composition at themidpoint of the each tie-line. The tie-triangles are input by giving an overall alloy composition at centre point of each triangle. In both cases, the phases use "ENTER" status so that PanOptimizer can easily find the corresponding equilibrium.

Perform Optimization:

• Load the database and experimental files (tdb and pop files) following the procedure in Pandat User's Guide 4.3.1;

User may check the parameters to be optimized by clicking the "Parameters" button on the optimization control panel, and check the difference between calculated equilibrium and experiments by clicking the "Experimental Data" button as shown in the red box in Figure 2.1.2;



Figure 2.1.2: PanOptimizercontrol interface for optimization setting
After several runs of optimization, the sum of squares will reach a minimum and does not change, which means PanOptimizer has found an optimal result for the parameters. User may calculate an isothermal section at 900 °C and compare to the experimental data. As shown in Figure 2.1.3, the calculated phase boundaries are in good agreement with the experimental data. And user may also need to check the values of the parameters and make sure that they are reasonable as shown in Figure 2.1.4. If there is noticeable difference between calculated boundary and the experimental data, user need to figure out new ternary parameters that need to be included in optimization or using more complicated model to describe the corresponding phases.



Figure 2.1.3: Comparison between calculated isothermal section at 900°C and experimental

data

🖳 Model Paramet	ters					-	- 🗆 X
Name		Low Bound	Up Bound	Value	Default Value	Std. Deviation	Relative S.D.
BCC0		-50000.0000	50000.0000	-38057.4000	0.0000	6061.1189	18.38%
BCCT		-50.0000	50.0000	24.1670	0.0000	5.1270	25.88%
FCC0		-50000.0000	50000.0000	-29506.7000	0.0000	6530.8798	27.20%
FCCT		-50.0000	50.0000	20.6101	0.0000	5.5677	35.10%
SIGMA0		-500000.0000	500000.0000	158595.0000	0.0000	16237.6317	11.10%
SIGMA1		-500000.0000	500000.0000	-77161.9000	0.0000	2119.0266	2.79%
Save TDB Se	t As D	efault Get Default	Include	Exclude		Apply	Done

Figure 2.1.4: Optimization results

3 PanEvolution/PanPrecipitation Examples

Example 3.1 : Precipitation Simulation of Ni-14AI (at%) Alloy

- Example 3.2 : TTT diagram of Ni-14AI (at%) Alloy
- Example 3.3 : Co-precipitation of γ' and γ'' in Ni-Al-Nb Ternary
- Example 3.4 : Simulation of Hardness of Aluminum Alloy 6005
- Example 3.5 : Simulation of Softening of Aluminum Alloy 6005
- Example 3.6 : Simulation of Yield Strength of Aluminum Alloy 356
- Example 3.7 : CCT diagram of Ni-14AI (at%) Alloy

Example 3.1 Precipitation Simulation of Ni-14AI (at%) Alloy

Purpose: Learn to perform a precipitation simulation of a binary alloy. In this example, precipitation simulation will be performed for Ni-14Al alloy during isothermal ageing at 550 °C, and experimental data will be added to the plots

Module: PanEvolution

Thermodynamic and Mobility Database: AlNi Prep.tdb

Kinetic Parameters Database: Ni-14Al Precipitation.kdb

Batch file: Example_#3.1.pbfx

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load AlNi Prep.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "Load KDB or EKDB", then select the Ni-14Al_Precipitation.kdb, a dialog will pop out as shown in Figure 3.1.1. This dialog shows the key information stored in the Ni-14Al_Precipitation.kdb, i.e, the matrix phase is Fcc, and the precipitate phase is L12_FCC;
- Click menu "File → Open File" to open the Ni-14Al_Precipitation.kdb. As shown in Figure 3.1.2, in addition to the matrix phase and precipitate phase, other parameters, such as, molar volume and interfacial energy are also defined in this file. Details on these parameters can be found in Pandat User's guide Section 5.3.;
- Click on PanEvolution/PanPrecipitation on the menu bar and click "Precipitation Simulation". A dialog will pop out as shown in Figure 3.1.1, set up the alloy chemistry on the left and the heat treatment condition on the right. In this setting, an isothermal ageing is performed at 550 °C assuming the initial state is pure Fcc phase; Add Intermediate PSD outputs at 1 hour, 10 hours and 50 hours.







Figure 3.1.2: Parameters defined in the Ni-14Al_Precipitation.kdb



Figure 3.1.3: Setup the alloy chemistry (Ni-14 at%Al) and heat treatment condition (isothermal ageing at 550 °C) for the simulation

- Right click the Default graph and rename it as vf;
- Create a new table as shown in Figure 3.1.4. A new table with two columns will be created with the first time in hour and the second size of L12_FCC in nanometer. Create a plot from this table and rename it as Size;
- Create a new table as shown in Figure 3.1.5. A new table with two columns will be created with the first log(time in minute) and the second the number density of L12_FCC in cm³. Create a plot from this table and rename it as nd;
- Import a table from a file as shown in Figure 3.1.6, and select Ni-14Al_Exp.dat;
- Open the Size graph, single click the Ni-14Al_Exp table and drag in the t (hr) as xaxis, press Ctrl and drag in the radius (nm) as y-axis. In the Property window set the "Plot Type" as Point, the plot with experimental data point is shown in Figure 3.1.7;
- Open the nd graph and add the experimental data on it as shown in Figure 3.1.8;

 Create a new table as shown in Figure Figure 3.1.9, select psd as the Table Type; select the psd_s(L12_FCC) and the psd_nnd(L12_FCC) two columns to create a new plot as shown in Figure 3.1.10;

Table Editor			×
Table Type: Default	Table Na	ame: generated	ОК
time		Columns	Cancel
log10(time)	t	/3600	
Т	./ s	(@L12_FCC)*1e9	 Clear All
vft	•		 Original Strs

Figure 3.1.4: Create a new table with two columns with the first column time (hour) and the

Table Editor × Table Name: generated Table Type: Default • OK time Cancel Columns log10(time/60) log10(time) Clear All log10(nd(@L12_FCC)*1e-6) т Original Strs . vft

second column the precipitate size (nm)



<i>i i i i</i>

Pandat Software by CompuTherm, LLC											- 0	×
File Edit View Databases Batch Calc Par	nPhaseDiagra	am PanEvolu	tion/PanPrecipitatio	on PanOptimizer	PanDiffusion	PanSolidificatio	n PanPhaseField	Property Ta	able Graph	Help		
🗔 🖬 📂 🗟 🎒 🖉 🚔 I X 🖕 🖄 🗙 💌	📰 🛃 g	. • = ×	۵ 🛐 🔝	🔀 🗹 🖂 🛣			🏭 🔛 ا 🔜 🕷	🧄 📓 ២ 🖪	1 😒 🔖	l 🖸 🖸	= 🕱 🥖	2
Workspace # ×	🖉 Ni-14AL	Precipitation.kd	b 💀 vf.gra	ph 😽 psd.	_100.graph	generated	table ×					-
Microstructure Evolution		time	s(@L12_FCC)									
recipitation	h	our ~	nanometer ~									
-R vf	1 0.0	000000	0.000000									
psd_100	2 1.	223183E-010	0.000000									
Add a New Table	3 7.3	339100E-010	0.000000									
Import Table from File	4 3.	791868E-009	0.000000									
	5 1.1	908166E-008	0.000000									
Frename P2	6 9.5	553062E-008	0.000000									
Collanse	7 4.3	777754E-007	0.000000									
× Delete	8 2.3	388999E-006	0.000000									
Workspace Databas	9 1.1	194512E-005	0.000000									
Property Property	10 5.9	972572E-005	0.000000									
	11 0.0	000299	0.000000									
	12 0.0	001493	0.000000									
	13 0.0	007466	0.258607									
	14 0.0	014931	0.209893									
	15 0.0	040555	0.295502									
	10 0.0	049000	0.303433									
	10 01	007710	0.401934									
	10 0.	126502	0.525389									
	20 0.	172935	0.694793									
	21 0.3	236567	0.891838									
				_	_	_	_	_	_	_	_	

Figure 3.1.6: Import an experimental data table from a file



Figure 3.1.7: Plot of size evolution with experimental data



Figure 3.1.8: Plot of number density evolution with experimental data

Table Editor	5	1283.	×
Table Type: psd 🔻	Tab	le Name: generated	ОК
index		Columns	Cancel
psd_id	•	psd_id	
psd_s(@*)		psd_s(@*)	Clear All
psd_nd(@*)		psd_nd(@*)	Original Strs
		psd_nnd(@*)	
	*		
psa_ns(@*)			
psd_nnd(@*)			

Figure 3.1.9: Create a new table for particle size distribution



Figure 3.1.10: Plot of particle size distribution

- It is common practice to plot the experimental data on the calculated diagram. When doing so, it is important to make unit consistency between the experimental data and the calculated property. In Pandat calculation, international standard unit is used, i.e., second for time, meter for length and cube meter for volume, and so on;
- Particle number density counts the number of particles in a unit volume. Default output from Pandat is number per m³, it was converted to number per cm³ in Figure 3.1.8;

- The psd_nnd (L12_FCC) in Figure 3.1.10 is normalized number density, which equals to the particle numbers of each size class divided by the total particle numbers;
- Figure 3.1.10 shows four distribution curves at four different times. The sharp one is at early nucleation stage which shows small particle size and high number density, the flat one shows the particle size distribution as final time (100 hours in this simulation). The corresponding time of each distribution can be found in the table. When create the table, simply put this time information in the table as shown in Figure 3.1.11;
- To only plot the particle size distribution curve at one time, set the inde x=1, or 2 ... or i. index=i means the final distribution. Figure 3.1.12 shows the table created for the final size distribution and Figure 3.1.13 shows the distribution curve.

