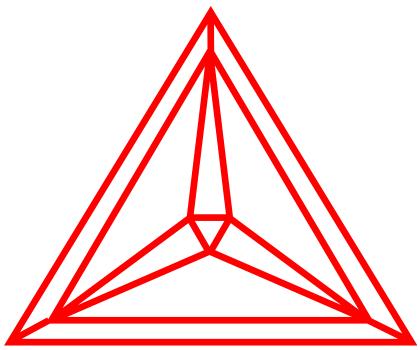
TCW

(Thermo-Calc[®] Windows)

Examples Book

Version 5.0



Thermo-Calc Software AB Stockholm Technology Park Björnnäsvägen 21 SE-113 47 Stockholm, Sweden

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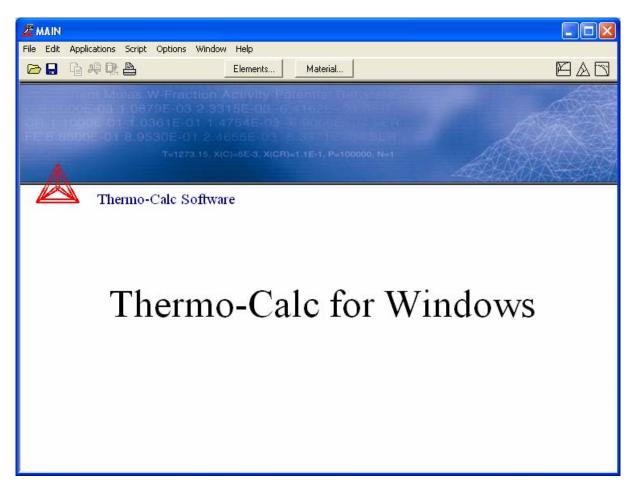
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CONTENT

1	Calculation of the Fe-Cr Phase Diagram	4
2	Plotting Thermodynamic Functions	6
3	Calculation of Single Equilibrium in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel	12
4	Isothermal Section of the Fe-Cr-C System at 1000 K	16
5	Calculation of Isopleth in Fe-8Cr-C System	16
6	Calculation of a Vertical Section for Mixing of Fe-1Cr-0.1C and Fe-20Cr-2C Alloys	24
7	Calculation of Property Diagram of a High Speed Steel	28
8	Calculate Heat and Heat Capacity Variation during Solidification of an Al-Mg-Si Alloy	35
9	Calculate Second Order Transition Line in Al-Fe System	40
10	Calculate CaO-SiO2 System	51
11	Calculate A3 Temperature and Its Dependence on Alloying Element	55
12	Mapping of Univariant Equilibria of Liquid in the Fe-C-Cr System	58
13	Plotting of Partial Pressure of Gas Species Along Solubility Lines in As-Ga Phase Diagram	61
14	Scheil-Gulliver Simulation of Solidification for an Al-based Alloy	65
15	Scheil-Gulliver Simulation of Solidification for a Steel with Back Diffusion of Carbon in Solid Phases	69
16	Calculation of Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel	75
17	Calculation of Speciation of a Gas	85
18	Calculation Using Script and how to Implement a Figure to a Word/PowerPoint file	90

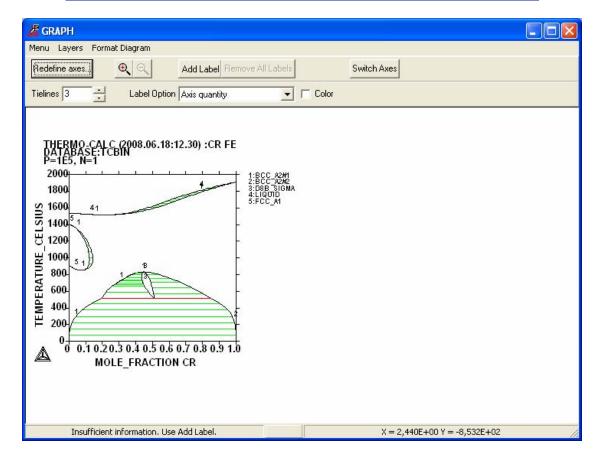
1 Calculation of the Fe-Cr Phase Diagram

- 1. Open the TCW program by double-clicking its shortcut icon.
- **2.** Click the \bowtie button.



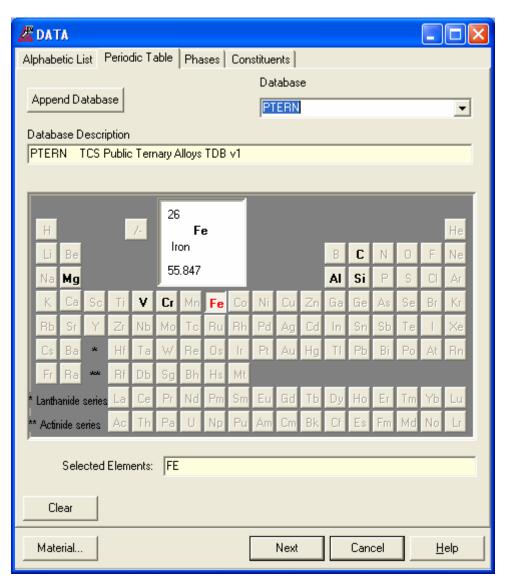
- 3. Select the elements *Fe* and *Cr* from the periodic table.
- 4. Click the *Phase Diagram* button.
- 5. The Fe-Cr binary phase diagram will be calculated and plotted automatically.

BINARY PHASE		AM													
eriodic Table Phases															
Database: TCB	N				7										
,															
TCBIN TC Binary Solutions Database v1															
			_	_	_	_	_	_	_	_	_	_	_		1
		24													
H		С	Cı hromi	-										He	
Li Be		51	.9961	1					В	С	Ν	0	F	Ne	
Na Mg						_	_	_	Al	Si	Ρ	S	CI	Ar	
K Ca Sc	Ti V	Cr	Mn		Co			_		Ge			Br	Kr	
	Zr Nb		_	Ru			-	Cd		Sn	Sb		-	Xe	
	Hf Ta		Re			Pt	Au	Hg	ΤI	Pb	Bi	Po	At	Rn	
	Яf Db .a Ce	Sg				Eve	Gd	Th	Du	Ua	E.	Tre	VE	Lu	
-	.a Ce No Th	_	Nd	Np		Am			_			Tm Md			
Actinide series		1.0		TYP:	1 01		- Conn	BIN	OI.	20		THIS.	110		
Phase Diagram	i-curves		A	\-cur	ves		Phas	e Fra	ction.			Can	cel	ŀ	<u>H</u> elp



2 Plotting Thermodynamic Functions

1. Choose the *Elements* button in the MAIN window. Select *Fe* from the *PTERN* database. Press *Next*.



2. For a unary system, all conditions are already predefined when the CONDITIONS window opens. Accept the present conditions and press *Next*.

Number of Missing Conditions	0	Set Reference Sta Components	te User Symbo Advanced Conditi	
Temperature	[1000 К		Compositio	on Unit Mass-percent 💌
Pressure	101325 Pa		nponent Value	Condition % Composition -
System Size Moles	1 m	bles	-	
All Defined Conditions in SI Units T=1000 P=1.01325E5 N=1 Delete Fixed Phases				
Back Script Managemen	t Show Value	Compute	Next	Cancel <u>H</u> elp

3. Define axis 1 as *T* and axis 2 as *NONE*. Enter min and max values as 27 resp. 1700 K. (The default temperature unit can be changed in the *Options* menu in the MAIN window.) Click *Next* to start the stepping.

A MAP/STEP DEFINITION	
Axis 1 Variable T Min (K) No of steps Max (K) 27 50 1700	Axis 2 Variable NONE Min (K) No of steps Max (K)
Image: Previous Calculation Image: Step Separate Image: Generate Automatic Start Points Image: Step Separate	arate
Back Script Management	Next Cancel <u>H</u> elp

4. In order to plot thermodynamic functions for the individual phases, select the *User Symbols* tab in the DIAGRAM window and type in following four functions and one table, using the *Type*, *Name* and *Expression* boxes. Click *Add Symbol* after each definition. Function GF=GM(FCC)

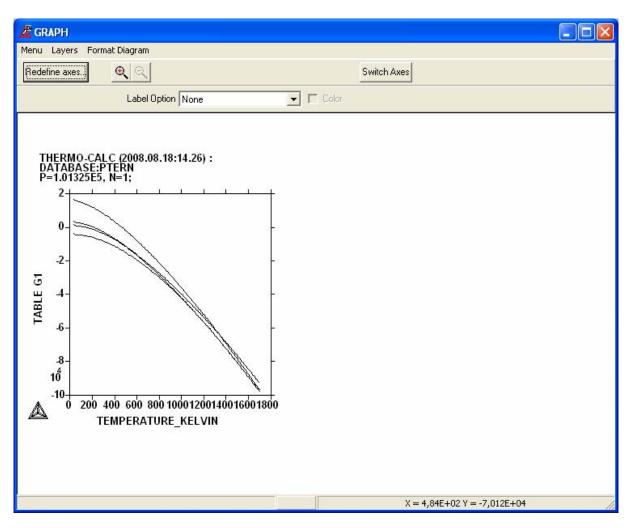
runcuo	$\Pi \cup \Pi - \cup M(\Pi \cup U)$
	GB=GM(BCC)
	GH=GM(HCP)
	GL=GM(LIQUID)
Table	G1=GF,GB,GH,GL

Z DIAGRAM DEFINITION		
Diagram Axes Scaling User Symbols Advanced Diagra	M Axes All Defined Symbols GF=GM(FCC_A1) GB=GM(BCC_A2) GH=GM(HCP_A3) GL=GM(LIQUID) G1=GF,GB,GH,GL	
	Type Name Table Expression Add Symbol Delete Symbol Tabulate	
X-Axis Text 🔽 Auto		Automatic
Back	☐ New Graph Window	Next Cancel <u>H</u> elp

5. Open the *Advanced Diagram Axis* tab and choose the table G1 for the Y-axis. The X-axis needn't be changed. Click *Next* to plot.

Z DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	
J	
X-Axis	Y-Axis
Temperature and Pressure Potential and Activity Temperature Kelvin	Temperature and Pressure Potential and Activity
Compositional Variables Phase Variables	Compositional Variables Phase Variables
Energy Variables Additional Quantities	Energy Variables Additional Quantities
Partial Derivatives	Partial Derivatives
User Symbols	User Symbols
X:Axis Text Automatic TEMPERATURE_KELVIN	Y-Axis Text 🔽 Automatic
Back	w Next Cancel <u>H</u> elp

6. Click *Redefine* to enter some other functions to make the small difference in Gibbs energy between the solution phases more visible.



