

Nb-Si-Ti 500
 fraction
 Tables, Default table
Batch Export

A screenshot of the Pandat software interface showing a table of calculated results. The window title is 'Pandat - [Pandat1]'. The menu bar includes File, Edit, View, Database, Batch, Calculation, Table, Graph, Window, and Help. The left sidebar shows a tree view with 'Batch File', 'Database', 'Components', 'Phases', 'Calculated Results', 'Section Calculation', 'Graphs', 'Default Graph', and 'Tables'. The 'Default Table' is selected. The table has the following columns: [C], x(Nb), x(Si), x(Ti), G [J], and phase. The data rows are as follows:

[C]	x(Nb)	x(Si)	x(Ti)	G [J]	phase
500.00	0.010000	0.886869	0.103131	-40215.76	DIAM
500.00	0.010193	0.884686	0.105121	-40598.67	DIAM
500.00	0.010579	0.880318	0.109103	-41364.48	DIAM
500.00	0.011351	0.871584	0.117065	-42896.10	DIAM
500.00	0.012895	0.854114	0.132991	-45969.33	DIAM
500.00	0.014440	0.836645	0.148916	-49022.57	DIAM
500.00	0.015984	0.819175	0.164841	-52085.81	DIAM

//

[Begin] [begin] [BEGIN]
[Begin] [End]

[Begin]

[End]
[Begin]

[End]

[Exit]

[Database]	{ "NbSiTi.tdb" }	
[Begin]	{ }	
[End]		
[Exit]		
[CalculationType]	{Point}	
	{Line}	
	{Section}	
	{Projection}	
	{Solidification}	

[Component]	{ Nb Si Ti }	
[Point]	{ T=1000 } { T=1000C } { x(Nb)=0.1 } { x%(Nb)=10 } { w(Nb)=0.05 } { w%(Nb)=5 }	x: mole fraction x%: mole percent w or wt : weight fraction w% or wt%: weight percent 100
[Steps]	{ 10 }	
[Model]	{ Scheil } { Lever }	Lever = equilibrium
[Interval]	{ 100K } { 100C }	100C 100 , 200 , 300 , ...
[Scanline]	{ dx = 0.2, dy = 0.3 }	
[Suspend]	{*}	{*}
[Restore]	{Liquid} {FCC_A1, BCC_A2}	

[Output]	{ fileName="hashi01.dat", format = "T, phaseName, fs, fl, Hm" }	<p style="text-align: center;">## hashi##.dat ##</p> <p>hashi00.dat hahsi01.dat hashi02.dat</p> <p>T : T(C) : phaseName :</p> <p>fs : fl : Hm :</p>
	{format = " f(phase_name), G(phase_name), H(phase_name), S(phase_name), Cp(phase_name) "}	f() : G() : H() : S() : Cp() :
	{format = " f(*), G(*), H(*), S(*) Cp(*) "}	
	{format = " x(comp), x%(comp), w(comp), w%(comp), mu(comp) "}	x() : x% : w : w% : mu() :

[Output]	{ format = “ x(*), x%(*), w(*), w%(*), mu(*) “}	x : x% : w : w% : mu :
	{ format = “ x(comp@phase), x%(comp@phase), w(comp@phase), w%(comp@phase), mu(comp@phase) “} x(Cu@liquid)	
	{ format = “ x(*@phase), x%(*@phase), w(*@phase), w%(*@phase), mu(*@phase) “}	
	{ format = “ x(*@*), x%(*@*), w(*@*), w%(*@*), mu(*@*) “}	
	a(Cu@fcc:liquid) a(*@fcc:liquid) a(*@*:liquid)	Liquid fcc Cu Activity
	Htot	{Solidification}
	ftot(fcc), ftot(*)	{Solidification} phase fraction
	f_tot(fcc), f_tot(*)	{Solidification} phase fraction

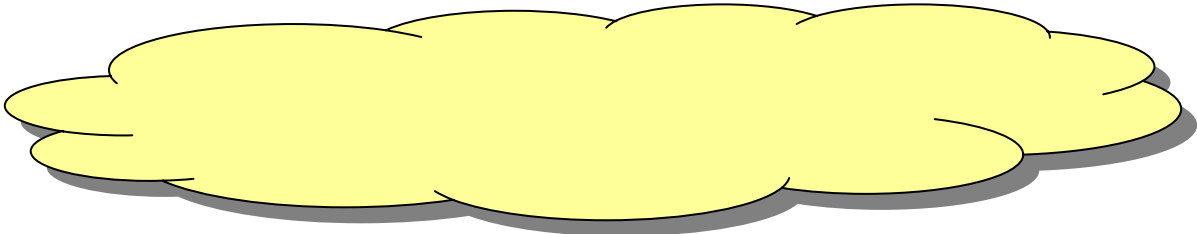
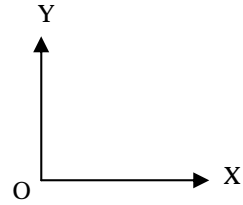
[CalculationType] {Line}