Table Editor		×
Table Type: psd	Table Name: psd	ок
index	Columns	Cancel
psd_id	▶ psd_id	
psd_s(@*)	psd_s(L12_FCC)	Clear All
psd_nd(@*)	psd_nd(L12_FCC)	Original Strs
psd gr(@*)	psd_nnd(L12_FCC)	-
nsd_ns(@*)	index	-
	time/3600	-
psu_inid(e)	log(time)	-
	*	
	Double click to enter edit mode:	J
	In edit mode, press 'Ctrl'+'m' to show list of	
Drag and drop available columns to setu Description: Index of the Particle Size Di	p a new table. Double click property cell to edit.	
Description, index of the Particle Size Di	anouton (r 50). Example, muex - i.	

Figure 3.1.11: List the index and corresponding time for each size distribution curve



Figure 3.1.12: Create the table for final size distribution



Figure 3.1.13: Plot for final size distribution and the plot

Example 3.2 TTT diagram of Ni-14AI (at%) Alloy

Purpose: Learn to calculate the TTT curve for a given alloy.

Module: PanEvolution

Thermodynamic and Mobility Database: AlNi_Prep.tdb

Kinetic Parameters Database: Ni-14Al_Precipitation.kdb

Batch file: Example #3.2.pbfx

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load AlNi Prep.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "Load KDB or **EKDB**", then select the Ni-14Al_Precipitation.kdb;
- Click on PanEvolution/PanPrecipitation on the menu bar and click "TTT Simulation". A dialog will pop out as shown in Figure 3.2.1, In this dialog, user needs to input the alloy chemistry (left), temperature range and step (bottom right) and the Target volume fraction (top right). If the "Relative Vol%" box is checked, it means the Target Vol% is relative to the equilibrium fraction of the precipitate phase at each temperature, otherwise it is the volume fraction of the precipitate phase.

All	oy Compos	ition	Target Volume Percent	
Value		Value	Relative Vol% = \/f(\/f_EO)	ОК
	x%(Al)	14		Cancel
•	x%(Ni)	86	20	Options
	x /0(141)	100	2.0	Extra Outputs
	Total:	100		Load Conditio
				Save Condition
			Time/Temperature Range	Select Comp
			Max Time [hr]: 1000	Parameters
			Max Temperature [C]: 1000	Load Chemistr
			Min Temperature [C]: 300	Save Chemist
			Steps	



• Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

- Figure 3.2.2 shows the default plot from the calculation. It should point out that this TTT curve represents the time-Temperature curve when 2% of the equilibrium precipitate at each temperature comes out. For example, the equilibrium fraction of L12_FCC precipitate phase is 16.56% at 650°C, 2% of it is 0.33%. In other words, it takes 6.5 second to precipitate 0.33% of L12_FCC at this temperature.
- Perform another calculation for 10% and merge the two plots as shown in Figure 3.2.3;
- Details on the time, temperature and fraction of precipitate can be found in the Default table;



Figure 3.2.2: TTT curve for Ni-14AI (at%) when 2% of equilibrium L12_FCC formed



Figure 3.2.3: Comparison of TTT curves for Ni-14AI (at%) when 2% or 10% of equilibrium L12_ FCC formed

Example 3.3 Co-precipitation of γ' and γ'' in Ni-Al-Nb Ternary

Purpose: Learn to calculate co-precipitation of γ' and γ'' for an alloy in a pseudo-ternary system.

Module: PanEvolution

Thermodynamic and Mobility Database: NiAlNb_Pseudo.tdb

Kinetic Parameters Database: Ni-2.4Al-3.8Nb.kdb

Batch file: Example #3.3.pbfx

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load NiAlNb Pseudo.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "Load KDB or EKDB", then select the Ni-2.4Al-3.8Nb.kdb; the pop-out window is shown in Figure 3.3.1 which include the alloy name, the matrix phase and the precipitates. Two precipitates are defined in this case. The phase name in the kdb file is L12_Fcc and gamma_double_ prime for γ' and γ", respectively;
- Open the Ni-2.4Al-3.8Nb.kdb from Pandat workspace through the menu "File →
 Open File", and view the kinetic parameters as shown in Figure 3.3.2;
- Click on the menu "PanEvolution/PanPrecipitation → Precipitation
 Simulation", and set up the calculation condition as shown in Figure 3.3.3.







Figure 3.3.2: Open the Ni-2.4AI-3.8Nb.kdb in Pandat workspace to view the kinetic parameters

of the two precipitate phases





- The default plot shows the total volume fraction of γ' (L12_Fcc) and γ'' as a function of time shown in Figure 3.3.4.
- Open the Default Table, create time vs sizes of γ' and γ" phases plots as shown in Figure 3.3.5;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;



Figure 3.3.4: Default plot showing the volume fraction evolution of the two precipitate phases



Figure 3.3.5: Calculated average size evolution of the two precipitate phases

- Figure 3.3.4 shows the calculated evolution of volume fraction of the two precipitate phases. It is seen that γ' precipitated quickly at very early stage, but gave way to γ" at later time;
- Figure 3.3.5 shows the calculated evolution of the average size of the two precipitate phases. It is seen that γ" is bigger than γ';
- Add a new table as shown in Figure 3.3.6 with the "Table Type" as psd. The Columns are particle sizes and number densities with (@*) means all precipitate phases. The default calculated size is in meter, which is converted to nm by multiplying the column by 1e+9. The default calculated number density is number/m³, which is converted to mol/m₃ by multiplying 1/6.02e+23. The inde x = i means to populate the size and number density at the final state t=10 h;
- Plot particle size distribution from the new table by selecting the particle size as x-axis and number density as y-axis. Plot it for L12 (γ') phase first and then add the one for γ'' as shown in Figure 3.3.7.







Figure 3.3.7: Particle number densities of γ' and γ'' at final stage

Example 3.4 Simulation of Hardness of Aluminum Alloy 6005

Purpose: Learn to calculate the particle size, number density and hardness of aluminum alloy 6005

Module: PanEvolution

Thermodynamic and Mobility Database: AlMgSi.tdb

Kinetic Parameters Database: AA6xxx.kdb

Batch file: Example_#3.4.pbfx

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load AlMgSi.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "Load KDB or **EKDB**", then select the AA6xxx.kdb; the pop-out window is shown in Figure 3.4.1 which include the alloy name, the matrix phase and the precipitate phase;
- Open the AA6xxx.kdb from Pandat workspace through the menu "File → Open
 File", and view the kinetic parameters;
- Click on the menu "PanEvolution/PanPrecipitation → Precipitation
 Simulation", and set up the calculation condition as shown in Figure 3.4.2. Note the alloy composition is wt% (click Option button to select the unit);







Figure 3.4.2: Setup alloy composition and heat treatment condition as ageing at 185°C for 1000

hours

- The default plot shows the total volume fraction of the Mg₅Si₆ phase as a function of time shown in Figure 3.4.3.
- Create a new table as shown in Figure 3.4.4, and plot the log10(time) vs. log(nd), log10 (time) vs. log(size), and log10(time) vs. hv;
- Right Click on the Table node below the Graph and choose "Import Table from File", import three tables: AA6005-nd_exp.dat, AA6005-size_exp.dat, and AA6005-hv exp.dat one by one;
- Plot the experimental data in the corresponding plot by drag in the x-axis and then press
 Ctrl and drag in the y-axis of the experimental data table;
- The default plot of the experimental data is a line instead of points. In the Property Window, change the Plot Type as Point;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;



Figure 3.4.3: Default plot of volume fraction evolution of the precipitate

Table Editor		×
Table Type: Default	Table Name: generated_1	ок
time	Columns	Cancel
log10(time)	log10(time)	
т	log10(nd(@*))	Clear All
	log10(s(@*)*1e10)	Original Strs
fv_tot	hv	
x(*)	ba di la construcción de la constru	
x(*@*)		

Figure 3.4.4: Create a new table

- Figure 3.4.3 shows the default plot of the simulation which is volume fraction evolution of the precipitate phase. The time is in second;
- Figure 3.4.5 shows the calculated number density evolution; Figure 3.4.6 shows the size evolution, and Figure 3.4.7 the hardness change with time. Experimental data are plotted on them for comparison;
- It is seen that the number density reaches the highest value at ~1000 s (~0.3 h), but the
 particle size is very small. The hardness reaches peak at ~10000 s (~2.8 h) when both the
 number density and the particle size are favorable.



Figure 3.4.5: Calculated evolution of the particle number density with experimental data



Figure 3.4.6: Calculated evolution of the particle size with experimental data



Figure 3.4.7: Calculated evolution of hardness with experimental data

Example 3.5 Simulation of Softening of Aluminum Alloy 6005

Purpose: Learn to calculate the particle size, number density and hardness of aluminum alloy 6005 during ageing and reheating

Module: PanEvolution

Thermodynamic and Mobility Database: AlMgSi.tdb

Kinetic Parameters Database: AA6xxx.kdb

Batch file: Example_#3.5.pbfx

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load AlMgSi.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "Load KDB or **EKDB**", then select the AA6xxx.kdb;
- Click on the menu "PanEvolution/PanPrecipitation → Precipitation
 Simulation", and set up the calculation condition as shown in Figure 3.5.1.