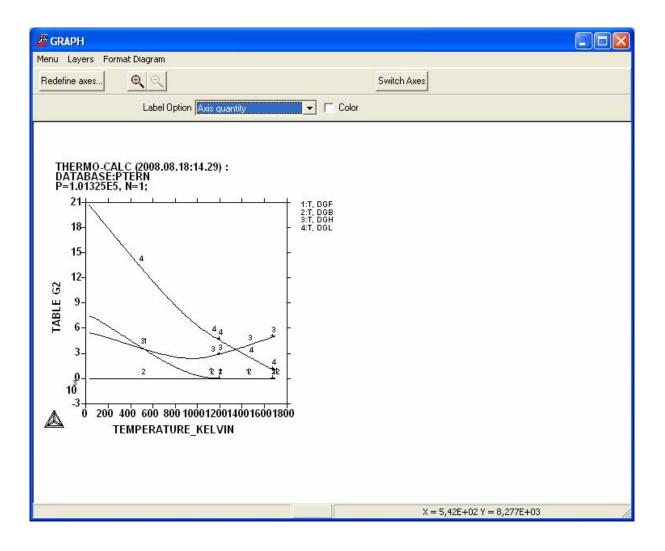
- 7. Type in new functions *DGF*, *DGH*, *DGL* which are the difference between the Gibbs energy for each phase compared with the Gibbs energy of the BCC phase. *DGB* will naturally be zero. Enter the functions in a table *G2*.
- Function DGF=GF-GB DGB=GB-GB DGH=GH-GB DGL=GL-GB

Table G2=DGF,DGB,DGH,DGL

Select Advanced Diagram Axis and change the Y-axis variable to G2 and click next to plot.

Z DIAGRAM DEFINITION		
Diagram Axes Scaling User Symbols Advanced Diagra	m Axes	
	All Defined Symbols GF=GM(FCC_A1) GB=GM(BCC_A2) GH=GM(HCP_A3) GL=GM(LQUID) DGF=GF-GB DGB=GB-GB DGI=GL-GB G1=GF,GB,GH,GL Type Name Function DGF,DGB,DGH,DGL Add Symbol	Tabulate
X-Axis Text 🔽 Autor		ext 🔽 Automatic
TEMPERATURE_KELVIN	NPM(*)	
Back	🦳 New Graph Window	Next Cancel <u>H</u> elp

8. Select *Axis quantity* from the *Label Option* list.



3 Calculation of Single Equilibrium in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel

- 1. Start TCW and click *Elements* on the MAIN window.
- 2. In the DATA window, choose the *TCFE6* database and select the following six elements; Fe, Mn, Si, C, Cr, Ni. Finish by clicking *Next*.

🖉 DATA																	×
Alphabetic List Periodic Table Phases Constituents																	
Append Database																	
Database Description TCFE6 TCS Steels/Fe-Alloys Database v6																	
	L3 3	leeis,	rre-A	noys	Data	nase	VD										
29 H /- Cu He																	
Li Be					oppe	ſ					B	C	N	0	F	Ne	
Na Mg				63	.546						AI	Si	Ρ	S	CI	Ar	
K Ca	Sc	Ti	v	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb Sr	Y	Zr	NЬ	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te		Xe	
Cs Ba	*	Hf	Ta	w	Re	Os	Ir	Pt	Au	Hg	ΤI	Pb	Bi	Po	At	Rn	
Fr Ra	skok	Rf	Db	Sg	Bh	Hs	Mt	_	_	_	_	_	_	_	_	_	
* Lanthanide :	series	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	ТЬ	Dy	Ho	Er	Tm	YЬ	Lu	
** Actinide se	eries	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	
Selected Elements: FE MN SI C CR NI																	
Clear	Clear																
Material									Next			Can	cel		H	elp	

3. To do an equilibrium calculation at 800 °C, enter this temperature in the *Temperature* box. (The default temperature unit can be changed in the *Options* menu in the MAIN window). Then enter the composition values in mass-percent for all the elements except the major Fe in the boxes on the right side of the CONDITIONS window: 0.4 Mn, 0.5 Si, 0.2 C, 1.5 Cr, and 3 Ni. Clicking *Next* will move you to the STEP/MAP DEFINITION window, choose instead *Compute* and look in the MAIN window.

Number of Missing Conditions 0 Temperature 800 Pressure 101325 System Size Moles 1 All Defined Conditions in SI Units	— c	Set Reference State Components	User Symbols Advanced Conditions		tart Values
T=1073.15 P=1.01325E5 N=1 W(MN)=4E-3 W(SI)=5E-3 W(CR)=1.5E-2 W(NI)=3E-2	Pa moles	Redefine Component FE MN SI C CR NI	Composition U Value 0,4 0,5 0,2 1,5 3	Jnit Mass % Co % Co % Co % Co % Co	Phases
Fixed Phases Back Script Management Show Value		Compute	Next	Cancel	Help

4. The result of this calculation is now shown in the MAIN window. The listing is equivalent to the output from the LIST-EQUILIBRIUM command in Thermo-Calc Classic. Under the present conditions, only fcc phase (austenite) is present as a stable phase. Note that the CONDITIONS window is still open for further calculations.

🖉 MAIN											
File Edit Applications	Script Options Window	/ Help									
	A	Elements Mate	erial								
🚜 Eq 1											
Database: TCFE6					^						
Number of moles of	K (800C, 1472F), Pri f components 1,000([,] -5,05909E+04, Ent	00E+00, Mass 5,51	867E+01	06							
Component	Moles	Mass-Fraction	Activity	Potential	Ref.State						
C CR FE MN NI SI	9,1894E-03 1,5920E-02 9,3284E-01 4,0181E-03 2,8209E-02 9,8246E-03	2,0000E-03 1,5000E-02 9,4400E-01 4,0000E-03 3,0000E-02 5,0000E-03	3,5852E-02 3,6447E-04 4,7357E-03 5,3430E-06 6,9330E-05 1,2756E-09	-2,9698E+04 -7,0642E+04 -4,7760E+04 -1,0832E+05 -8,5450E+04 -1,8274E+05	SER SER SER SER SER SER SER						
FCC_A1#1 STATUS ENTERED Driving force 0,0000E+00 Number of moles 1,0000E+00, Mass 5,5187E+01 Mass fractions: FE 9,44000E-01 CR 1,50000E-02 NI 3,00000E-02 SI 5,00000E-03											
5					× ≥ .::						

5. A more interesting calculation is to find out at what temperature bcc (ferrite) becomes stable for this steel (the A3 line). Go back to the CONDITIONS window and take away the condition on temperature (mark T=800 in the list and click *Delete*, or clear the *Temperature* box). The degrees of freedom will change from zero to one.

Number of Missing Conditions	1	Set Reference State Components	User Symbols	Start Values Phases
Number of Missing Conditions Temperature Pressure System Size Moles All Defined Conditions in SI Units P=1.01325E5 N=1 W(NI)=4E-3 W(SI)=5E-3 W(CR)=1.5E-2 W(NI)=3E-2 Delete Fixed Phases	1 C 101325 Pa 1 moles	Components Redefine Component	Advanced Conditions	
				1 1
Back Script Managemen	t Show Value	Compute	Next Cano	el <u>H</u> elp

6. Now select the *Phases* tab on the right hand side of the window. Click the *BCC_A2* phase and select the status *FIXED* in the *Phase Status* box. Type the value θ (zero) in the box right next to it. This will specify that the bcc phase must take part in the equilibrium, which changes the degrees of freedom back to zero again. Zero amount of the bcc phase will find the bcc/bcc+fcc phase diagram line, which is where bcc start to form. Press *Compute*.

Number of Missing Conditions	0		Set Reference State Components	User Symbols Advanced Condition	5	Start Values Phases
Temperature Pressure System Size Moles 💌	101325	C Pa moles	Phases LIQUID AL4C3 BCC_A2 CEMENTITE CHI A12	Status ENTERED ENTERED FIXED ENTERED ENTERED	Moles 0.00 0.00 0.00 0.00 0.00	
All Defined Conditions in SI Units P=1.01325E5 N=1 W[MN]=4E-3 W[SI]=5E-3 W[C]=2E-3 W[C]=2E-3 W[C]=3E-2 W[NI]=3E-2			CH1_A12 CR3SI DIAMOND_FCC_A4 FCC_A1 FCC_A1#2 FE2SI FE4N_LP1 FE8SI2C FECN_CHI GRAPHITE Phase Status:	ENTERED ENTERED ENTERED ENTERED ENTERED ENTERED ENTERED ENTERED	0.00 0.00 1.00 0.00 0.00 0.00 0.00 0.00	
Fixed Phases BCC_A2 = 0.00				Phase Conditions Add Composition		
Back Script Managemen	t Show Value		Compute	Next	Cancel	<u>H</u> elp

7. The new equilibrium is shown in the MAIN window. Use the scrollbar to view the entire listing. The A3 temperature for this steel is 756 °C.

🔏 MAIN							
	Script Options Window	/ Help					
	4	Elements Mate	rial				
🖉 Eg 2							
Conditions: P=1.01325E5, N=1, W(MN)=4E-3, W(SI)=5E-3, W(C)=2E-3, W(CR)=1.5E-2, W(NI)=3E-2 DEGREES OF FREEDOM 0 Temperature 1029K (756C, 1393F), Pressure 1,013250E+05							
Number of moles (of components 1,000(y -4,73427E+04, Ent	00E+00, Mass 5,518	367E+01	D6			
Component	Moles	Mass-Fraction	Activity	Potential	Ref.State		
C CR FE MN NI SI	9,1894E-03 1,5920E-02 9,3284E-01 4,0181E-03 2,8209E-02 9,8246E-03	2,0000E-03 1,5000E-02 9,4400E-01 4,0000E-03 3,0000E-02 5,0000E-03	4,6760E-02 4,3309E-04 5,4708E-03 5,8404E-06 7,6121E-05 7,5297E-10	-2,6209E+04 -6,6274E+04 -4,4570E+04 -1,0312E+05 -8,1153E+04 -1,7977E+05	SER SER SER SER SER SER		
Number of moles (Mass fractions: FE 9,67624E-01	Number of moles 0,0000E+00, Mass 0,0000E+00						
Mass fractions:	STATUS ENTERED 1,0000E+00, Mass 5,5 CR 1,50000E-02 M	5187E+01	orce 0,0000E+00		_		
NI 3,00000E-02	SI 5,00000E-03 C	2,00000E-03			▼ ≥		

4 Isothermal Section of the Fe-Cr-C System at 1000 K

- 1. Here we use the ternary module in TCW, which is opened by clicking \triangle
- 2. Select the *PTERN* database in the *Database* box and click the three elements in the periodic table; Cr, Fe, and C.
- 3. Click *Isothermal Section* to continue.