[Point]

1

[CalculationType] {Section}

[Point]

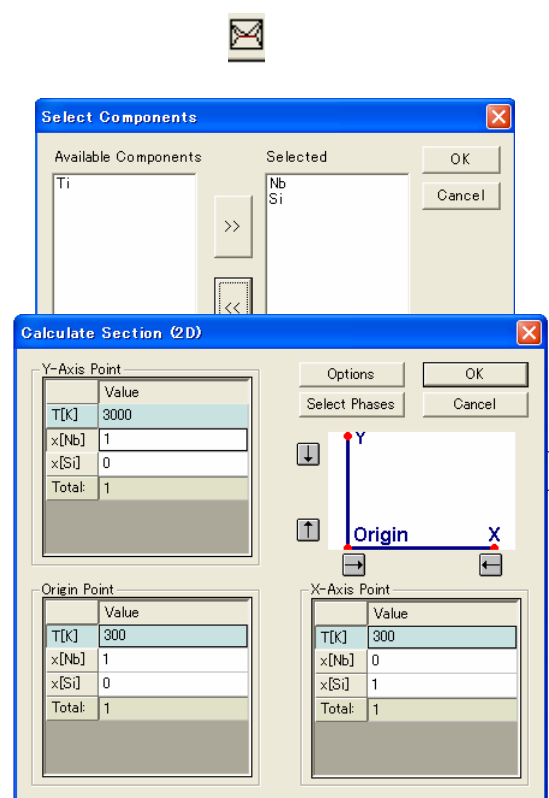


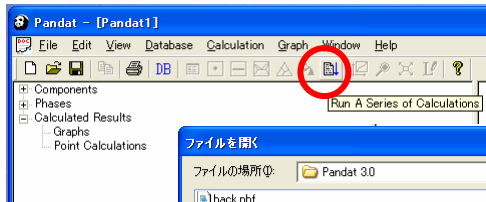
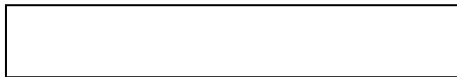
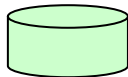
```
[begin] {Nb-Si binary phase diagram}
  [CalculationType] {SECTION}

  [COMPONENT] {Nb Si}

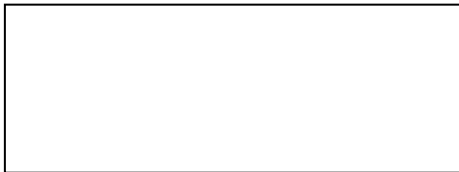
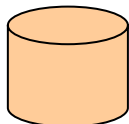
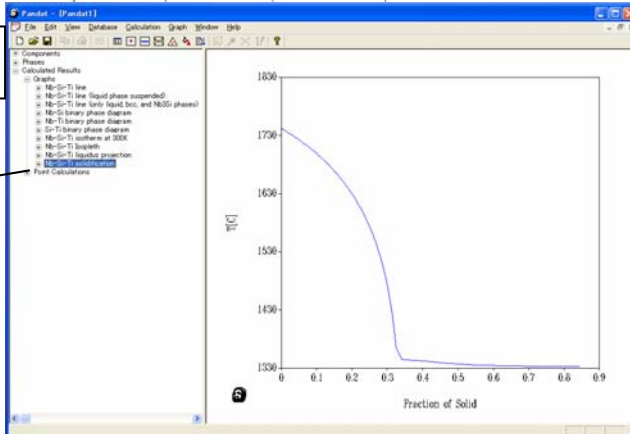
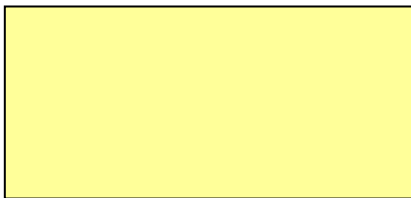
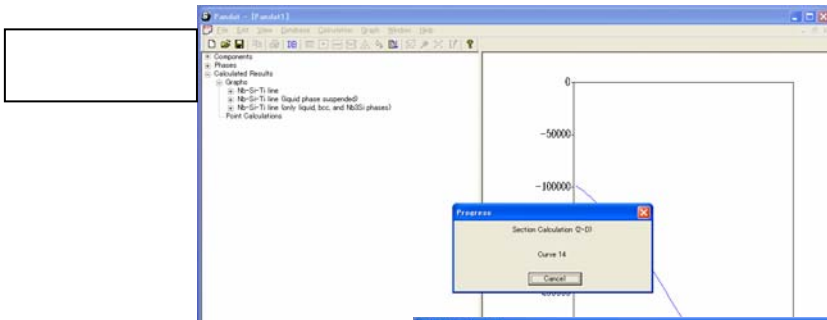
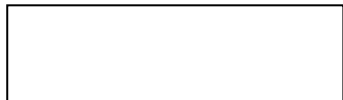
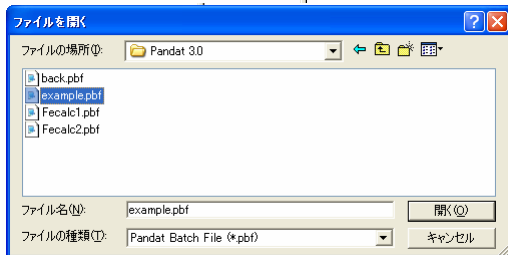
  [POINT] {T = 3000, x(Nb) = 1}
  [POINT] {T = 300, x(Nb) = 1}
  [POINT] {T = 300, x(Si) = 1}

[end]
```