	Value	Therr	nal History:	U Use Rat	te? 🐢 📟 🔤	OK
w%(Al)	98.63		time[hour]	Temperature[C]		Cancel
w%(Ma)	0.55		0.0	00000	185.00	Options
w%(Qi)	0.82		4.0	00000	185.00	Extra Output
w /6(01)	100		4.0	00000	350.00	Load Conditi
l otal:	100	Ma	5.0	00000	350.00	Save Conditi
		C	350 267.5			Load Chemi Save Chemi
		Tem	185_0	2.5 time[hour]	5	
			185_0	2.5 time[hour]	5 PSD Outputs:	•
tial Structure	sulation O Terms Int-	2000 (For	185	2.5 time[hour] Intermediate	5 PSD Outputs:	.
tial Structure Equil. Cale	culation O Temp. [C]:	2000 (Equ	ilibrium phases will not evolve)	2.5 time[hour] Intermediate	5 PSD Outputs:	•
al Structure Equil. Cale Define throu	sulation O Temp. [C]: ligh GUI O	2000 (Equ Set Initia	185 0	2.5 time[hour] Intermediate	5 PSD Outputs:	(
ial Structure Equil. Cale Define throu mport from	sulation O Temp. [C]: ligh GUI O	2000 (Equ Set Initia	ilibrium phases will not evolve)	2.5 time[hour] Intermediate	5 PSD Outputs:	.

Figure 3.5.1: Setup heat treatment condition as ageing at 185°C for four hours and then quickly heat up to 350°C and hold for 1 hour

- Create a new table as shown in Figure 3.5.2, and plot the time vs. log10(nd), time vs. log(size), and time vs. hv;
- Right Click on the Table node below the Graph and choose "Import Table from File", import table: AA6005-reheat_exp.dat;
- Plot the experimental data in the corresponding plot by drag in the x-axis and then press
 Ctrl and drag in the y-axis of the experimental data table;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;

Table Editor			>
Table Type: Default	✓ Tab	le Name: generated	ОК
s_range(@*,lb,ub)		Columns	Cancel
D(@*)		time	
1(@*)		log10(nd(@Mg5Si6))	Clear All
A_R(@*)		log10(s(@Mg5Si6)*1e10)	Original Strs
nd(@*)		hv	
log10(nd(@*))	*		

Figure 3.5.2: Create a new table

- Figure 3.5.3 shows the calculated evolution of particle number density with experimental data, time is in second. It is seen that the particle number density increases quickly within the first hour and then decreases slightly during ageing at 185 °C. It decreases drastically when heating up to 350 °C;
- Figure 3.5.4 shows the calculated evolution of particle size with experimental data. It is seen that the particle size increases gradually during ageing at 185 °C. It increases drastically when heating up to 350 °C;
- Figure 3.5.5 shows the calculated evolution of hardness with experimental data. It is seen that the hardness increases gradually during ageing at 185 °C. It drops quickly when heating up to 350 °C.



Figure 3.5.3: Calculated evolution of the particle number density with experimental data



Figure 3.5.4: Calculated evolution of the particle size with experimental data



Figure 3.5.5: Calculated evolution of hardness with experimental data

Example 3.6 Simulation of Yield Strength of Aluminum Alloy 356

Purpose: Learn to calculate yield strength including intrinsic, solid solution, and precipitation strengthening of aluminum alloy 356 during the process of ageing

Module: PanEvolution

Thermodynamic and Mobility Database: AlMgSi.tdb

Kinetic Parameters Database: AA3xx.kdb

Batch file: Example_#3.6.pbfx

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load AlMgSi.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "Load KDB or **EKDB**", then select the AA3xx.kdb;
- Click on the menu "PanEvolution/PanPrecipitation → Precipitation
 Simulation", and set up the calculation condition as shown in Figure 3.6.1. Note that the "Equilibrium Calculation" button under Initial Structure (bottom) should be checked and the solution temperature (540 °C in this case) should be given;



Figure 3.6.1: Setup calculation condition for aluminum alloy 356

- Create a new table as shown in Figure 3.6.2, and select all the columns in the newly created table to create a plot;
- Right Click on the Table node below the Graph and choose "Import Table from File", import table: AA356-ys_exp.txt; Note that the extension of a data file can be either txt or dat;
- Plot the experimental data in the corresponding plot by drag in the logt as x-axis and then press Ctrl and drag in the experimental data ys as the y-axis, then repeat it to add experimental data of ysp, ysi and yss;
- Create a new table as shown in Figure 3.6.4, select log10(time/3600) as x-axis, and x% (Mg@_Fcc) and x%(Si@_Fcc) as y-axis to create a plot as shown in Figure 3.6.5;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;

Table Editor		×
Table Type: Default ~	Table Name: generated	ОК
s_range(@*,lb,ub)	Columns	Cancel
D(@*)	log10(time/3600)	
1(@*)	sigma_y	Clear All
A R(@*)	sigma_p(@Mg5Si6)	Original Strs
	sigma_ss	
nd(@')	sigma_i	
log10(nd(@*))	*	
nr(@*)		

Figure 3.6.2: Create a new table for yield strength plot



Figure 3.6.3: A comparison of the calculated yield strength (lines) with the experimental data

(symbols)

Table Editor				×
Table Type: Default	\sim	Table	e Name: generated	ОК
time			Columns	Cancel
log10(time)		•	log10(time/3600)	
т			x(*@*)	Clear All
fv_tot		*		Original Strs

Figure 3.6.4: Create a new table to show the evolution of phase compositions



Figure 3.6.5: Evolution of elemental solubility in the matrix Fcc

- Example 3.6 shows a comparison of the calculated yield strength (lines) with the experimental data (symbols). The orange line (symbols) represents the intrinsic contribution; the green line (symbols) represents the solid solution strengthening; the red line (symbols) represents the precipitation strengthening; and the blue line (symbols) is the total from all three contributions;
- It is clearly seen from Figure 3.6.3 and Figure 3.6.5 that with the formation of Mg₅Si₆ precipitate, the solubility of Mg and Si in Fcc decreases and solution strengthening also decreases.

Example 3.7 CCT diagram of Ni-14Al (at%) Alloy

Purpose: Learn to calculate the CCT curve of a given alloy.

Module: PanEvolution

Thermodynamic and Mobility Database: AlNi_Prep.tdb

Kinetic Parameters Database: Ni-14Al_Precipitation.kdb

Batch file: Example_#3.7.pbfx

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load AlNi Prep.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "Load KDB or **EKDB**", then select the Ni-14Al_Precipitation.kdb;
- Click on PanEvolution/PanPrecipitation on the menu bar and click "CCT Simulation". A dialog will pop out as shown in Figure 3.7.1, In this dialog, user needs to input the alloy chemistry (left), temperature range, cooling rate range and step (bottom right) and the Target volume fraction (top right).

Alloy Compo	osition	Target Volume Percent	
	Value		ОК
x(Al)	0.14		Cancel
v(Nii)	0.86		Options
X(INI)	0.00		Extra Outputs
Total:	1		Load Conditio
			Save Conditio
			Select Comp
			Parameters
			Load Chemist
			Save Chemist
		Temperature Range	
		Start Temperature [C]: 800	
		End Temperature [C]: 400	
		Cooling Rate Range	
		Slowest [K/S]: 0.1000	
		Fastest [K/S]: 100.0000	
		Steps	
		# of Cooling Bate Steps: 50	



• Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

- Figure 3.7.2 shows the default plot from the calculation. On this diagram, the green lines are the cooling curves with different cooling rate, the blue line is the CCT curve represents the temperature when 0.2 vol% of L12_Fcc phase is precipitated under different cooling rates.
- Perform another calculation for 1% and merge the two plots as shown in Figure 3.7.3;
- Details on the time, temperature and fraction of precipitate can be found in the Default table;


Figure 3.7.2: CCT curve for Ni-14AI (at%) when 0.2% of L12_FCC is precipitated under different cooling rates.



Figure 3.7.3: Comparison of CCT curves for Ni-14AI (at%) when 0.2% or 1% of L12_FCC precipitated under different cooling rates

4 PanDiffusion Examples

- Example 4.1 : Diffusion within a Single Phase: Uniform Initial Compositions
- Example 4.2 : Diffusion within a Single Phase: Linear Initial Compositions
- Example 4.3 : Diffusion between Two Phases: Uniform Initial Compositions
- Example 4.4 : Diffusion between Two Phases at Varied Temperatures
- Example 4.5 : Diffusion among Multiple Regions
- Example 4.6 : Carburization with Fixed Composition at Boundary
- Example 4.7 : Carburization with Input Flux
- Example 4.8 : Carburization of a Tube with Fixed Environmental Activity
- Example 4.9 : Dissolution of y' Particle in y Matrix
- Example 4.10 : Transformation from γ to α
- Example 4.11 : Fe-Si-C Uphill Diffusion
- Example 4.12 : Dissolution of a Single θ-Al2Cu Particle in FCC Matrix
- Example 4.13 : Dissolution of Multiple Particles
- Example 4.14 : Decarburization of Fe-C Matrix

Example 4.1 Diffusion within a Single Phase: Uniform Initial Compositions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion couple with both sides having the same single phase structure and uniform composition through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: FeCrNi.tdb

Batch file: Example #4.1.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load FeCrNi.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.1.1. First select "Region Composition Distribution" as Uniform, which means that composition in each region is uniform before diffusion. Click on Region_1 and set the composition of the left side of the diffusion couple as 30Cr-10Fe-60Ni (at%), then click on Region_2 and set the composition of the right side of the diffusion couple as 10Cr-20Fe-70Ni (at%) (which is not shown in Figure 4.1.1).
- The length of both Region_1 and Region_2 is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 1000 hours.
- The default output includes composition profiles of the initial and final stages. Composition profiles can also be plotted and listed in the table for intermediate times. By clicking the blue "+" next to the "Moments for Profile Outputs" composition profiles for number of intermediate stages can be outputted. As shown in Figure 4.1.1, those at 200 hour and 500 hour will be outputted. Click OK to start calculation.

- User can define the "Geometry" as "Planar, Cylindrical, and Spherical";
- User can also select "Interface Flux Model" and set "boundary conditions". Details on these options can be found in Pandat User's Guide sections 6.3.11 and 6.3.12.