🖉 TER	RNARY	1																	k
Periodic Table Phases																			
	tabase: ERN	PT TCS F	'ERN Public		nary A	Alloys	TDB												
	H				6	C arbor											Не		
	Li Be											В	C	Ν	0	F	Ne		
1	Na Mg	,										AI	Si	Ρ	S	CI	Ar		
	K Ca	Sc	Ti	۷	Cr	Mn	Fe	Co	Ni	Си	Zn	Ga	Ge	As	Se	Br	Kr		
E F	Rb Sr	Y	Zr	NЬ	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	-	Xe		
	Cs Ba	*	Hf	Ta	W	Re	Os	lr.	Pt	Au	Hg	ΤI	Pb	Bi	Po	At	Rn		
- IL	Fr Ra	state	Bf	DЪ	Sg	Bh	Hs	Mt		_	_		_	_	_	_	_		
* La	anthanide	e series			Pr	Nd		Sm			ТЬ	_	Ho	_	Tm				
** /	Actinide :	series	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		
	Selected Elements: CR FE C																		
Isoth	ermal S	ectior		Mon	ovaria	ant Li	nes	Li	quidu	is Pro	ijectio	on			Canc	el	Ŀ	<u>l</u> elp	

4. When the temperature box appears the temperature is set to 726.85 °C (1000 K). The default unit may be changed to K in the *Options/Units* menu in the MAIN window. Click *Next* to proceed.

🔏 TEMPERATURE
Temperature 726.85 C
Use Global Minimization Next Cancel

5. To plot the isothermal section click *next*. By placing the mouse cursor at a certain region in the diagram the name of the phase(s) stable in that region is displayed in the lower left corner of the GRAPH window.

Caraph Caraph	
Menu Layers Format Diagram	
Redefine axes. Add Label Remove All Labels	Switch Axes
Tielines 2 📩 Label Option None 💌 🔽	Color
THERMO-CALC (2008.06.18:15.00) :CR-FE-C at T=1000 K DATABASE:PTERN T=1000, P=1E5, N=1; 1.0+ 0.9-	
0.82 0.72 0.65 0.65 0.65 0.0.7 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.63 0.64 0.14	
CEMENTITE+GRAPHITE+M7C3	X = 4,069E-01 Y = 4,167E-01

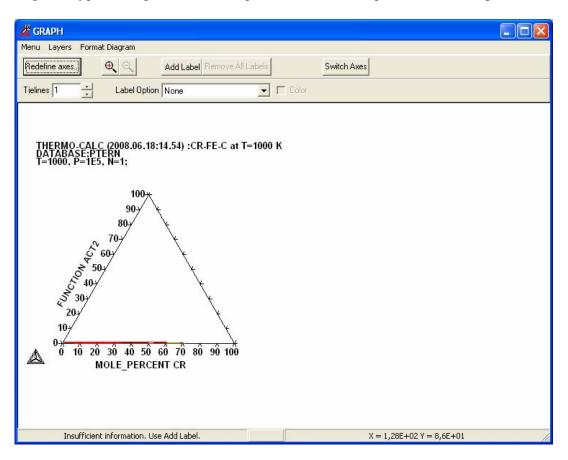
6. Press *Redefine* to plot amount of Cr vs. activity of carbon instead. To get easily understandable activity values, open the User Symbols tab and enter a function for the activity of carbon referred to the current temperature: ACT2=ACR(C,GRAPHITE).

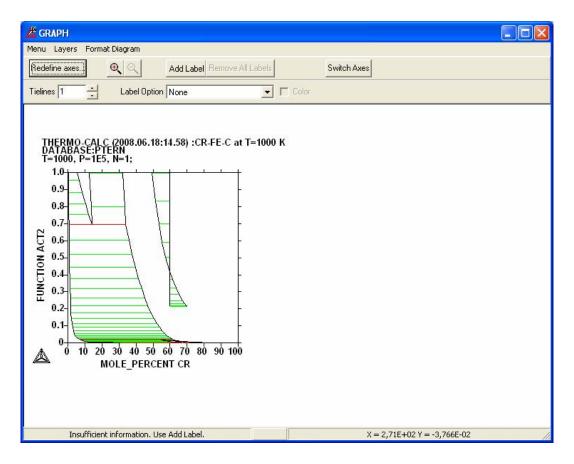
Z DIAGRAM DEFINITION			
Diagram Axes Scaling User Symbols Advanced Diag	am Axes		
	All Defined Symbols		
	Type Function	Name	
	Add Symbol Delete	Symbol Tabulate	
X-Axis Text IV Aut	omatic	Y-Axis Text MOLE_FRACTION C	V Automatic
Back	🔲 New Graph Window		Next Cancel <u>H</u> elp

7. Next select *Advanced Diagram Axis* and set the X-Axis variable to Mass Percent Cr and the Y-Axis variable to the function ACT2. Click next to plot.

A DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	
CR-FE-C at T=1000 K	
-X-Axis	Y-Axis
Temperature and Pressure Potential and Activity	Temperature and Pressure Potential and Activity
For Component	
Compositional Variables Phase Variables CR	Compositional Variables Phase Variables
Mole-percent v	
Energy Variables Additional Quantities	Energy Variables Additional Quantities
	T T
Partial Derivatives	Partial Derivatives
User Symbols	User Symbols
	ACT2
X-Axis Text 🔽 Automatic	Y-Axis Text TAutomatic
MOLE_PERCENT CR	FUNCTION ACT2
· · ·	
Back	W Next Cancel Help

8. Change the type of diagram from triangular to normal using the *Format Diagram* menu.





5 Calculation of Isopleth in Fe-8Cr-1C System

- **1.** Open the TCW program.
- 2. Click *Elements*.
- **3.** Select *PTERN* from the *Database* list and then click alloy elements *C*, and *Cr*, *and Fe* in the periodic table. Click *Next*.
- **4.** Specify the concentrations of C and Cr as *1* and *8 mass-percent*, respectively and accept the default temperature. Click *Next*.

Number of Missing Conditions	0	Set Reference State Components		Values hases
Temperature	1000 к		Composition Unit Mass-perc	ent 💌
Pressure	101325 Pa	Redefine Component	Value Con	dition sition 💌
System Size Moles 💽	1 mole	s CR FE	8 % Compo % Compo	sition 💌
-All Defined Conditions in SI Units T=1000 P=1.01325E5 N=1 W(C)=1E-2 W(CR)=8E-2 Delete	1			
-Fixed Phases		_		
Back Script Managemen	t Show Value	Compute	Next Cancel	Help

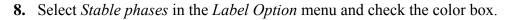
5. The default mapping axis, W(C) and T are just what we are interested in and the minimum and maximum values for them are OK. Click *Next*.

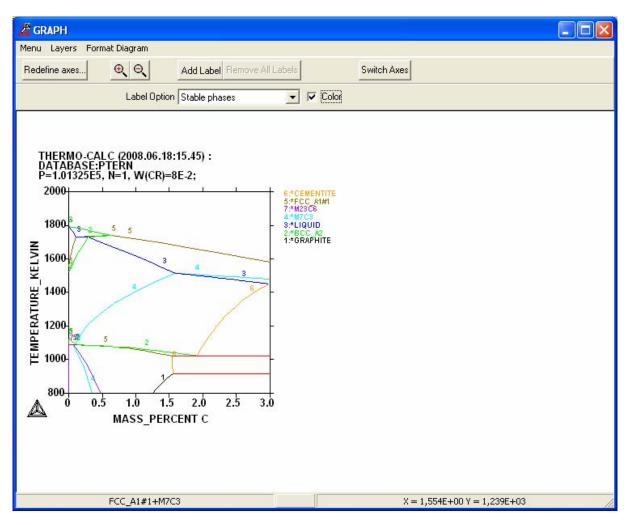
A MAP/STEP DEFINITION	
Axis 1 Variable W(C) Min (%) No of steps Max (%) 0 50 100	Axis 2 Variable T Min (K) No of steps Max (K) 773,1 50 2273
Image: Overwrite Previous Calculation Image: Step Separate Automatic Start Points Image: Back Script Management	rate Next Cancel <u>H</u> elp

6. After the calculation is finished, the DIAGRAM DEFINITION window pops up. The mapping axes are shown as the default plotting X-axis and Y-axis now. Click *Next*. The following diagram is plotted.

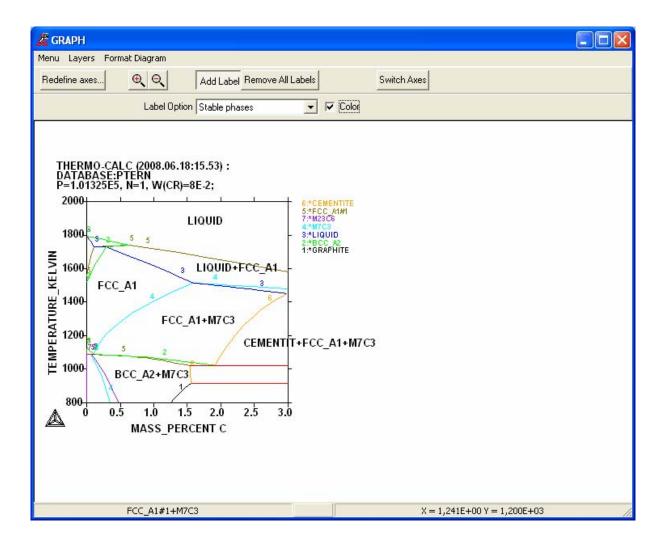
🖉 GRAPH	
Menu Layers Format Diagram	
Redefine axes. Add Label Remove All Labels	Switch Axes
Label Option None	Color
THERMO-CALC (2008.06.18:15.12) : DATABASE:PTERN P=1.01325E5, N=1, W(CR)=8E-2; 2400 2000 1800 1400 1200 1400 1200 0 10 20 30 40 50 60 70 80 90 100 MASS_PERCENT C	
CEMENTITE+GRAPHITE+M7C3	X = 5,5E+01 Y = 1,200E+03

7. Choose *Scaling* from the *Format Diagram* menu to open the Scaling tab on the DIAGRAM DEFINITION window. Specify the min value for X-axis as θ and max as 3, and for Y-axis as 800 and 2000. Click *Next*.