Pandat



Microsoft Excel - Scheil_BSD.dat

1	phaseName	T	B	fs	f1	D	E	F	G	H	I
2											
235	Liquid+NiSi2	1648.18	0.322123	0.677877	37482.1	0.677877	0.322123				
236	Liquid+NiSi2	1646.58	0.322378	0.677622	37419.9	0.677622	0.322378				
237	Liquid+NiSi2	1644.98	0.322629	0.677371	37356.1	0.677371	0.322629				
238	Liquid+NiSi2	1643.39	0.322877	0.677123	37292.4	0.677123	0.322877				
239	Liquid+NiSi2	1641.78	0.323122	0.676878	37229.0	0.676878	0.323122				
240	Liquid+NiSi2	1640.18	0.323384	0.676636	37166.6	0.676636	0.323384				
241	Liquid+NiSi2	1639.59	0.323644	0.676396	37104.4	0.676396	0.323644				
242	Liquid+NiSi2	1638.99	0.323911	0.676159	37042.4	0.676159	0.323911				
243	Liquid+NiSi2	1638.39	0.324184	0.675925	36980.6	0.675925	0.324184				
244	Liquid+NiSi2	1637.79	0.324462	0.675694	36919.1	0.675694	0.324462				
245	Liquid+NiSi2	1637.18	0.324745	0.675466	36857.8	0.675466	0.324745				
246	Liquid+NiSi2	1636.58	0.325032	0.675241	36796.8	0.675241	0.325032				
247	Liquid+NiSi2	1635.98	0.325323	0.675018	36736.0	0.675018	0.325323				
248	Liquid+NiSi2	1635.38	0.325618	0.674798	36675.4	0.674798	0.325618				
249	Liquid+NiSi2	1634.78	0.325916	0.674580	36615.0	0.674580	0.325916				
250	Liquid+NiSi2	1634.18	0.326217	0.674364	36554.8	0.674364	0.326217				
251	Liquid+NiSi2	1633.58	0.326521	0.674151	36494.9	0.674151	0.326521				
252	Liquid+NiSi2	1632.98	0.326827	0.673941	36435.2	0.673941	0.326827				
253	Liquid+NiSi2	1632.38	0.327136	0.673733	36375.7	0.673733	0.327136				
254	Liquid+NiSi2	1631.78	0.327447	0.673528	36316.4	0.673528	0.327447				
255	Liquid+NiSi2	1631.18	0.327760	0.673325	36257.3	0.673325	0.327760				
256	Liquid+NiSi2	1630.58	0.328075	0.673124	36198.4	0.673124	0.328075				
257	Liquid+NiSi2	1629.98	0.328392	0.672925	36139.7	0.672925	0.328392				
258	Liquid+NiSi2	1629.38	0.328711	0.672728	36081.2	0.672728	0.328711				
259	Liquid+NiSi2	1628.78	0.329032	0.672533	36022.9	0.672533	0.329032				
260	Liquid+NiSi2	1628.18	0.329355	0.672340	35964.8	0.672340	0.329355				
261	Liquid+NiSi2	1627.58	0.329680	0.672149	35906.9	0.672149	0.329680				
262	Liquid+NiSi2	1626.98	0.330007	0.671960	35849.2	0.671960	0.330007				
263	Liquid+NiSi2	1626.38	0.330336	0.671773	35791.7	0.671773	0.330336				
264	Liquid+NiSi2	1625.78	0.330667	0.671588	35734.4	0.671588	0.330667				
265	Liquid+NiSi2	1625.18	0.331000	0.671405	35677.3	0.671405	0.331000				
266	Liquid+NiSi2	1624.58	0.331335	0.671224	35620.4	0.671224	0.331335				