Figure 4.1.1: Setting of the simulation condition

- Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.1.2
- In addition to Default table, composition profiles at selected times are given in separated tables under Table, which can be plotted separately as shown in Figure 4.1.3.

- In this example, the initial compositions of the two regions of the diffusion couple are both in the single Fcc phase field as shown in the isotherm of Fe-Cr-Ni at 1000°C in Figure 4.1.4;
- Composition profiles at selected times can be obtained.



Figure 4.1.2: Calculated composition profiles after diffusion for 200, 500 and 1000 hours,

respectively



Figure 4.1.3: Calculated composition profiles after diffusion for 200 hours



Figure 4.1.4: Isothermal section of Ni-Cr-Fe at 1000 °C, the initial compositions of both sides locate in the single Fcc phase field

Example 4.2 Diffusion within a Single Phase: Linear Initial Compositions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion couple with both sides having the same single phase structure and composition varies linearly through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: FeCrNi.tdb

Batch file: Example #4.2.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load FeCrNi.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure Figure 4.2.1. First select "Region Composition Distribution" as Linear, which means that composition in each region varies linearly from the left edge to the right edge. Click on Region_1 and set the composition of the left side of the diffusion couple as 30Cr-10Fe-60Ni (at%), then click on Region_2 and set the composition of the left edge as 30Cr-10Fe-60Ni (at%), which is not shown in Figure 4.2.1).
- The length of both Region_1 and Region_2 is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 1000 hours.
- The output composition profiles include the initial and final stages and one intermediate stage at 100 hours. Click or

II Regions (clie	ck on each individua	al region for se	ttings):	Therm	Cance			
Region_1 linear Comp.			Region 2			time[hour]	Temperature[C]	Option
			unifor	n Comp.	▶	0.000000	1000.00	Extra Out
					·	1000.000000	1000.00	Load Con
Settings for the Selected Region [Region_1]:						0.000000	0.00	Save Con
Region Comp	osition Distribution:	linear	~	Select Phases				Select Ph
Loft End			Dight End					Select Co
Leit End	Value	_	Right Enu	Value		1010		
★ x%(Cr)	30		★ x%(Cr)	10	ģ	1010		
	10	-		20	Len	1000-		
x /0(1 C)		_	x /0(1 C)	70		990	i i i i i i i i i i i i i i i i i i i	
x%(NI)	60		x%(Ni) 70 tir		time	(hour)		
Total:	100		Total:	100				
					Momer	its for Profile Outputs:		
					time [hr	l		
					100			
Diff. Length	um]	100						
Boundary Conc	litions		Sim	ulation Conditions				
Upper Bour	dary Condition: clo	osed	~					

Figure 4.2.1: Setting of the simulation condition

• Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.2.2

- Composition shows linear distribution in both regions at the beginning;
- After holding the diffusion couple at 1000 °C for 1000 hours, the diffusion couple becomes nearly homogenized.



Figure 4.2.2: Calculated composition profiles at 100 hour and 1000 hour

Example 4.3 Diffusion between Two Phases: Uniform Initial Compositions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion couple with the two sides having different phase structure and uniform composition through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: FeCrNi.tdb

Batch file: Example_#4.3.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load FeCrNi.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.3.1. First select "Region Composition Distribution" as Uniform, which means that composition in each region is uniform before diffusion. Click on Region_1 and set the composition of the left side of the diffusion couple as 30Cr-10Fe-60Ni (at%), then click on Region_2 and set the composition of the right side of the diffusion couple as 55Cr-40Fe-5Ni (at%) (which is not shown in Figure 4.3.1).
- The length of both Region_1 and Region_2 is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 200 hours.
- In the settings shown in Figure 4.3.1, composition profiles only at the initial and final stages will be outputted. Click OK to perform calculations.

• Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.3.2

- The two sides of the diffusion couple locate at different phase fields, one in Fcc and the other in Bcc as shown in the isotherm of Fr-Cr-Ni at 1000°C in Figure 4.3.3, therefore diffusion between them pass through the Fcc+Bcc two-phase field;
- After holding the diffusion couple at 1000 °C for 200 hours, boundary between the Fcc and Bcc moved.



Figure 4.3.1: Setting of the simulation condition



Figure 4.3.2: Calculated composition profiles after diffusion at 1000°C for 200 hours



Figure 4.3.3: Isothermal section of Ni-Cr-Fe at 1000 °C, the initial compositions of the two sides locate in different phase fields, one in Fcc and the other in Bcc

Example 4.4 Diffusion between Two Phases at Varied Temperatures

Purpose: Learn to perform diffusion simulation at varied temperatures for a diffusion couple with the two sides having different phase structure and uniform composition through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: FeCrNi.tdb

Batch file: Example #4.4.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load FeCrNi.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.4.1. First select "Region Composition Distribution" as Uniform, which means that composition in each region is uniform before diffusion. Click on Region_1 and set the composition of the left side of the diffusion couple as 30Cr-10Fe-60Ni (at%), then click on Region_2 and set the composition of the right side of the diffusion couple as 55Cr-40Fe-5Ni (at%) (which is not shown in Figure 4.4.1).
- The length of both Region_1 and Region_2 is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000°C for 200 hours, then the temperature decreases from 1000°C to 900°C linearly in the next 100 hours.
- Click "Select Phase" and set Fcc and Bcc as the entered phases.
- In the settings shown in Figure 4.4.1, composition profiles only at the initial and final stages will be outputted. Click OK to perform calculations.

• Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.4.2

Information obtained from this calculation:

 After holding the diffusion couple at 1000 °C for 200 hours, the temperature decreases gradually in the next 100 hours to 900 °C. Composition profiles after the entire thermal history can be obtained;



• Learn to set up multi-step thermal history for a diffusion simulation.

Figure 4.4.1: Setting of the simulation condition



Figure 4.4.2: Calculated composition profiles at 300 hours

Example 4.5 Diffusion among Multiple Regions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion sandwich with different phase structure but uniform composition through each region before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: FeCrNi.tdb

Batch file: Example_#4.5.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load FeCrNi.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.5.1. First click the blue "+" above Regions to add another region, Region_3. Select "Region Composition Distribution" as Uniform.
- Click on Region_1 and set the composition of the left region of the diffusion couple as 30Cr-10Fe-60Ni (at%), Select Fcc as the entered phase in "Select Phases" of "Settings for the Selected Region [Region 1]".
- Click on Region_2 and set the composition of the middle region of the diffusion couple as 55Cr-40Fe-5Ni (at%). Select Bcc as the entered phase in "Select Phases" of "Settings for the Selected Region [Region_2]".
- Click on Region_3 and set the composition of the right region of the diffusion couple as 10Cr-20Fe-70Ni (at%). Select Fcc as the entered phase in "Select Phases" of "Settings for the Selected Region [Region_3]".
- The length of each region is set to be 100 $\mu m,$ and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 500 hours.

- Click "Select Phase" and set Fcc and Bcc as the entered phases.
- In the settings shown in Figure 4.5.1, composition profiles at the initial and final stages, as well as that at 200 hour will be outputted. Click OK to perform calculations.

• Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.5.2

- The three regions of the diffusion triple locate at different phase fields, the one in Bcc is sandwiched between two regions in the Fcc as shown in Figure 4.5.3;
- After holding the diffusion couple at 1000°C for 500 hours, composition profiles can be viewed at final stage (500h) and intermediate stage (200h). The phase boundaries are moved;



Figure 4.5.1: Setting of the simulation condition



Figure 4.5.2: Calculated composition profiles for the diffusion sandwich at 1000°C for 200h and

500h



Figure 4.5.3: Isothermal section of Ni-Cr-Fe at 1000 °C, the initial compositions of the left and right regions locate in the single Fcc phase field, while the middle region locates in the Bcc phase field

Example 4.6 Carburization with Fixed Composition at Boundary

Purpose: Learn to perform diffusion simulation at constant temperature for a carburization process with a fixed chemical composition at boundary.

Module: PanDiffusion

Thermodynamic and Mobility Database: Fe-Si-C.tdb

Batch file: Example_#4.6.pbfx

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load Fe-Si-C.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.6.1. First click the red "X" above Regions to delete Region 2 and leave one Region only.
- Click on Region_1 and set the composition as 0.5C-99.5Fe (at%), the Diff. Length as 100 μm, and the # of Grids as 100.
- The Thermal History is set as 1200 K for 25 seconds;
- Click on Lower Boundary Condition (left edge of Region_1) and select "fixed_ composition", and set the Value as "x%(C)=3.0";
- In the settings shown in Figure 4.6.1, composition profiles at the initial and final stages will be outputted. Click OK to perform calculations.

Post Calculation Operation:

• Enlarge the composition range between 0 and 4 (at%) to clearly display Carbon composition. The calculated plot is show in Figure 4.6.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

- Carbonization process in Fcc phase in the Fe-C system. Lower boundary condition is a fixed carbon composition;
- After holding the material at 1200K for 25 seconds, composition profiles can be viewed at final stage (25 s). The carbon gradually diffused into the Fcc phase from the boundary;

Regione (elis	k on each individual	region for or	tinge):	J. V	Therm	al History	× 🗉 🗈	Car
Regions (clic	x on each individual	region for se	stungs):		timefeeeend	Temperature [K]		
		Region_1			Þ	ume[second]	1200 00	Extra C
			np.			25.00	1200.00	Data C
ettings for i	the Selected Reg	ion [Regior	_1):	•	0.00	0.00	Load Co Save Co	
egion Comp	osition Distribution:	uniform	~	Select Phases				Select
Region Composition			Right End					Select
	Value			Value		1210 T		
x%(Fe)	99.5		▶ x%(Fe)	99.5	đ	1200		
x%(C)	0.5		x%(C)	0.5	_ ⊢	1190		
Total:	100		Total:	100		0	12.5 25	
				Mome	nts for Profile Outputs:	+ \chi	-	
					time (se	ec]		
Diff. Length [um]	100						
oundary Cond	litions		Sir	nulation Conditions				
Upper Boun	dary Condition: clos	sed	\sim					
Value: 0.0			G	eometry: planar	\sim	Inner Radius [um]:	0.000000	
Lower Boun	dary Condition: fixe	d compositi	on 🗸					
						4 - 1	10.11.0	

Figure 4.6.1: Setting of the simulation condition



Figure 4.6.2: Calculated C composition profile for diffusion at 1200K for 25s

Example 4.7 Carburization with Input Flux

Purpose: Learn to perform diffusion simulation at constant temperature for a carburization process with an input flux as boundary condition.