9. The phase regions can also be labeled by first clicking *Add Label* and then clicking in the phase fields you want to label. In the following diagram, the *Liquid*, *Fcc_A1*, *Liquid*+*Fcc_A1*, *Fcc_A1*+*M7C3*, *Cementite*+*Fcc_A1*+*M7C3*, *Bcc_A2*+*M7C3* phase regions have been labeled.



6 Calculation of a Vertical Section for Mixing of Fe-1Cr-0.1C and Fe-20Cr-2C Alloys

- **1.** Open the TCW program.
- 2. Click *Elements*.
- **3.** Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *C*, and *Cr* in the periodic table. Click *Next*.
- 4. A vertical section across the Fe-1Cr-0.1C and Fe-20Cr-2C alloys can be mapped by varying either Cr or C content and temperature and keeping the constraint condition between W(CR) and W(C): W(CR)/W(C)=(20-1)/(2-0.1)=19/1.9=10, i.e. W(CR)-10W(C)=0. Supposing we are varying Cr content, first set an arbitrary concentration of Cr between these two alloys, say 15, then click the *Advanced Conditions* tab, enter the equation W(CR)-10W(C)=0 in the User Defined Conditions box. Click Next.

Number of Missing Conditions	1	Set Reference State Components	User Symbols Advanced Conditions	Start Values
Temperature	1000 K	Bedefine Componen		Mass-percent 💌 Condition
Pressure System Size Moles 💽	101325 Pa	FE		Composition -
	T. moles	CR	15 %	Contraction of the local division of the loc
All Defined Conditions in SI Units				
=1000 P=1.01325E5 N=1 ₩(CR)=0.15				
Delete]			
-Fixed Phases				
Back Script Managemen	t Show Value	Compute	Next Ca	ncel <u>H</u> elp

Number of Missing Conditions	1	Set Reference State Components	User Symbols	Start Values Phases
Temperature Pressure	1000 K 101325 Pa 1 moles	Gibbs Energy Helmholtz Energy Enthalpy Entropy Volume User Defined Conditions W(CR)-10W(C)=0	Normalization: per mole per mole per mole per mole per mole	 J/mol J/mol J/mol/K m3/mol
Back Script Management	Show Value	Compute	Next Cancel	<u>H</u> elp

5. Define the mapping ranges: from 0 to 20%Cr and 600 to 1900 K. Click Next.

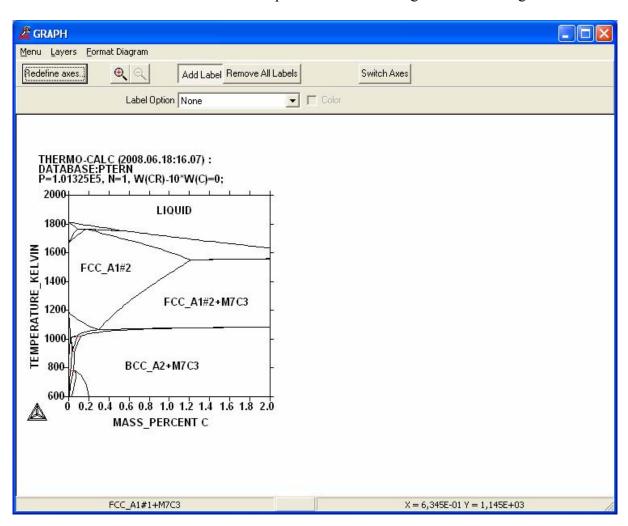
A MAP/STEP DEFINITION	
Axis 1 Variable W(CR) • Min (%) No of steps • Max (%) 0 50 20	Axis 2 Variable T Min (K) No of steps Max (K) 600 50 1900
✓ Overwrite Previous Calculation ☐ Step Sepa ✓ Generate Automatic Start Points	arate
Back Script Management	Next Cancel <u>H</u> elp

6. Click *Next* and the vertical section is plotted. One can label phase regions by first clicking *Add Label* and clicking in the phase regions one wants to label. The following is a labeled diagram.

Z GRAPH	
Menu Layers Format Diagram	
Redefine axes. (Add Label Remove All Labels	Switch Axes
Label Option None	Color
THERMO-CALC (2008.06.18:16.03) : DATABASE:PTERN P=1.01325E5, N=1, W(CR)-10°W(C)=0; 1000 1600 1600 $FCC_A1#2$ $FCC_A1#2$ $FCC_A1#2 + M7C3$ 1000 $BCC_A2 + M7C3$ 600 0 2 4 6 8 10 100 10000 10000 10000 10000 1	
BCC_A2+M7C3	X = 1,5E+01 Y = 7,57E+02

7. Of course, one can now also plot C wt.% vs T. Click *Redefine* to change the X-Axis.

A DIAGRAM DEFINITION			
Diagram Axes Scaling User Symb	ols 🛛 Advanced Diagram Axes 📄		
Temperature L	Init © Celsius © Kelvin © Fahrenheit	Composition Unit Moles Mass	Percent
Diagram Title			
X-Axis Variable Composition	•	Y-Axis Variable Temperature	•
For Compone	nt For Phase For Phase SYSTEM	For Component	For Phase
X-Axis Text MASS_PERCENT C	V Automatic	Y-Axis Text TEMPERATURE_KELVIN	, ✓ Automatic
Back	🥅 New Graph W	/indow Next	Cancel <u>H</u> elp



8. Click *Next* and the vertical section is plotted. The following is a labeled diagram.

7 Calculation of Property Diagram of a High Speed Steel

- 1. Click the *Elements* button in the MAIN window, and select *TCFE6* in the *Database* box in the DATA window. Select the eight elements Fe, C, Cr, Si, Mn, W, Mo and V. Then click *Next*.
- 2. Define a single equilibrium in the CONDITIONS window. Put the temperature to 1000 °C (the default settings for the temperature unit can be changed under the *Options* menu in the MAIN window), and the compositions to 0.9 % C, 4 % Cr, 0.3 % Mn, 5 % Mo, 0.3 % Si, 2 % V and 8 % W (mass %). Fe is the balance, leave the box empty. Now click *Next*.

Number of Missing Conditions	0	Set Reference Components		User Symbols Advanced Conditions	1	Start Values Phases
Temperature	1000 0	2			Init Ma	ass-percent 💌
Pressure	101325 F	Pa Redefine	Component FE	Value	%	Condition
System Size Moles 💌	1 r	noles	C	0,9	%	Composition -
	N		CR	4	%	Composition 💌
			SI	0,3	%	Composition -
All Defined Conditions in SI Units			MN	0,3	%	Composition 💌
T=1273.15			W	8	%	Composition 💌
P=1.01325E5	<u>^</u>		MO V	5	%	Composition 💌
N=1 W(C)=9E-3 W(CR)=4E-2 W(SI)=3E-3 W(M)=3E-3 W(W)=8E-2 W(MO)=5E-2 W(MO)=5E-2 W(MO)=5E-2			45	-	*	Composition <u></u>
Fixed Phases						
Back Script Managemen	t Show Value	Compute		Next	Cancel	

3. Before the axes are defined in the MAP/STEP window, it is useful to take a look at the calculated equilibrium in the MAIN window to see that it is reasonable. In this case we have a metallic fcc phase (85 mole percent) and two carbides: FCC_A1#2 and M6C. The second fcc phase is a MC carbide with mostly vanadium on the metal sublattice. Tungsten is the majority element in the M6C phase.

Eile Edit Application	ns <u>S</u> cript Options <u>W</u> ind	1	laterial		
🚜 Eg 1					
MO SI V W	3,0187E-02 6,1870E-03 2,2741E-02 2,5205E-02	5,0000E-02 3,0000E-03 2,0000E-02 8,0000E-02	2,2544E-04 6,3355E-09 3,8343E-06 2,7611E-04	-8,8892E+04 -1,9983E+05 -1,3202E+05 -8,6746E+04	SER SER SER SER SER
Mass fractions: FE 9,17022E-01	STATUS ENTERE 8,5093E-01, Mass 4 MO 1,30455E-02 V 4,12902E-03 MN 3,66663E-03	7339E+01 SI 3,49220E-03	g force 0,0000E+00		
Mass fractions: V 5,33934E-01 W 1,59272E-01	STATUS ENTERE 3,0461E-02, Mass 1 MO 9,91495E-02 . CR 4,70296E-02 FE 2,58603E-02	,2205E+00 MN 1,58070E-04	g force 0,0000E+00		
Mass fractions: W 4,04913E-01 FE 2,78325E-01	S ENTERED 5 1,1861E-01, Mass 9 . V 3,32498E-02 CR 3,04407E-02 1 C 2,17364E-02	SI 9,02531E-04			
<		(0)			×

4. The most common property diagram calculation is obtained by stepping in temperature for a given composition. Various temperature dependent quantities can then be used on the Y-axis in the DIAGRAM DEFINITION window. Change axis 1 to *T* and axis 2 to *NONE*. The limits for the temperature axis can be 600 – 1500 °C. Click *Next*.

A MAP/STEP DEFINITION	
Axis 1 Variable T Min (C) No of steps Max (C) 600 50 1500	Axis 2 Variable NONE • Min (C) No of steps Max (C)
Overwrite Previous Calculation Step Separate Generate Automatic Start Points	arate
Back Script Management	Next Cancel <u>H</u> elp

- 5. When the step calculation is finished, the DIAGRAM DEFINITION window appears with two axes already defined, let's use these. Press *Next*.
- 6. Select *Axis quantity* in the *Label Option* menu and check the color box. The y-axis quantity means the fraction of each phase expressed in moles. We can see that in addition to the phases stable at T=1000 °C, also bcc and M23C6 are stable at low temperature and liquid at high T. The cursor can be used to get an estimate of the values in the diagram. In the plot window below the cursor is placed on the liquidus temperature, 1417 °C.

<u> </u>	
Menu Layers Format Diagram	
Redefine axes 🔍 🔍	Switch Axes
Label Option Axis quantity	
THERMO-CAL C (2008.08.18:15.04) : DATABASE:TCFE6 P=1.01325E5, N=1, W(C)=9E-3, W(CR)=4E-2, W W(MO)=5E-2, W(V)=2E-2; 1.0 0.9 0.9 0.9 0.8 0.7- 0.6- 0.5- 0.4- 0.3- 0.2- 0.1 $\frac{5}{2}$ $\frac{22}{2}$ $\frac{2}{2}$ $\frac{2}$	1:T-273:15.NPM(FCC_A1#1) 2:T-273:15.NPM(FCC_A1#2) 3:T-273:15.NPM(LQUID) 5:T-273:15.NPM(BCC_A2) 6:T-273:15.NPM(M23C6)
NPM(LIQUID)	X = 1,417E+03 Y = 1,000E+00

7. Another example of a property diagram is the activity of carbon vs. temperature. Click *Redefine* and open the *Advanced Diagram Axis* tab. Change the Y-axis variable to *Activity* for component *C*. Click *Next* to plot.