Excel

```

////////////////////////////////////
//   Pandat Batch File Example   //
//                               //
//   Copyright 2005 CompuTherm LLC //
//                               //
//           October  1, 2005     //
////////////////////////////////////

```

```

// Refer Pandat 5 manual on the batch command keywords for detail
// any line beginning with "/" is a comment line and will be ignored
// General: [command] {value list}
// All [commands] may be written in upper or lower case,
// [Begin], [begin], [BEGIN], etc are all equivalent

```

```

// [DATABASE] define a database file with extension name as "tdb" or "pdb"
// [DATABASE] is usually put at the beginning of the batch file.
// It can be anywhere in a batch file, but at least before the first [end].
// Different calculations may use different databases.
// A calculation uses the most recently defined database.
[DATABASE] {"NbSiTi.tdb"}

```

// Desine a point calculation

```

// begin the definition of a calculation, with the title of the calculation
// the title will shown on the tree view in PANDAT interface
[begin] {Nb-Si point}

```

```

// point calculation type
[CalculationType] {point}

```

```

// select subsystem components
[COMPONENT] {Nb Si}

```

```

// define the point to be calculated
[POINT] {T = 1000, x(Nb) = 0.2, x(Si) = 0.8}

```

```

//      Other example points:
//      Set units:
//      Temperature: use C or K(default)
//      Composition: use x, x%, w (or wt), w% (or wt%)
//      [POINT] {T = 1000c, x%(Nb) = 30,   x%(Si) = 70}
//      [POINT] {T = 1000C, w(Nb) = 0.2,   w(Si)  = 0.8}
//      [POINT] {T = 1000K, w%(Nb) = 20,   w%(Si) = 80}
//      [POINT] {T = 1000K, wt(Nb) = 0.23, wt(Si) = 0.77}

```

```

//      If composition is not defined for all components,
//      the balance will be equally distributed to the remaining components:
//      [POINT] {T = 1000c, x(Nb) = 0.24}
//      in this case, x(Si) = 0.76

```

```

// end of the definition of calculation
[end]

```

// Define a line calculation with output files

```

[begin] {Nb-Si-Ti line}
// line calculation type
[CalculationType] {line}

// select components
[COMPONENT] {Nb Si Ti}

```

```

// set endpoints of the line
[POINT] {T = 1000C, x(Nb) = 0.2, x(Si) = 0}
[POINT] {T = 1000C, x(Nb) = 0.2, x(Si) = 0.8}

// number of calculation steps
[steps] {80}

// Optional:
[output] {FileName = "line_1.dat", format = "T, x(Nb), x(Si), mu(Nb), f(Liquid)}
// FileName and format are required. In format, fields are separated by ","
[output] {FileName = "line_2.dat", format = "T, x(Nb), x(Si), mu(Nb), f(*)}
// x(component) means overall mole fraction
// f(*) means phase fractions of all related phases
// Separator in output file = TAB
[output] {FileName = "line_3.dat", format = "T, phaseName, x(Nb), x(Si), mu(Nb),
act(*@*:liquid)}
// phaseName: names of phases in the system in equilibrium
// act(*@*:liquid) outputs activities of all components in any phase in
// equilibrium, with liquid as reference
// act(componentName@phaseName:referencePhaseName) is also acceptable

[end]

// Define a line calculation with liquid phase suspended
[begin] {Nb-Si-Ti line (liquid phase suspended)}
  [CalculationType] {line}
  [COMPONENT] {Nb Si Ti}

  // suspend the liquid phase
  [suspend] {liquid}

  [POINT] {T = 3000C, x(Nb) = 0.2, x(Si) = 0.5, x(Ti) = 0.3}
  [POINT] {T = 1000C, x(Nb) = 0.2, x(Si) = 0.5, x(Ti) = 0.3}
  [steps] {50}

[end]

// Define a line calculation with specific phases selected
[begin] {Nb-Si-Ti line (only liquid, bcc, and Nb3Si phases)}
  [CalculationType] {line}
  [COMPONENT] {Nb Si Ti}

  // suspend all phases
  [suspend] {*}

  [restore] {liquid, bcc_a2, NB3SI}
  // restore these phases
  // no need for [restore] {*} since all phases are included before using [suspend]

  [POINT] {T = 3000C, x(Nb) = 0.2, x(Si) = 0.5, x(Ti) = 0.3}
  [POINT] {T = 1000C, x(Nb) = 0.2, x(Si) = 0.5, x(Ti) = 0.3}
  [steps] {50}

[end]

// Define a section calculation
// calculate a binary phase diagram
[begin] {Nb-Si binary phase diagram}
  [CalculationType] {SECTION}
  [COMPONENT] {Nb Si}