Module: PanDiffusion

Thermodynamic and Mobility Database: Fe-Si-C.tdb

Batch file: Example_#4.7.pbfx

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load Fe-Si-C.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.7.1. First click the red "X" above Regions to delete Region 2 and leave one Region only;
- Click on Region_1 and set the composition as 0.15C-99.85Fe (wt%), the Diff. Length as 3 mm, and the # of Grids as 200;
- The Thermal History is at 1173 K for 18000 seconds;
- Click on Lower Boundary Condition (left edge of Region_1) and select "flux", and set the Value as "J(C) =-8.25E-9* (a (C:Graphite[*])-0.64) /7e-006";
- In the settings shown in Figure 4.7.1, composition profiles at the initial and final stages, as well as at 100s, 1000s and 5000s, will be outputted. Click OK to perform calculations.

Post Calculation Operation:

• Enlarge the composition range between 0 and 1 (wt%) to clearly display Carbon composition. The calculated plot is show in Figure 4.7.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

- Carbonization process in Fcc of the Fe-C system. Lower boundary condition is an input flux. This setting provides user an option when the flux of C is known in the environment;
- After holding the material at 1173K for 18000 seconds, composition profiles can be viewed at selected stages. The carbon composition gradually diffused from the boundary to the body;



Figure 4.7.1: Setting of the simulation condition



Figure 4.7.2: Calculated C composition profiles for diffusion at 1173 K for 100s, 1000s, 5000s, and 18000s

Example 4.8 Carburization of a Tube with Fixed Environmental Activity

Purpose: Learn to perform diffusion simulation at constant temperature for a carburization process with an input flux as boundary condition.

Module: PanDiffusion

Thermodynamic and Mobility Database: Fe-Si-C.tdb

Batch file: Example_#4.8.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load Fe-Si-C.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.8.1. First click the red "X" above Regions to delete Region 2 and leave one Region only;
- Click on Region_1 and set the composition as 0.05C-98.65Fe-1.3Si (wt%), the Diff.
 Length as 10 mm, and the # of Grids as 200;
- Click "Select Phase" and set Fcc as the entered phase;
- The Thermal History is at 1273 K for 2E5 seconds;
- Click on Upper Boundary Condition and select "activity", and set the activity value at the right edge of Region_1 as "a (C:graphite [*])=1E-5". Click on Lower Boundary Condition and select "activity", then set the activity value at the left edge of Region_1 as "a (C:graphite[*])=0.9";
- In order to set a tube geometry, select "cylindrical" in "Geometry", and apply 20 mm to "Inner Radius";
- In the settings shown in Figure 4.8.1, composition profiles at the initial and final stages, as well as at 1E4 s, will be outputted. Click OK to perform calculations.

• Enlarge the composition range between 0 and 1.4 (wt%) to clearly display Carbon composition. The calculated plot is show in Figure 4.8.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

 Learn to set up Boundary conditions for a tube geometry, and fixed activities at both inner and outer surfaces;



• Observe carbon diffusion from inner surface (high activity) into the tube;

Figure 4.8.1: Setting of the simulation condition



Figure 4.8.2: Calculated composition profiles at 1273 K for 1E4s, and 2E5s

Example 4.9 Dissolution of y' Particle in y Matrix

Purpose: Learn to perform diffusion simulation at constant temperature where a γ' particle (L12, Ni3AI) dissolve into γ matrix (Fcc, Ni-AI). Learn to select entered phase(s) in each region.

Module: PanDiffusion

Thermodynamic and Mobility Database: AlNi_Diff.tdb

Batch file: Example_#4.9.pbfx

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load AlNi_Diff.tdb following the procedure in Pandat User's Guide 3.2.1;
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.9.1;
- Click on Region_1 and set the composition as 25A1-75Ni (at%), and select L12_FCC as the entered phase in "Select Phases" of "Settings for the Selected Region [Region_1]". In Region_1, set the Diff. Length as 5 um. Click on Region_2 and set the composition as 15A1-85Ni (at%) and select Fcc as the entered phase in "Select Phases" of "Settings for the Selected Region [Region_2]". In Region 2, set the Diff. Length as 10 um.
- The Thermal History is at 1473 K for 100 seconds;
- In order to set a tube geometry, select "spherical" in "Geometry", The total number of grids (# of Grids) is 100;
- In the settings shown in Figure 4.9.1, composition profiles at the initial and final stages, as well as at 10s, 30s, 50s and 70s, will be outputted. Click OK to perform calculations.

Post Calculation Operation:

• The calculated plot is show in Figure 4.9.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

- · Learn to set up simulation for dissolution of spherical particles;
- After holding the material at 1473K for 100s, composition profiles can be viewed at selected stages. The interface moving from γ phase to γ' indicates the dissolution of γ' particles.



Figure 4.9.1: Setting of the simulation condition



Figure 4.9.2: Calculated composition profiles at 1473 K for 10s, 30s, 50s, 70s and 100s



Figure 4.9.3: Ni-Al phase diagram. The initial composition of left-hand side locates in the single L12-FCC phase field. The initial composition of right-hand side locates in the single Fcc phase

field

Example 4.10 Transformation from γ to α

Purpose: Learn to perform diffusion simulation at constant temperature where a $\gamma \rightarrow \alpha$ transformation happens in Fe-C alloy. Learn to select entered phase(s) in each region.

Module: PanDiffusion

Thermodynamic and Mobility Database: Fe-Si-C.tdb

Batch file: Example_#4.10.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load Fe-Si-C.tdb following the procedure in Pandat User's Guide 3.2.1 and select elements Fe and C.
- Click on the menu "PanDiffusion → Diffusion Simulation" and set up the calculation condition as shown in Figure 4.10.1;
- Click on Region_1 and set the composition as 100Fe-OC (wt%), and select Bcc as the entered phase in "Select Phases" of "Settings for the Selected Region [Region_1]". In Region_1, set the Diff. Length as 1E-5 mm. Click on Region_2 and set the composition as 99.85Fe-0.15C (wt%) and select Fcc as the entered phase in "Select Phases" of "Settings for the Selected Region [Region_2]". In Region 2, set the Diff. Length as 2 mm;
- The Thermal History is at 1050 K for 1E6 seconds;
- The total number of grids (# of Grids) is 100;
- In the settings shown in Figure 4.10.1, composition profiles at the initial and final stages, as well as at 1E3 seconds and 1E5 seconds, will be outputted. Click OK to perform calculations.

• Enlarge the composition range between 0 and 0.5 (wt%) to clearly display Carbon composition. The calculated plot is show in Figure 4.10.2 Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

• Observe composition profiles of C and interface movement from α to γ which indicates the $\gamma \rightarrow \alpha$ phase transformation.



Figure 4.10.1: Setting of the simulation condition



Figure 4.10.2: Calculated composition profiles at 1050 K for 1E3 seconds, 1E5 seconds and 1E6 seconds

Example 4.11 Fe-Si-C Uphill Diffusion

Purpose: Learn to perform uphill diffusion simulation in a Fcc matrix at a constant temperature.

Module: PanDiffusion

Thermodynamic and Mobility Database: Fe-Si-C.tdb

Batch file: Example_#4.11.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load Fe-Si-C.tdb following the procedure in Pandat User's Guide 3.2.1 and select all three elements;
- Click on the menu "PanDiffusion → Diffusion Simulation" or click the icon []] and set up the calculation condition as shown in Figure 4.11.1;
- Click on "Select Phases" and make Fcc the entered phase, while other phases are suspended;
- Click on Region_1 and set the composition as Fe-3.8Si-0.49C (wt%). In Region_1, set the length (Diff. Length) as 25 mm.
- Click on Region_2 and set the composition as Fe-0.05Si-0.45C (wt%). In Region_2, set the length (Diff. Length) as 25 mm;
- The **Thermal History** is a period of 312 hours (13 days) with a constant temperature at 1050 °C;
- The total number of grids (# of Grids) is 100;
- In the settings shown in Figure 4.11.1, composition profiles at the initial and final stages, as well as 100 and 200 hours, will be outputted. Click OK to perform calculations;
- Details on these options can be found in Pandat User's Guide sections 6.3.11 and 6.3.12.