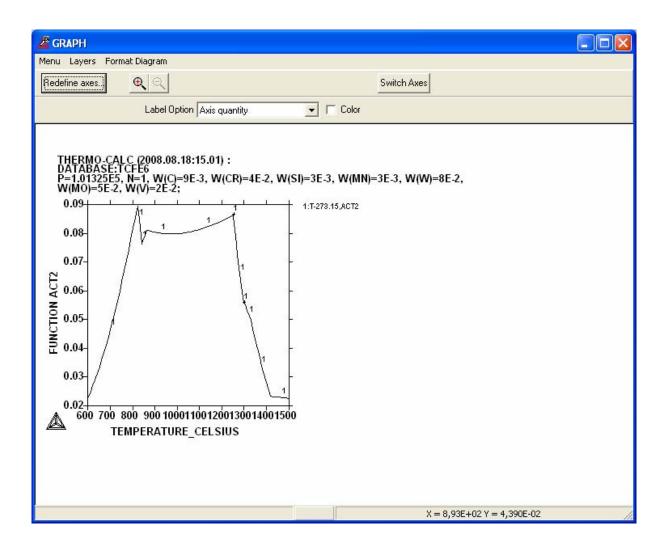
Z DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	_
-X-Axis	Y-Axis
Temperature and Pressure Potential and Activity	Temperature and Pressure Potential and Activity
Temperature Celsius	Activity
	For Component
Compositional Variables Phase Variables	Compositional Variables Phase Variables C
Energy Variables Additional Quantities	Energy Variables Additional Quantities
Partial Derivatives	Partial Derivatives
User Symbols	User Symbols
X-Axis Text 🔽 Automatic	 Y-Axis Text ☐ Automatic
TEMPERATURE_CELSIUS	ACR(C)
· -	,
Back 📃 New Graph Window	Next Cancel <u>H</u> elp

A GRAPH	
Menu Layers Format Diagram	
Redefine axes 🔍 🔍 Switch Axes	
Label Option 🗛 guantity 🗾 🔽 Color	
THERMO-CALC (2008.08.18:14.59) : P-101325E5; N-1, W(C)=9E3, W(CR)=4E2, W(SI)=3E3, W(MN)=3E3, W(W)=8E2, W(J)=2E-2; W(J)=2E-2; U(J)=0 (1:7273.15, ACR(C)) (1:7273.15,	
N = 1,0152+03 + = 3,9762-03	111

8. The magnitude of the carbon activity may seem strange in the last plot. This is because the default reference state for carbon is at room temperature in this database. Enter a function to refer the C activity to graphite at the temperature of the calculation. Click *Redefine* and open the *User Symbols* tab. Define the function (ACT2=ACR(C,GRAPHITE)) and move to *Advanced Diagram Axes* where you select the new function for the Y-axis. Click *Next* to plot.

A DIAGRAM DEFINITION			
Diagram Axes Scaling User Symbols Advanced Diagr	am Axes		
	All Defined Symbols		
	Type Function	Name	
	[Add Symbol] Delete Syr	nbol Tabulate	
X-Axis Text I Auto	matic	Y-Axis Text ACR(C)	T Automatic
Back	🔲 New Graph Window		Next Cancel <u>H</u> elp

Z DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	
-X-Axis	Y-Axis
Temperature and Pressure Potential and Activity	Temperature and Pressure Potential and Activity
Compositional Variables	Compositional Variables Phase Variables
Energy Variables Additional Quantities	Energy Variables Additional Quantities
Partial Derivatives	Partial Derivatives
User Symbols	User Symbols ACT2
X-Axis Text 🔽 Automatic	Y-Axis Text 🦳 Automatic
TEMPERATURE_CELSIUS	FUNCTION ACT2
Back	indow Next Cancel <u>H</u> elp



9. Click *Redefine* to plot yet another property diagram, this time the composition of the M6C phase. Open the *Advaced Diagram Axes* tab and select *Phase Composition (moles)* for all components in the M6C phase as the Y-axis variable. Click *Next* to plot. In the diagram below, note that the M6C phase is stable for temperatures below 1304 °C and at larger temperatures the metastable composition is shown.

Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	
-X-Axis	Y-Axis
Temperature and Pressure Potential and Activity	Temperature and Pressure Potential and Activity
	For Component
Compositional Variables Phase Variables	Compositional Variables Phase Variables ALL
	Phase Composition (mc T For Phase
	M6C
Energy Variables Additional Quantities	Energy Variables Additional Quantities
Partial Derivatives	Partial Derivatives
User Symbols	User Symbols
<u> </u>	
X-Axis Text 🔽 Automatic	Y-Axis Text 📃 Automatic
TEMPERATURE_CELSIUS	×(M6C,*)
Back	Next Cancel <u>H</u> elp

10. Select *Axis quantity* in the *Label Option* menu and check the color box.

Z GRAPH	
Menu Layers Format Diagram	
Redefine axes.)	Switch Axes
Label Option Axis quantity	▼ I⊽ Color
THERMO-CAL C (2008.08.18:15.11) : DATABASE: TCFE6 P=1.01325E5. N=1. W(C)=9E-3. W(CR)=4E-2. W(S) W(MO)=5E-2. W(V)=2E-2: 0.50 0.45 0.40 0.35 0.30 0.20 0.20 0.15 0.20 0.15 0.10 0.15 0.10 0.50 0.10 0.50 1 11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	D)=3E-3, W(MN)=3E-3, W(W)=8E-2, 1:T-273 15, X MSC,CP) 3:T-273 15, X MSC,FE) 4:T-273 15, X MSC,FE) 4:T-273 15, X MSC,KI) 7:T-273 15, X MSC,KI) 7:T-273 15, X MSC,W) 8:T-273 15, X MSC,W)
Х(М6С,МО)	X = 1,052E+03 Y = 1,888E-01

8 Calculate Heat and Heat Capacity Variation during Solidification of an AI-15%Mg-9%Si Alloy

- 1. Click the *Elements* button in the MAIN window. Select database *PTERN* and elements *Al*, *Mg* and *Si* from the periodic table.
- 2. Click *Next* to come to the CONDITIONS window. Enter compositions in mass-fraction; 0.15 Mg and 0.09 Si, and the temperature 1000 K.

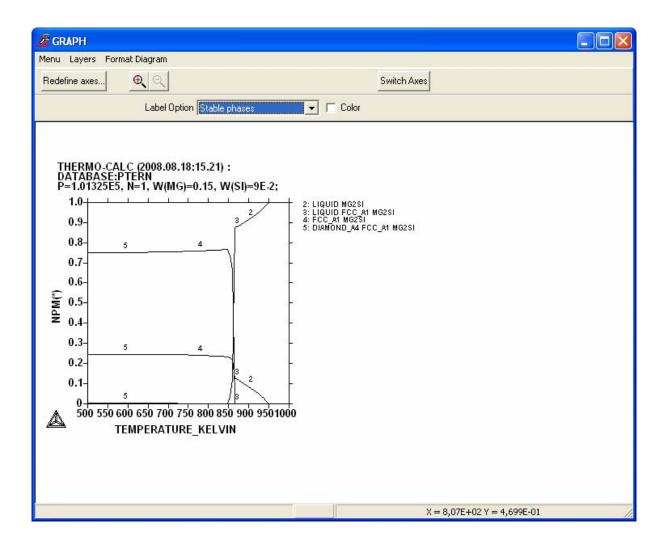
Number of Missing Conditions	0	Set Reference State Components	e User Symbols Advanced Conditions	Start Values
Temperature	1000 K			Mole-fraction
Pressure	101325 Pa	Al		Condition Composition - Composition -
System Size Moles 👤	1 mo	les SI		Composition -
All Defined Conditions in SI Units				
T=1000 P=1.01325E5 N=1 X(MG)=0.15				
X(SI)=9E-2				
1	-			
Delete				
Fixed Phases	2			
Back Script Managemen	t Show Value	Compute	Next Ca	ancel <u>H</u> elp

3. Click next to open the MAP/STEP DEFINITION window. Set *T* as axis variable and step between *500 K* and *1000 K* with step length *12.5*. Click *Next*.

MAP ISTEP DEFINITION	
Axis 1 Variable T Min (K) Step length Max (K) 500 12.5 1000	Axis 2 Variable NONE • Min (K) No of steps • Max (K)
Source 12.5 1000 Image: Display the Display the Previous Calculation Image: Step Separate Image: Display the D	Next Cancel <u>H</u> elp

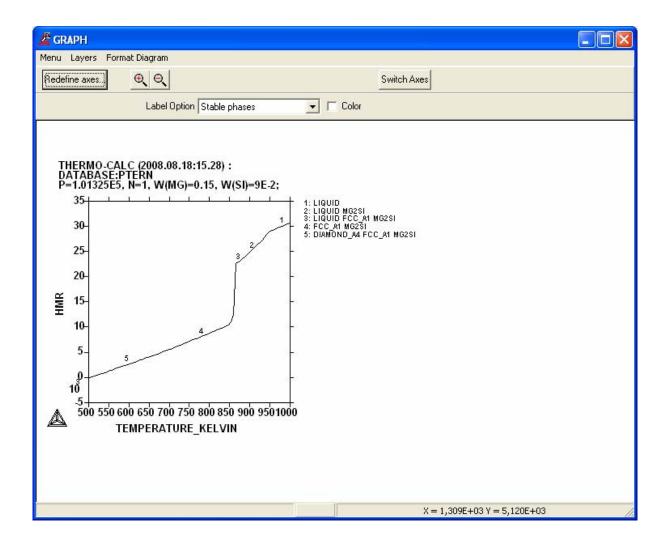
4. Set diagram axis as *Temperature Kelvin* on X-axis and *Phase fraction* of all phases on Y-axis, default values. Click *Next* to plot. Choose *Stable phases* in the *Label Option* menu.