```

```

// Specify three points that define the section to be calculated
// Y
// |
// |
// |
// |
// O-----X
    [POINT] {T = 3000, x(Nb) = 1}
    [POINT] {T = 300, x(Nb) = 1}
    [POINT] {T = 300, x(Si) = 1}

    // scanline definition, same as the calculation option in PANDAT interface
    // if this is not given, PANDAT will use internal default value:
    // 1% from the four borders of the section
    [scanline] {dx = 0.01, dy = 0.01, dx = 0.99, dy = 0.99}

    [output] {FileName = "binary_##.dat", format = "phaseName, T, x(Nb), x(Si), f(*)"}
// "binary_##.dat" means file name will be automatically numbered as "binary_00.dat",
// "binary_01.dat", "binary_02.dat", ...
// existing files in the current working folder will not be overwritten.
[end]

[begin] {Nb-Ti binary phase diagram}
    [CalculationType] {SECTION}
    [COMPONENT] {Nb Ti}
    [POINT] {T = 3000, x(Nb) = 1}
    [POINT] {T = 300, x(Nb) = 1}
    [POINT] {T = 300, x(Ti) = 1}
    [output] {FileName = "binary_##.dat", format = "phaseName, T(C), x(Nb), x(Ti), f(*)"}
    // in format, the unit of T can be defined as T(C) or T(K), default is in K
[end]

[begin] {Si-Ti binary phase diagram}
    [CalculationType] {SECTION}
    [COMPONENT] {Si Ti}
    [POINT] {T = 3000, x(Si) = 1}
    [POINT] {T = 300, x(Si) = 1}
    [POINT] {T = 300, x(Ti) = 1}
    [output] {FileName = "binary_##.dat", format = "phaseName, T(K), x(Si), x(Ti), f(*)"}
[end]

// calculate a ternary phase diagram: Nb-Si-Ti Isotherm at 1500K

// Phase diagram: Nb-Si-Ti Isotherm at 1500K
[begin] {Nb-Si-Ti isotherm at 1500K}
    [CalculationType] {SECTION}
    [COMPONENT] {Nb Si Ti}
    [POINT] {T = 1500, x(Nb) = 1}
    [POINT] {T = 1500, x(Si) = 1}
    [POINT] {T = 1500, x(Ti) = 1}
[end]

// Phase diagram: Nb-Si-Ti Isopleth
[begin] {Nb-Si-Ti Isopleth}
    [CalculationType] {SECTION}
    [COMPONENT] {Nb Si Ti}
    [POINT] {T = 3000, x(Nb) = 1}
    [POINT] {T = 300, x(Nb) = 1}
    [POINT] {T = 300, x(Si) = 0.5, x(Ti) = 0.5}
[end]

```

```
// calculate a ternary phase diagram: Nb-Ti-Si liquidus projection
```

```
[begin] {Nb-Si-Ti liquidus projection}
  [CalculationType] {Projection}
  [COMPONENT] {Nb Si Ti}
  [Interval] {T = 200C}
//   [Interval] {T = 200K}
//     // with interval value, PANDAT will calculate the isotherm lines
//     // with given interval value
//     // without interval value, only liquidus projection will be calculated
//     // interval value of T can be defined in unit K or C, default is in K
[end]
```

```
// calculate solidification sequence of a ternary alloy
```

```
[begin] {Nb-Si-Ti solidification}
  [CalculationType] {solidification}
  [COMPONENT] {Nb Si Ti}
  [POINT] {T = 3000, x(Si) = 0.8, x(Ti) = 0.1, x(Nb) = 0.1}
  [model] {Scheil}
//   [model] {Lever}
//     two options for solidification model: scheil or lever

  [output] {FileName = "Scheil_###.dat", format = "phaseName, T, fs, fl, Hm,
ftot(*), f_tot(*)"}
// for solidification simulation, fs is total accumulated fraction of solid, fl is fraction of liquid,
// ftot(*) is accumulated fraction of individual solid phase given in the
// same sequence as "phaseName"
// accumulated only for Scheil, otherwise f(*)=equilibrium fraction.
// f_tot is same as ftot, except that only the phases that solidified
// at the temperature are shown.
[end]

// exit: end of batch calculation
[exit]
```