 Set the scale of the Y axis to be 0.3-0.6 (wt%); Remove composition profiles of Fe and Si; Add grid to the graph by setting "Show Major Grid" as "True" in the property window; The calculated plot is show in Figure 4.11.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

- Diffusion Simulation × Diffusion Conditions OK 💥 🖅 🗈 Cancel All Regions (click on each individual region for settings) 🕂 🎇 Thermal History: Temperature[C] Options time[hour] Region_1 uniform Comp. Region_2 uniform Comp. 0.00 1050.00 Extra Outputs 1050.00 315.00 Load Condition 0.00 0.00 as for the Selected Region [Region 2]: Save Condition Composition Distribution: uniform Select Phases Select Phases Select Comps Region Composition Right End Value Value 1060 Temp... w%(C) 0.45 ▶ w%(C) 0.45 1050 99.5 99.5 w%(Fe) w%(Fe) 1040 0.05 0.05 ົດ 157.5 315 w%(Si) w%(Si) Σ time(hour) Total 100 \leq + 🗙 Moments for Profile Outputs time [hr] 100 200 Diff. Length [mm] 25 Boundary Conditions Simulation Conditions Upper Boundary Condition: closed Geometry: planar \sim Inner Radius (mm): Lower Boundary Condition: closed Interface Flux Model: automatic ~ # of Grids: 100 Value:
- Composition profile of carbon in Fcc Matrix after an uphill diffusion.

Figure 4.11.1: Setting of the simulation condition



Figure 4.11.2: Composition profile of Carbon

Example 4.12 Dissolution of a Single θ-Al2Cu Particle in FCC Matrix

Purpose: Learn to perform single-particle dissolution simulation.

Module: PanDiffusion

Thermodynamic and Mobility Database: AlCu_MB.tdb

Batch file: Example_#4.12.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide section 2.1;
- Load AlCu_MB.tdb following the procedure in Pandat User's Guide section 3.2.1 and select both two elements;
- Click on the menu "PanDiffusion → Dissolution Simulation" or click the icon and set up the calculation condition as shown in Figure 4.12.1;
- Click on "Select Phases" and make Fcc and AlCu_Theta the entered phases, while other phases are suspended;
- In Alloy Composition set a composition of Al-1.55Cu (at%);
- The total number of grids (# of Grids) is 100;
- The Geometry of particles is set to "Spherical";
- In "Phase Information", select Fcc as "Matrix Phase".
- To add a particle, click the blue "+" button in the "Particle" field, then select AlCu_
 Theta in "Phase Name". "Particle Size" is set to 3.0 μm. "Vol. Fraction" is set to
 0.008;
- The "Thermal History" is a period of 35 minutes at 550°C;
- Click OK to start calculation;
- By default, dissolution simulation gives time-evolution of particle size as output. In order to display composition profile at desired moments, click the blue "+" button next to the "Moments for Profile Outputs" and input a time value. As shown in Figure 4.12.1, profiles at 10 minutes and 15 minutes will be outputted. Click OK to start calculation;
- Details on these options can be found in Pandat User's Guide section 6.4.

Dissolu	tion Simulatio	on						×
Allo	y Compositio	n		Therm	al History:		X 🗐 🗈	ОК
		Value			time[minute]		Temperature[C]	Cancel
•	x%(Al)	98.45		⊳		0.00	550.00	Options
	x%(Cu)	1.55				35.00	550.00	Extra Outputs
	Total:	100				0.00	0.00	Load Condition
								Save Condition
								Select Phases
								Select Comps
					560			
Ph	ase Informati	on						
Ma	trix Phase:	Fcc	~	S.				
Pa	rticles:		+ 💥	emi	550 -			
P	hase Name	Particle Size[um]	Vol. Fraction	⊢ .				
AI	Cu_Theta	3	0.008		0	10	7.5 35	
						time(n	ninute)	
				Mome	nts for Profile Ou	utputs:	+ 💥	
				time [m	in]			
				10	-			
Sir	nulation Cond	ditions		15				
Ge	eometry: sph	nerical \vee 🛛 # of Grid	ls: 100					
Int	erface Flux M	lodel: automatic	~					

Figure 4.12.1: Setting of the simulation condition

- The calculated particle dissolution with time is shown in Figure 4.12.2 User can modify it by changing the title, the scale and so on from the Property Window. User can also add experimental data by clicking menu "Table → Import Table From Files", and select Example_#4.12.txt, and then follow Example 3.1 : Precipitation Simulation of Ni-14AI (at%) Alloy to add the experimental data on the plot. More information about change graph appearance can be found in Pandat User's Guide Section 2.3.1.
- Click and open the Default table and select "distance", "x% (Al)" and "x% (Cu)" to plot the composition profiles at starting, ending and the two selected intermediate times as shown in Figure 4.12.3.



Figure 4.12.2: The simulation result of particle-size evolution



Figure 4.12.3: The simulation result of composition-profile evolution

Example 4.13 Dissolution of Multiple Particles

Purpose: Learn to perform multi-particle dissolution simulation. Two Al2Cu particles, with different sizes and volume fractions, dissolve into the Fcc matrix.

Module: PanDiffusion

Thermodynamic and Mobility Database: AlCu_MB.tdb

Batch file: Example_#4.13.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide section 2.1;
- Load AlCu_MB.tdb following the procedure in Pandat User's Guide section 3.2.1 and select both two elements;
- Click on the menu "PanDiffusion → Dissolution Simulation" or click the icon and set up the calculation condition as shown in Figure 4.13.1;
- Click on "Select Phases" and make Fcc and AlCu_Theta the entered phases, while other phases are suspended;
- In Alloy Composition set a composition of Al-1.55Cu (at%);
- The total number of grids (# of Grids) is 75;
- The Geometry of particles is set to "Spherical";
- In "Phase Information", select Fcc as "Matrix Phase".
- To add the first particle, click the blue "+" button in the "Particle" field, then select AlCu_Theta in "Phase Name". "Particle Size" is set to 3.0 μm. "Vol. Fraction" is set to 0.008;
- To add the second particle, click the blue "+" button in the "Particle" field, then select AlCu_Theta in "Phase Name". "Particle Size" is set to 1.0 μm. "Vol. Fraction" is set to 0.001;
- The "Thermal History" is a period of 35 minutes at 550 °C;

Click OK to start calculation;

•	Details on	these	options	can b	e found	in	Pandat	User's	Guide	section	6.4
---	------------	-------	---------	-------	---------	----	--------	--------	-------	---------	-----

ssolu	ition Simula	atio	n						>
Alle	Composi	tion						¥ 📼 🛋	01
	y composi	uon			Therm	nal History:			OK
<u> </u>		-	Value			time[min	ute]	Temperature[C]	Cancel
▶	x%(Al)		98.45				0.00	550.00	Options
	x%(Cu)		1.55		▶		35.00	550.00	Extra Outputs
	Total:		100				0.00	0.00	Load Condition
									Save Condition
									Select Phases
									Select Comps
						_			
	_					560 _T		·,,	
Ph	ase Inform	atio	n		5				
Ma	atrix Phase:	F	cc	~)d	550			
Pa	rticles:			+ 🗙	Tem	550			
Р	hase Name	e	Particle Size[um]	Vol. Fraction		F40			
AI	Cu_Theta	\sim	3.0	0.008		0	1	7.5 35	
AIC	Cu_Theta	~	1.0	0.001			time(r	ninute)	
					Mome	nts for Prof	ile Outputs:	+ 💥]
					time (m	in]			
Sir	nulation Co	ondi	tions						
6				da. 75					
Ge	sometry.	pne	ancal • # or Gn	ds. 75					
Int	terface Flux	c Mo	odel: automatic	~					

Figure 4.13.1: Setting of the simulation condition

Post Calculation Operation:

 The calculated particle dissolution with time is shown in Figure 4.13.2 User can modify it by changing the title, the scale, and add grid to the graph by setting "Show Major Grid" True in the Property Window.More information about change graph appearance can be found in Pandat User's Guide Section 2.3.1.



Figure 4.13.2: The simulation result of particle-size evolution

Example 4.14 Decarburization of Fe-C Matrix

Purpose: Learn to perform decarburization simulation at constant temperature with a fixed activity at boundary.

Module: PanDiffusion

Thermodynamic and Mobility Database: Fe-Si-C.tdb

Batch file: Example_#4.14.pbfx

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load Fe-Si-C.tdb following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "PanDiffusion → Diffusion Simulation" or click the icon []] and set up the calculation condition as shown in Figure 4.14.1.
- First click the red "X" above Regions to delete **Region** 2 and leave one Region only.
- Click on Region_1 and set the composition as 0.5C-99.5Fe (at%), The length (Diff. Length) as 100 μm, and the # of Grids as 100.
- The Thermal History is a period of 10 seconds with a constant temperature at 1000 °C;
- Click on Lower Boundary Condition (left edge of Region_1) and select fixed "activity", and set the Value as "a(C:graphite[*])=0.01";
- In the settings shown in Figure 4.14.1, composition profiles at the initial and final stages will be outputted. Click OK to perform calculations.
- By default, dissolution simulation gives time-evolution of particle size as output. In order to display composition profile at desired moments, click the blue "+" button next to the "Moments for Profile Outputs" and input a time value. As shown in Figure 4.14.1, profiles at 1 second and 5 second will be outputted. Click OK to start calculation;
- Details on these options can be found in Pandat User's Guide section 6.4.

• Set the scale of the Y axis to be 0.1-0.6 (at%). Remove composition profile of Fe. The calculated composition profiles are displayed in Figure 4.14.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

• Decarburization process in Fcc phase in the Fe-C system. Lower boundary condition is a fixed carbon activity (0.01, Graphite as the reference state).



Figure 4.14.1: Setting of the simulation condition



Figure 4.14.2: Simulation result of carbon composition profile

5 PanSolidification Examples

Example 5.1 : Solidification Simulation of a Mg-Al alloy under a Given Cooling Rate

Example 5.2 : Prediction of Hot Cracking Susceptibility of an Al-Cu-Mg Alloy

Example 5.3 : Hot Cracking Susceptibility Map of Al-Cu-Mg at Al-Corner

Example 5.1 Solidification Simulation of a Mg-Al alloy under a Given Cooling Rate

Purpose: Learn to perform solidification simulation of a Mg-Al binary alloy under specified solidification conditions using PanSolidification Module. Learn to use the features in PanSolidification Module.