Z DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Temperature Unit C Celsius C Kelvin C Fahrenheit	Composition Unit Moles Percent Mass
Diagram Title	
X-Axis Variable Temperature	Y-Axis Variable Phase Fraction
For Component For Phase	For Component For Phase
X-Axis Text IV Automatic	Y-Axis Text
Back	ndow Cancel Help



5. Now plot the total enthalpy (heat) as a function of temperature. Click *Redefine axes* in the GRAPH window to return to the DIAGRAM DEFINITION window. Open the *Advanced Diagram Axes* tab and select *Enthalpy* normalized *per mole* as variable on the Y-axis and select *SYSTEM*. Click *Next* to plot.

Z DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	_
-X-Axis	Y-Axis
Temperature and Pressure Potential and Activity	Temperature and Pressure Potential and Activity
Temperature Kelvin 🔽	SER Reference State
Compositional Variables Phase Variables	Compositional Variables Phase Variables
	For Phase
Energy Variables Additional Quantities	SYSTEM Energy Variables Additional Quantities
	Enthalou Victoria Vi Victoria Victoria
, _, _	per mole
Partial Derivatives	Partial Derivatives
User Symbols	User Symbols
X-Axis Text 🔽 Automatic	Y-Axis Text Catomatic
TEMPERATURE_KELVIN	HMR
Back New Graph Windo	
Back	W Next Cancel <u>H</u> elp



6. Next we want to plot the heat capacity. Click *Redefine axes* in the GRAPH window to return to the DIAGRAM DEFINITION window. Open the *Advanced Diagram Axes* tab and select *Heat capacity for system* as the Y-axis variable. Click *Next* to plot. Use the *zoom in* button to change the scaling of the plot.

Z DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	
-X-Axis	Y-Axis
Temperature and Pressure Potential and Activity Temperature Kelvin	Temperature and Pressure Potential and Activity
Compositional Variables	Compositional Variables Phase Variables
Energy Variables Additional Quantities	Energy Variables Additional Quantities
Partial Derivatives	Partial Derivatives Heat capacity for system (HM.T)
User Symbols	User Symbols
X-Axis Text I Automatic TEMPERATURE_KELVIN	Y-Axis Text Capacity for System (Cp)
Back	w Next Cancel Help

🖉 GRAPH	. 🗆 🔀
Menu Layers Format Diagram	
Redefine axes	
THEDMO CALC (2008 08 19:16 20) ·	
THERMO-CALC (2008.08.18:16.20) : DATABASE:PTERN P=1.01325E5, N=1, W(MG)=0.15, W(SI)=9E-2;	
160 + 10152553, $100 + 100$	
140-	
<u>कि</u> 120-	
₣ 100-	
Heat Capacity for System (Cp)	
2 60-	
ਿੰਦ 40-	
te 20-	
TEMPERATURE_KELVIN	
X = 1,245E+03 Y = 8,7E+01	11.

9 Calculate Second Order Transition Line in AI-Fe System

- 1. Click the *Elements* button in the MAIN window and select database *SSOL4* and elements *Al* and *Fe* from the periodic table.
- 2. Reject all phases and select *LIQUID*, *B2_BCC*, *BCC_A2* and *A2_BCC* (disordered part of the *B2_BCC*).

Z DATA		
Alphabetic List Periodic Table	Phases Constituents	
Rejected Phases:	Selected Phases:	
L12_FCC BCC_B2 IONIC_LIQUID:Y FCC_A1 HCP_A3 HCP_ZN DIAMOND_A4 BCT_A5 TETRAGONAL_U CBCC_A12 CUB_A13 ORTHORHOMBIC_A20 LAVES_C14 LAVES_C15 LAVES_C36 FE4N ALM_D019 ALCE_AMORPHOUS ALCU_THETA ALCUZN_T AL2FE	 LIQUID:L B2_BCC A2_BCC BCC_A2 X X	
Material	Next Cancel	Help

3. Click *Next* to come to the CONDITIONS window. Select the composition unit mole-fraction and set the amount of Al to 0.4, and the temperature to 400 K.

Number of Missing Conditions	1	ł	Set Reference State Components	User Symbols Advanced Conditions	Start Values
Temperature	400	к		Composition Unit	Mole-fraction
Pressure	101325 F	Pa	Redefine Component	Value	Condition Composition 💌
System Size Moles	1 r	moles	FE		Composition
All Defined Conditions in SI Units T=400 P=1.01325E5 N=1 Delete	1				
-Fixed Phases	21				
Back Script Managemen	Show Value		Compute	Next Ca	ncel <u>H</u> elp

4. To see how Al and Fe distribute on the sublattices click the *Options* in the MAIN window and select *Output*. Select *Constitution and Composition* and click *Ok*, then click *Compute*.

🖉 ΟυΤΡυΤ 📃 🗖 🔀					
Reset to Default					
Save equlibrium output to file:					
Every output in new window					
Fraction Order					
 Value Order 					
C Alphabetical Order					
Fraction Type					
 Mass Fraction 					
Mole Fraction					
Composition Only?					
C Composition					
Constitution and Composition					
Stable Phases Only?					
Stable Phases Only					
C All Non-suspended Phases					
OK Cancel <u>H</u> elp					

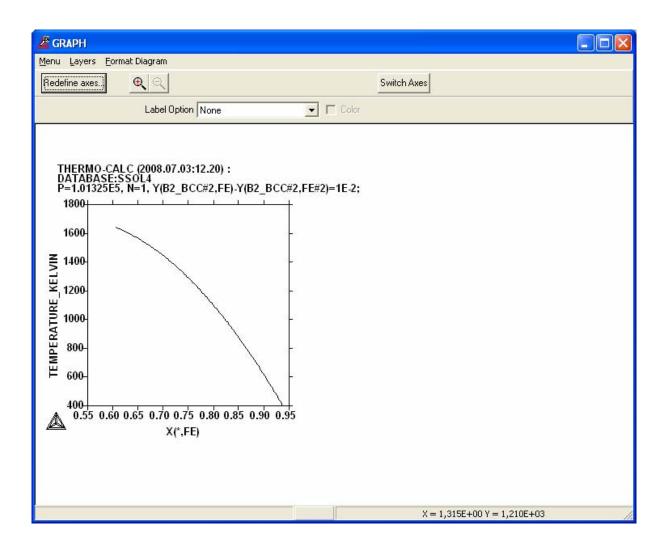
🖉 MAIN						
Eile Edit Applications	Script Options Window		erial		M	AS
🖉 Eq 1						
Output from POLY- to jul 03 2008 12:1						^
Database: SSOL4						
Conditions: T=400, P=1.01325 DEGREES OF FREED	E5, N=1, X(AL)=0.4 DOM 0					
Number of moles o	(127C, 260F), Press f components 1,000(-3,81486E+04, Ent	00E+00, Mass 4,43	010E+01	E+00		
Component	Moles	Mass-Fraction	Activity	Potential	Ref.State	
AL FE	4,0000E-01 6,0000E-01	2,4362E-01 7,5638E-01	4,1974E-08 4,1248E-04	-5,6493E+04 -2,5919E+04	SER SER	=
Mass fractions: FE 7,56376E-01 Constitution: Sublattice 1 Numb FE 1,0000E+00 A Sublattice 2 Numb	oer of sites 0,5 AL 4,2288E-06 VA ber of sites 0,5 E 2,0000E-01 VA 1	+301E+01 1,8447E-10	force 0,0000E+00			

- 5. Change the condition for the amount of Al to be that of a difference in site-fractions in the two sublattices. Remove the X(AL)=0.4 condition and enter $Y(B2_BCC\#2,FE\#1)$ - $Y(B2_BCC\#2,FE\#2)=1E-2$ under the *Advanced Conditions* tab in the CONDITIONS window.
- 6. Click *Next* to open the MAP/STEP DEFINITION window. Set one axis variable to *T* with min and max values 400 K and 2000 K, and step length 10. Then click *Next*.

MAP/STEP DEFINITION	
Axis 1 Variable T Min (K) Step length Max (K) 400 10 2000	Axis 2 Variable NONE
Overwrite Previous Calculation Step Separate Generate Automatic Start Points Back Script Management Script Management	Next Cancel <u>H</u> elp

7. Select *Mole-Fraction* of *Fe* in *All* phases and *Temperature* as diagram axes. Click *Next* to plot.

Charles and the second	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Temperature Unit	Composition Unit
C Celsius	🖸 Moles 🔲 Percent
Kelvin	C Mass
C Fahrenheit	
Diagram Title	
X-Axis	Y-Axis
Variable	Variable
Composition	Temperature
For Component For Phase	For Component For Phase
FE V ALL V	NONE ALL
X-Axis Text 🔽 Automatic X(°.FE)	Y-Axis Text Cutomatic TEMPERATURE_KELVIN
1 × × − ×	,
Back New Graph V	Vindow Next Cancel Help



8. To plot the transition line in the Al-Fe phase diagram save the plot on an experimental file (e.g. example9.exp).

Save As					? ×
Save in	TCW5		• 🗢 🖲	• 🖬 🍅 🖬	
My Recent Documents Desktop					
My Documents My Computer					
My Network Places	File name: Save as type:	example9 Experimental File (*.exp)		-	Save Cancel

9. Close the GRAPH window and select *Elements* in the MAIN window. Reject all phases and select *LIQUID*, *FCC_A1*, *B2_BCC*, *BCC_A2*, *A2_BCC*, *AL13FE4*, *AL2FE*, *AL5FE2* and *AL5FE4*. Finally, click *Next*.

🖉 DATA		
Alphabetic List Periodic Table	Phases Constituents	
Rejected Phases:	Selected Phases:	
LAVES_C14 LAVES_C15 LAVES_C36 FE4N ALM_D019 ALCE_AMORPHOUS ALCU_THETA ALCUZN_T ALLU AL4MN AL11MN4 AL12MN AL11MN4 AL12MN ALNB3 AL3NB AL3NB AL3NB AL3NB AL3NB AL3NI2 ALTI FESB FEU6 FE2U	 LIQUID:L FCC_A1 B2_BCC BCC_A2 A2_BCC AL13FE4 AL2FE AL5FE2 AL5FE4 >>> 	
Material	Next Cancel	<u>H</u> elp

10. Enter T=1300 K and X(AL)=0.3. Click *Next*.

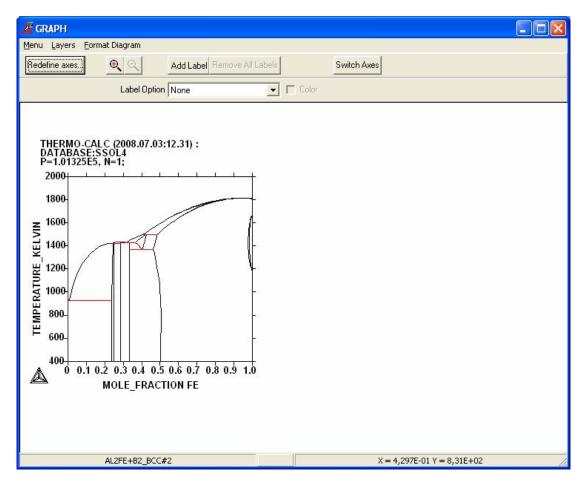
Number of Missing Conditions	0	Set Reference State Components	User Symbols Start Values Advanced Conditions Phases
Temperature	1300 K		Composition Unit Mole-fraction 💌
Pressure	101325 Pa	Redefine Component	t Value Condition 0.3 Composition
System Size Moles	1 mole	es FE	Composition
All Defined Conditions in SI Units T=1300 P=1.01325E5 N=1 X(AL)=0.3 Delete]		
-Fixed Phases			
Back Script Managemen	t Show Value	Compute	Next Cancel <u>H</u> elp

11. Set X(AL) as axis variable for x-axis and T as axis variable for y-axis and click *Next* to map the phase diagram.

A MAP/STEP DEFINITION	
Axis 1 Variable X(AL)	Axis 2 Variable T
Min No of steps Max 0 50 1	Min (K) No of steps Max (K) 400 50 2273
Image: Overwrite Previous Calculation Image: Step Sep Image: Overwrite Previous Calculation Image: Step Sep	arate
Back Script Management	Next Cancel <u>H</u> elp

12. Select *Mole Fraction* of *Fe* and *Temperature* as diagram axes and click *Next* to plot.

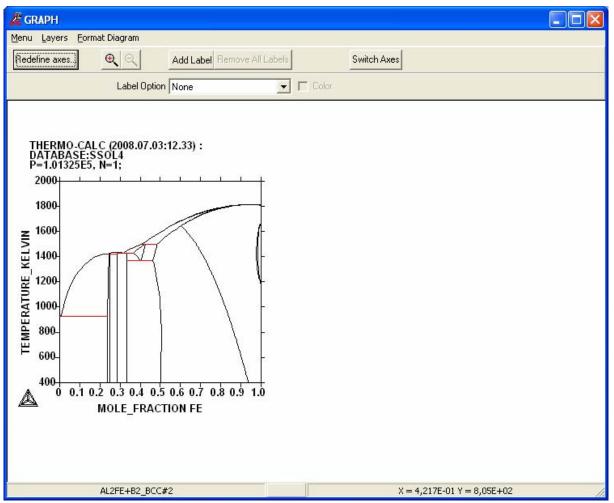
Z DIAGRAM DEFINITION		
Diagram Axes Scaling User Symbols Advanced Diagram Axe	15	
Temperature Unit C Celsius C Kelvin C Fahrenheit		Moles 🥅 Percent Mass
Diagram Title		
X-Axis Variable Composition	Y-Axis Variable Temperature	
For Component For Ph FE SYST		For Phase
X-Axis Text V Automatic MOLE_FRACTION FE	Y-Axis Text TEMPERATURE_KELV	Automatic
,	New Graph Window	Next Cancel Help



13. To plot the transition line in the phase diagram select *Append* under *Menu* and find the experimental plot file created earlier (example9.EXP).

APPEND / REMOVE	
Append files:	
 Files with checked boxes will be appended.	2
Uncheck the box to remove the file.	Add
Click Add to add more files to the list.	
	OK Cancel





10 Calculate the CaO-SiO2 System

- 1. Click the *Elements* button in the MAIN window.
- 2. Select database *PION* and elements *Ca*, *Si* and *O* from the periodic table.
- **3.** Reject all phases and select only those we know should be stable in this system; CRISTOBALITE, TRIDYMITE, QUARTZ, LARNITE, HATRURITE, RANKINITE, PSEUDO_WOLLASTONITE, WOLLASTONITE, HALITE:I, OLIVINE, and IONIC_LIQ:Y.

Z DATA	
Alphabetic List Periodic Table Phases	Constituents
Rejected Phases:	Selected Phases:
LIQUID:L GAS:G FCC_A1 BCC_A2 DIAMOND_FCC_A4 ALPHA_CA2SIO4 ALPHA_PRIME_CA2SIO4 HCP_A3 CBCC_A12 CUB_A13 CA2SI CASI CASI CASI2 CR3SI CRSI2	 CRISTOBALITE TRIDYMITE QUARTZ LARNITE HATRURITE RANKINITE PSEUDO_WOLLASTONITE WOLLASTONITE HALITE:I OLIVINE IONIC_LIQ:Y
	<< >>
Material	Next Cancel <u>H</u> elp

4. Next, reject the following constituents from the IONIC_LIQ:Y phase: VA#2 and SI+4#1.

ATA DATA		
Alphabetic List Periodic Table	Phases Constituents	
Selected Phases: (CA+2,SI+4)1(0-2,SI04-4,VA) 		Selected Constituents:
CRISTOBALITE TRIDYMITE QUARTZ LARNITE HATRURITE RANKINITE PSEUDO_WOLLASTON WOLLASTONITE HALITE:I OLIVINE IONIC_LIQ:Y	SI+4#1 VA#2	CA+2#1 0-2#2 SI04-4#2 SI02#2
	<	
Material	Next	Cancel <u>H</u> elp

- **5.** Click *Next* to come to the CONDITIONS window. Define more convenient components than the elements. Click *Redefine* and enter *CAO*, *SIO2* and *O*. Click *Ok* to return to the CONDITIONS window.
- 6. Enter temperature (2000 K), pressure (1E5 Pa) and size of the system (1 moles). Enter oxygen activity equal to one (ACR(O)=1) and mass-fraction 4E-1 for the SIO2 component.

Number of Missing Conditions	0	Components Advanced Conditions Phases Set Reference State User Symbols Start Values
Temperature Pressure System Size Moles ▼ All Defined Conditions in SI Units T=2000 P=1E5 N=1 ACF(0)=1 X(SI02)=0.4	2000 K 100000 Pa 1 moles	Phase IONIC_LIQ (CA+2)6(0-2,SI04-4,SI02)2 Amount 0 moles Major Constituent(s) Minor Constituents Sublattice Major Constituents Minor Constituents Sublattice #1 0-2 SI04-4 Sublattice #2 > SI04-4 SI02
 Fixed Phases		K X Force Start Values Phase Constituents
Back Script Managemen	t Show Value	Compute Next Cancel <u>H</u> elp

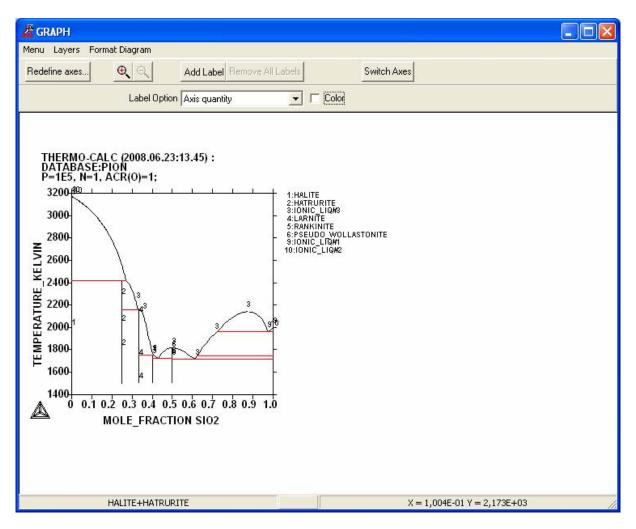
- **7.** Click *Start Values* tab and change the major constituent in sublattice 2 in IONIC_LIQ to O-2.
- 8. Click *Compute* to perform an equilibrium calculation for the given conditions.

A MAIN					
File Edit Applications	Script Options Window	v Help			
	A	Elements Mate	rial		
🔏 Eg 1					
Database: PION					~
Conditions: T=2000, P=1E5, N DEGREES OF FREE	=1, ACR(O)=1, X(SIO DOM 0	2)=0.4			
Number of moles of	K (1727C, 3140F), P f components 1,000(′ -9,93143E+05, Ent	00E+00, Mass 5,768	306E+01	E+00	
Component	Moles	Mass-Fraction	Activity	Potential	Ref.State
CAO O SIO2	6,0000E-01 0,0000E+00 4,0000E-01	5,8334E-01 -3,1312E-17 4,1666E-01	2,4259E-23 1,0000E+00 1,1989E-31	-8,6593E+05 0,0000E+00 -1,1840E+06	SER SER SER
Mass fractions: CAO 5,83340E-01 Constitution: Sublattice 1 Num CA+2 1,0000E+00 Sublattice 2 Num)	7681E+01 1 O -3,13116E-17	orce 0,0000E+00		1
5					►

- 9. Click *Next* to come to the MAP/STEP DEFINITION window.
- **10.** Select X(SIO2) and T as axis variable 1 and 2 respectively. Enter 0 and 1 as limits for axis 1 and 1500 and 3500, with step length 50, as limits for axis 2.

MAP/STEP DEFINITION	
Axis 1 Variable X(SIO2)	Axis 2 Variable T
Min No of steps Max 0 50 1	Min (K) No of steps Max (K) 1500 50 3500
✓ Overwrite Previous Calculation ☐ Step Sepa ✓ Generate Automatic Start Points	arate
Back Script Management	Next Cancel <u>H</u> elp

- 11. Click *Next* to execute the map command.
- **12.** In the DIAGRAM DEFINITION window the suitable diagram axes should appear automatically (X(SIO2) on x-axis and Temperature Kelvin on y-axis). Just click *Next* to plot and choose *Axis quantity* in the *Label Option* menu.



11 Calculate A3 Temperature and Its Dependence on Alloying Element

- 1. Click the *Elements* button in the MAIN window.
- 2. Select database TCFE6 and elements C, Cr, Fe, Mn, Nb and Si from the periodic table.
- **3.** Click *Next* to come to the CONDITIONS window. Enter compositions in mass-fraction and the temperature: W(Cr)=1.5E-2, W(C)=3E-3, W(Mn)=5E-3, W(Nb)=1E-3, W(Si)=3E-3, T=1100 K.