Module: PanSolidification

Thermodynamic and Mobility Database: $AlMg_MB.tdb$

Kinetic Parameters Database: Mg_Alloys.sdb

Batch file: Example_#5.1.pbfx

- Create a workspace and select the PanSolidification module following Pandat User's Guide section 2.1;
- Load SDB file Mg_Alloys.sdb through menu "PanSolidification → Load SDB" or by click icon , select the available alloys: Mg alloys, as shown in Figure 5.1.1;
- Set Solidification simulation conditions as shown in Figure 5.1.2. The alloy composition is Mg-9wt.% Al. The cooling rate is 0.38 K/s is setting in Thermal History solidifying from 680 °C to 300 °C with 1000 second. Solidification rate is set as 50 μm/s. Please pay attention to the units of the time and length when set conditions;
- Then Click OK to perform Solidification simulation. (Detailed description also in Pandat User's Guide 1.17.4).







Figure 5.1.2: Set up conditions for solidification simulation

- The default plot presents the relationship between fraction of solid (fs) and temperature during solidification as shown in Figure 5.1.3.
- The Default table contains many more calculated results as different columns: such as the secondary dendrite arm spacing (arm_space), the amount of Al₁₂Mg₁₇ phase (f_tot (@Al12Mg17)) column, and the composition of Al in the solid phase (w S(Al)). Users

can create other plots from these data.

- The evolution of secondary dendrite arm spacing during solidification is shown in Figure 5.1.4.
- Experimental data can be imported through menu "Table → Import table from File". The comparison of the calculated and experimentally measured Al composition in solid is shown in Figure 5.1.5.



Figure 5.1.3: Default plot showing fraction of solid as a function of Temperature



Figure 5.1.4: The evolution of secondary dendrite arm spacing



Figure 5.1.5: Comparison of the calculated and experimentally measured AI composition profile vs. fs in the primary (Mg) dendrites

Example 5.2 Prediction of Hot Cracking Susceptibility of an Al-Cu-Mg Alloy

Purpose: Learn to perform solidification simulation to predict the hot cracking susceptibility index of an alloy in PanSolidification Module.

Module: PanSolidification

Thermodynamic and Mobility Database: PanAl_TH+MB.pdb

Kinetic Parameters Database: Al Alloys.sdb

Note: In Pandat 2022 version, the property CSI is defined as "-T//sqrt(fs)". In the "Table editor" window, users can directly select CSI or simply type in CSI rather than using the math operation of "-T//sqrt(fs)".

Hot tearing or hot cracking is a serious defect occurred in welding and casting solidification. Cracking usually generated at the end stage of solidification along grain boundaries. Prof. Kou [2005Kou] proposed a criterion to describe the crack susceptibility by using a simple crack susceptibility index (CSI), which is the maximum value of $|dT/d(f_s)^{1/2}|$ at $(f_s)^{1/2} < 0.99$. The CSI criterion has been successfully applied in several AI alloy systems. In this example, users will learn how to perform solidification simulation of an AI-Cu-Mg alloy and output the relationship of $|dT/d(f_s)^{1/2}|$ vs $(f_s)^{1/2}$ directly from Pandat, and thus determine the CSI value of the alloy. Users will also learn to set extra output tables with some specified properties and extra output plots from this example. Commercial database of PanAl_TH+MB.pdb including the thermodynamic and mobility data is required to perform the calculation of this example.

- Create a workspace and select the PanSolidification module following Pandat User's Guide 1.1 section 2.1;
- Load PanAl_TH+MB.pdb through menu "Database → Load TDB or PDB" or by click icon , and then select Al, Cu and Mg three components;
- Load SDB file Al_Alloys.sdb through menu "PanSolidification → Load SDB" or by click icon , select the available alloys: Al alloys.

- Set Solidification simulation conditions as shown in Figure 5.2.1. The alloy composition is AI-5wt.%Cu-2wt.%Mg. The cooling rate is 20 K/s is setting in Thermal History solidifying from 680 °C to 380 °C with 15 second. Temperature gradient is set as 10⁻³ °C/μm. Please pay attention to the units of the time and length when set conditions.
- Set "Extra Outputs table". Click the "Extra Outputs" in Figure 5.2.1, a new interface as shown in Figure 5.2.2 will appear. Click the blue "+" symbol in Figure 5.2.2 to pop out the Table Editor as shown in Figure 5.2.3. From this Table Editor, users can specify and type in properties to output, such as sqrt(fs), -T//sqrt(fs) in this example. -T//sqrt(fs) refers to $-dT/d(f_s)^{1/2}$, as the syntax // means derivative in Pandat software. Note that with this setting, a "generated" table will be created in addition to the Default table (In Pandat 2022, the CSI property is introduced to replace the "-T//sqrt(fs)".)
- Set "Extra Outputs graph". Click the icon "Graph" in "Set extra output" interface as shown in Figure 5.2.2, then click the blue "+" symbol to add extra Graph. An interface as shown in Figure 5.2.4 will appear. Select the "generated" table generated by the previous step. Drag sqrt(fs) from the left column to X axis in the right column; drag T//sqrt(fs) from the left column to Y axis in the right column. Then click OK. Note that with this setting, a "graph" of -T//sqrt(fs) vs. sqrt(fs) will be plotted automatically in addition to the Default graph.
- Then Click OK to perform Solidification simulation. (Detailed description also in Pandat User's Guide 7.4).



Figure 5.2.1: Set up conditions for solidification simulation



Figure 5.2.2: Extra Output interface

Table Editor					×
Table Type: Default ~		Table	Name:	generated	ок
time	^		Colur	nns	Cancel
arm_space			time		
x_S(*)			т		Clear All
w S(*)			fs		
			w(*)		
1. L		<u> </u>	sqrt(fs)		
			-T//sqr	t(fs)	
H_tot		F #			
H_Latent					
Q					
f_tot(@*)					
fw_tot(@*)					
x_tot(*@*)					
w_tot(*@*)					
dTdx(*)					
dxdT(*@*)					
dwdT(*@*)		Doul	ble clic	to enter edit mode;	1
dxdT_L(*@*)	~	In eo Math	lit mode functio	e, press 'Ctrl'+'m' to show list of ons	
Drag and drop available columns to Description: The time of the Particle Example: 'time=100' gets the psd at	setu Size 100	up a ne e Distrit)s. 'time	w table. oution (P e=time' g	Double click property cell to edit. SD). Use 'time' to get all PSDs. jets the last available psd.	

Figure 5.2.3: Define properties in the extra output table

Graph Options				×
Table Source: generated	→ Graph	Name: graph	Is Triangle?	OK Cancel
Available Columns:	Plots:			
T	X Axis	Y Axis	Source	
sart(fs)	sqrt(fs)	-T//sqrt(fs)	generated	
-T//sqrt(fs)				
phase_name				

Figure 5.2.4: Define the axes of the extra graph

- The default plot presents the relationship between fraction of solid (fs) and temperature during solidification as shown in Figure 5.2.5.
- The extra graph specified is plotted automatically as shown in Figure 5.2.6.
- Rescale Figure 5.2.6. as shown in Figure 5.2.7. The hot cracking susceptibility index (CSI) is defined as the maximum value of $-dT/d(f_s)^{1/2}$ with $(f_s)^{1/2} < 0.99$.



Figure 5.2.5: : Default plot showing the relation between temperature and fraction of solid



Figure 5.2.6: Extra plot specified by Extra Graph setting



Figure 5.2.7: Rescale of Figure 5.2.6 showing the maximum point of -T//sqrt(fs) with sqrt(fs) < 0.99.

Example 5.3 Hot Cracking Susceptibility Map of Al-Cu-Mg at Al-Corner

Purpose: In the Example 5.2 : Prediction of Hot Cracking Susceptibility of an Al-Cu-Mg Alloy, Users have learned how to obtain the crack susceptibility index (CSI) value of a single alloy under certain solidification conditions. In this example, users will learn to use High Throughput Calculation (HTC) calculations to obtain a susceptibility index map in Al-Cu-Mg ternary system.

Module: PanSolidification

Thermodynamic and Mobility Database: PanAl TH+MB.pdb

Kinetic Parameters Database: Al_Alloys.sdb

Note: In Pandat 2022 version, the property **CSI** is defined as "-T//sqrt(fs)". In the "Table editor" window, users can directly select CSI or simply type in CSI rather than using the math operation of "-T//sqrt(fs)".

- Create a workspace and select the PanSolidification module. Before calculation, save the workspace in a user assigned folder different from the default workspace. The HTC calculation results will be saved automatically under this folder. (Detailed description also in the Pandat User's Guide section 2.1;
- Load PanAl_TH+MB.pdb through menu "Database → Load TDB or PDB" or by click icon , and then select Al, Cu and Mg three components;
- Load SDB file Al_Alloys.sdb through menu "PanSolidification → Load SDB" or by click icon , select the available alloys: Al alloys;
- Start HTC function through menu "Batch Calc → High Throughput Calculation (HTC)";
- Choose calculation type from the drop-down list of HTC pop-up window and select "pan_ solidification" as shown in Figure 5.3.1;

High Throughput Calculation	×
Choose Calculation Type:	OK
choose calculation type.	OK
pan_solidification ~	Cancel
Max time for each calculation (minutes): 15.0 The calculation will be automatically skipped after timeout.	

Figure 5.3.1: Dialog to choose calculation type of HTC in PanSolidification

- Define the compositional space for HTC simulation. The composition range is set to 0-5 wt.% Cu and 0-5 wt.% Mg, and mouse right click on the composition field of AI to set as the remaining composition, which is shown as -1 in all the composition field of AI, as shown in Figure 5.3.2.;
- Define the solidification conditions for HTC simulation. The solidification conditions with cooling rate of 20 K/s and Temperature gradient is set as 10⁻³ °C/μm, as shown in Figure 5.3.2;
- Set "Extra Outputs table". Click the "Extra Outputs" in Figure 5.3.2, a new interface as shown in Figure 5.3.3 will appear. Click the blue "+" symbol in Figure 5.3.3 to pop out the Table Editor as shown in Figure 5.3.4. From this Table Editor, users can specify and type in properties to output, such as sqrt(fs), -T//sqrt(fs) in this example. -T//sqrt(fs) refers to -dT/d(f_s)^{1/2}, as the syntax // means derivative in Pandat software. Note that with this setting, a "generated" table will be created in addition to the Default table;
- Set "Extra Outputs graph". Using the procedure described in Example 5.2, click the icon "Graph" in "Set extra output", set sqrt(fs) as X axis and -T//sqrt(fs) as Y axis. Then click OK;
- Click "Run HTC" button to perform HTC simulations. (Detailed description also in Pandat User's Guide section 10.2.3).



Figure 5.3.2: Dialog to setup compositional space and solidification conditions for



PanSolidification HTC

Figure 5.3.3: Extra Output interface

Table Editor				×
Table Type: Default ~		Table Name:	generated	ок
time	^	Colur	nns	Cancel
arm_space		time		
x_S(*)		Т		Clear All
w_S(*)		fs		-
fl		w(*)		-
fs		sqrt(fs)	(f _)	-
H tot		-1//sqr	(#\$)	
H Latent		PR		
f tot(@*)				
f_lot(@)				
x_tot("@")				
w_tot(*@*)				
dTdx(*)				
dxdT(*@*)				
dwdT(*@*)		Double click	to enter edit mode;	-
dxdT_L(*@*)	~	Math function	e, press "Ctrl"+"m" to show list of ons	
Drag and drop available columns to	setu	up a new table. I	Double click property cell to edit.	
Description: The time of the Particle Example: 'time=100' gets the psd at	Size	e Distribution (P)s. 'time=time' g	SD). Use 'time' to get all PSDs. ets the last available psd.	

Figure 5.3.4: Define properties in the extra output table

Post Calculation Operation: Result Analysis

- After all calculations have been finished, analyze the results through menu "Batch Calc
 - \rightarrow Result Analysis". User can then analyze the results of the selected HTC calculation

by opening the corresponding workspace as shown in Figure 5.3.5.

Result Analysis -> Cho	oose Workspace	×
Choose Target Workspace	D:_Work\3_Calculations\1_Pandat\PanSolidfication \20191118_T440\20191113_PanSolidfication_HTC\AlCuMg_20K_New \AlCuMg_20K_New.pndx	Continue Cancel
	There are 121 calculations for analysis.	

Figure 5.3.5: : "Result Analysis" popup dialog to choose target workspace

 Define the criteria of the properties as filters for result analysis. As shown in the following Figure 5.3.6, analysis the "generated table", set the condition to find the CSI for each alloy composition, i.e., CSI = MAX(-T//sqrt(fs)) at sqrt(fs)< 0.99;

esult Analysis -> Set Rules				
Target Workspace: D:_Work\3_Calculations\1_Pandat\PanSolidit \AlCuMn 201K New\default	fication\20191118_T440\201	91113_PanSolidific	ation_HTC	Analyze
				Cancel
Common Tables for All Calculations: (only one table can be cho	osen for analysis at one tin	ne)	K New\default\S	
	0/20151115_PariSolidilication	_HTC WCuMg_20		
Common Columns for the Target Table: (drag and drop to char	nge the oder)		Sel/Cir All	
Ts ✓ -17/sqt(ts) T ✓ phase_name ✓ sqt(fs) ✓ arm_space ✓ w(M) ✓ w(Mg) ✓ w(Cu) ✓ -T ✓ sqt(fs)_1				
1. Set an Expression to Select Rows: (choose a template text	and insert)		Insert Selected Column Name	
sqrt(fs)<0.99	└ Insert lext			
2. Get Min/Max Value from Selected Row (choose a template T=MIN(T) CSI=MAX(-T//sqrt(fs))	text and insert) V Insert Text			
Examples: 1. finding the rows with values in a certain range: fl < 1.0 AND f 2. finding the row with minimum T with T=MIN(T).	fl > 0.9;	Empty Row	v Between Results	



- After results analysis, a table which list CSI = MAX(-T//sqrt(fs)) for each alloy composition is generated as shown in Figure 5.3.7;
- Select w%(Cu) as X-axis, press Ctrl then select w%(Mg) and (-T//sqrt(fs)) as Y-axis and Z-axis, respectively, click and the tool bar to generate Figure 5.3.8 which shows the crack susceptibility map for Al-Cu-Mg alloys with cooling rate of 20 K/s;
- The simulated result is comparable with the experimental results shown in Figure 5.3.9.

Pandat Software by CompuTherm, LLC												– 🗆 🗡
Eile Edit View Databases Batch Calc BanPhaseDia	gram <u>P</u> anPr	ecipitation <u>P</u> anO	ptimizer <u>P</u> anDiff	usion PanSolidif	ication Propert	y Jable <u>G</u> raph	Help					
🗔 🖬 🖆 🖬 🕼 🤉 🚔 🖄 🖒 🖄 🗶 🗑 📑 🖲	i 🛃 🗉 🚍	2 🛆 🖸 🕼		1 I I I I I I I I I I I I I I I I I I I	🛐 i 🕞 😹 🌉 i	ا 🛞 🖍 🖳 🥰	🛓 🔍 ព 🔳 🗉	1 🗰 🖉				
Workspace 7 >	🛛 🚅 тов	Viewer 🖉	result_analysis.rep	iont" 🖉 r	esult_analysis_1.re	port* 🖉 I	esult_analysis_2.rep	iort* 🛛 🖉 i	result_analysis_3.rep	port* 🗙 🔝 g	araph_g.graphx	- <u>-</u>
Solidification Simulation_99		CalculationName	AlloyChemistry	т	ts	w(AI)	w(Mg)	w(Cu)	sqrt(fs)	-т	sqrt(fs)_1	-T//sqrt(fs)
Solidification Simulation_100				c ~	mole/mole	% ∽	56 V	% v				
Solidification Simulation_102	P 1	olidification Si	100Al+0Cu+0	660.3200	0.000000	100.0000			0.000000	-933.4700	0.000000	0.000000
Solidification Simulation_103	2											
Solidification Simulation_104	3	olidification Si	99.5AI+0Cu+0	650.1186	0.973761	99.500000	0.500000		0.986793	-923.2686	0.986793	198.4887
Solidification Simulation 106	4											
Solidification Simulation_107	5	olidification Si	99AI+0Cu+1M	642.4693	0.961605	99.000000	1.000000		0.980615	-915.6193	0.980615	220.9515
Solidification Simulation_108	6											
Solidification Simulation 109	7	olidification Si	98.5Al+0Cu+1	629.7008	0.977782	98.500000	1.500000		0.988829	-902.8508	0.988829	459.4995
Solidification Simulation_111	8											
Solidification Simulation_112	9	kolidification Si	98AI+0Cu+2M	619.4919	0.975603	98.000000	2.000000		0.987726	-892.6419	0.987726	520.3589
Solidification Simulation_113	10											
Solidification Simulation 115	11	kolidification Si	97.5Al+0Cu+2	609.2811	0.974813	97.500000	2.500000		0.987326	-882.4311	0.987326	590.3968
Solidification Simulation_116	12											
Workspace Databases	13	Iolidification Si	97Al+0Cu+3M	599.0674	0.974725	97.000000	3.000000		0.987281	-872.2174	0.987281	663.2440
Property 8.2	14											
AL 53	15	kolidification Si	96.5AI+0Cu+3	588.8493	0.974991	96.500000	3.500000		0.987416	-861.9993	0.987416	736.4674
X Annearance	16											
BackgroundColor AppWorkspace	17	kolidification Si	96AI+0Cu+4M	578.6257	0.975449	96.000000	4.000000		0.987648	-851.7757	0.987648	808.8810
GridColor ControlDark	18											
BorderStyle FixedSingle	19	konditication St	95.5AI+0Cu+4	568.3953	0.976033	95.500000	4.500000		0.987944	-841.0403	0.987944	879.7254
DefaultCellStyle DataGridViewCellStyle { BackCe	20	alidžestice Si	0551400-4535	559 1571	0.076716	95,000000	5.000000		0.022200	.921 2071	0.022200	049 2722
✓ Layout	21	Kondin Carolin Gr	adminious annual	330.1371	0.370710	23.000000	3.000000		0.8002.80	-031.3071	0.0002.00	340.3722
AutoSizeColumnsMode None	22	Initidification Si	00 54H+0 5Curt	651 3961	0.969184	99,500000			0.984471	-924 5461	0.984471	217.9860
	2.0			001.0001	0.000101		_		0.001111	0210101		
	25	iolidification Si	994I+0 5Cu+0	641 1777	0.977626	99.000000	0.500000		0.988750	-914 3277	0.988750	444 6552
	26											-
	27	olidification Si	98.5AI+0.5Cu+	630.9614	0.975540	98.500000	1.000000		0.987694	-904,1114	0.987694	600.1732
	28											
	29	olidification Si	98AI+0.5Cu+1	618.1857	0.979015	98.000000	1.500000		0.989452	-891.3357	0.989452	844.6077
	30											
	<											· · · · ·

Figure 5.3.7: A table which lists the CSI = MAX(-T//sqrt(fs)) for each alloy composition is generated after the results analysis



Figure 5.3.8: AI-Cu-Mg crack susceptibility map with cooling rate of 20 K/s



Figure 5.3.9: Experimental crack susceptibility test results