Number of Missing Conditions	0	Set Reference Sta Components	ate User Symbols Advanced Conditions	Start Values
Temperature	1100 K		Composition Unit	Mass-fraction
Pressure	101325 PA	neuenne	nponent Value C 3E-3	Condition
System Size Moles	1 m	oles	CR 1.5E-2	Composition
			FE 5E-3	Composition Composition
All Defined Conditions in SI Units	2.		NB 1E-3 SI 3E-3	Composition - Composition -
T=1100 P=1.01325E5 N=1 W(C)=3E-3 W(MN)=5E-3 W(NB)=1E-3 W(SI)=3E-3 W(CR)=1.5E-2 Delete]			
Fixed Phases	20.1			
Back Script Managemen	t Show Value	Compute	Next Ca	ncel <u>H</u> elp

- 4. Click *Compute* to perform an equilibrium calculation for the given conditions.
- 5. Fix the BCC_A2 phase with zero moles and remove the temperature condition.

Degrees of freedom	-1		Set Reference State Components	User Symbo Advanced Condit		Start Values Phases
Temperature	1100	К	Phases LIOUID	Status ENTERED	Moles	~
Pressure	101325	Pa	ALAC3 BCC_A2	ENTERED FIXED	0.00	
System Size Moles	[1 	moles	CEMENTITE CHI_A12 CR3SI DIAMOND_FCC_A4 FCC_A1 FCC_A1#2 FE2SI FE4N_LP1 FE8SI2C FECN_CHI GRAPHITE Phase Status:	ENTERED ENTERED ENTERED ENTERED ENTERED ENTERED ENTERED ENTERED ENTERED	0.00 0.00 0.00 1.00 0.00 0.00 0.00 0.00	
Delete						
Fixed Phases				Phase Conditi Add Compositi		
Back Script Managemen	t Show Value		Compute	Next	Cancel	Help

- 6. Click *Compute* once more.
- **7.** To get the A₃ temperature click *Show Value* button and choose *Temperature Kelvin* in the SHOW VALUE window. Click *Show* to see the value.

Set Reference State User Symbols Stat Values Temperature K Components Advanced Conditions Phases System Size 101325 Pa Component Value Condition System Size Moles 1 moles CR 15E-2 Composition V All Defined Conditions in SI Units Image: Size Size Size Size Size Size Size Size					
Pressure 101325 Pa Pressure 101325 Pa System Size Moles 1 moles C CR 1.5E-2 Composition • CR 1.5E-2 Composition • MN 5E-3 Composition • MN Si 3E-3 Composition • MN Si Si Si Delete	Number of Missing Conditions	0		and a set of the one	
	Temperature Pressure System Size Moles ✓ All Defined Conditions in SI Units P=1.01325E5 N=1 W[C]=3E-3 W[M]=5E-3 W[N]=5E-3 W[N]=3E-3 W[CR]=1.5E-2 Delete Fixed Phases	Г К 101325 Ра	Redefine Cor	Composition Unit mponent Value C 3E-3 CR 1.5E-2 FE	Condition Composition • Composition • Composition • Composition • Composition •
Back Script Management Show Value] Compute Next Cancel Help	Back Script Managemer	it	Compute	Next Ca	ancel Help

A SHOW VALUE		
Temperature and Pressure	Potential and Activity	
Temperature Kelvin		•
Compositional Variables	Phase Variables	
· ·		-
Energy Variables	Additional Quantities	
		-
Partial Derivatives		
		<u> </u>
User Symbols		Show
· ·		L. Show
Show Value of: T-K		
, Variable	Mnemonic	Value
,	Mnemonic T-K	Value 1071,61
, Variable		

8. To investigate the dependence of the A₃ temperature on alloy composition, try changing one of the mass-fractions and click *Compute* after each change. Click *Show* in the SHOW VALUE window to see the new temperature.

12 Mapping of Univariant Equilibria of Liquid in the Fe-C-Cr System

- 1. Click *Elements* in the MAIN window.
- 2. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *C*, and *Cr* in the periodic table. Click *Next*.
- **3.** Specify the concentrations of C and Cr as *1* and *5 mass-percent*, respectively and change the temperature to *2000 K*. Click *Next*.

Number of Missing Conditions	0	Set Referen Component		User Symbols Advanced Condition		Start Values Phases
Temperature	2000 K			Composition	Unit Mass	-percent 💌
Pressure	101325 P	a Redefine	Component FE	Value	× 0	Condition omposition 💌
System Size Moles	[1 m	noles	С	1	% C	omposition 💌
			CR	5	% C	omposition 💌
All Defined Conditions in SI Units	9.5					
T=1000 P=1.01325E5						
N=1 W(C)=1E-2 W(CR)=5E-2						
Delete						
Fixed Phases	-51					
			2			
Back Script Managemen	t Show Value	Compute		Next	Cancel	Help

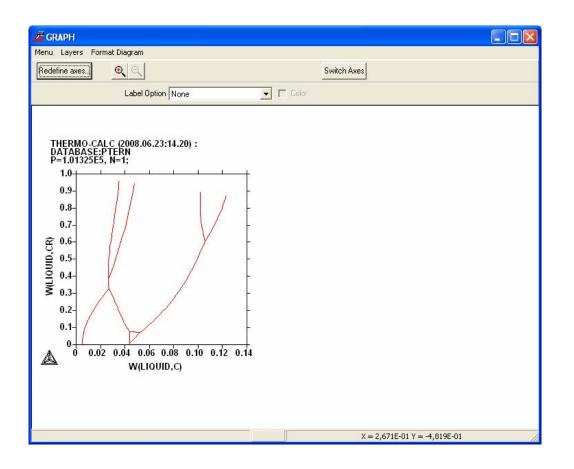
4. Set the variable for *Axis 1 to W(C)* and the variable for *Axis 2* to *W(CR)*. Click the arrow on the right of the window, and the panel for *Axis 3* appears. Choose *T* as the variable for the third axis and select *LIQUID* as the *Present Phase* since we are going to map the univariant equilibrium lines for the liquid phase. Click *Next*.

A MAP/STEP DEFINITION	
Axis 2 Variable W(CR) • Min (%) No of steps • Max (%) 0 50 100	Axis 3 Variable Set Present Phase T ILIQUID Min (K) No of steps Max (K) 773,15 50 2273,15
 ✓ Overwrite Previous Calculation ✓ Generate Automatic Start Points 	e
Back Script Management	Next Cancel <u>H</u> elp

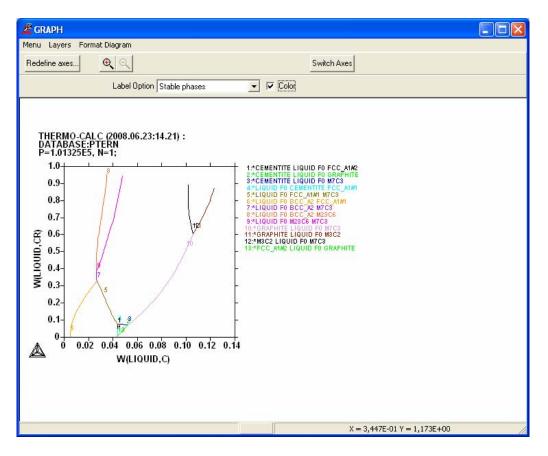
5. The default axes are mass-fraction of C and CR in the LIQUID phase. Accept this choice and click *Next*.

A DIAGRAM DEFINITION			
Diagram Axes Scaling User Syr	mbols Advanced Diagram Axes		
Temperatur	e Unit C Celsius C Kelvin C Fahrenheit	Composition Unit C Moles T Percent I Mass	
Diagram Title			
X-Axis Variable Compositio	on 💌	Y-Axis Variable Composition	
For Compo	nent For Phase	For Component For Phase	
X-Axis Text [W(LIQUID,C)	i ✓ Automatic	Y-Axis Text 🔽 Au W(LIQUID,CR)	utomatic
Back	🦵 New Graph Win	ndow Cancel	Help

6. The univariant lines of the liquid phase are plotted.



7. To identify the regions of different primary phases, choose *Stable phases* in the *Label option* menu and check the color box.



13 Plotting of Partial Pressure of Gas Species Along Solubility Lines in As-Ga Phase Diagram

- 1. Click Elements in the MAIN window. Select database *PG35* and elements *As* and *Ga* in the periodic system.
- 2. Reject all phases and select phases *LIQUID*, *RHOMBO_A7*, *ORTHO*, *FCC_B3* and *GAS*. Click *Next*.
- **3.** Enter the conditions T=1200 K and X(GA)=0.3. Put the *GAS* phase as *DORMANT*, which means that the phase is not considered in the equilibrium calculation but the driving force is calculated.

Number of Missing Conditions	0	E	Set Reference State Components	User Symbols Advanced Conditions	Start Val s Phas	
Temperature	1200	к	Phases	Status	Moles	
Pressure	101325	Pa	GAS FCC_B3 LIQUID	DORMANT ENTERED ENTERED	0.00	
System Size Moles 💌	1	moles	ORTHO RHOMBO_A7	ENTERED ENTERED	0.00 0.00	
-All Defined Conditions in SI Units T=1200 P=1.01325E5 N=1 X(GA)=0.3 Delete Fixed Phases			Phase Status:	Phase Conditions	noles	
				Add Composition S		
Back Script Managemen	t Show Value		Compute	Next	Cancel <u>H</u>	lelp

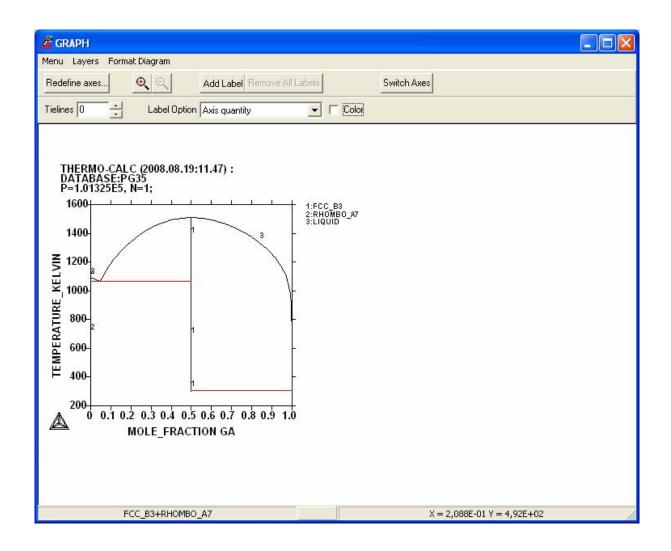
- 4. Click Compute.
- 5. From the equilibrium calculation it can be seen that the GAS phase would like to be stable (positive driving force) but it is not allowed to form as it is dormant. Click *Next*.

🖉 MAIN					
File Edit Applications	Script Options Window	Help			
	A	Elements Mater	ial		
🔏 Eg 1					
Component	Moles	Mass-Fraction	Activity	Potential	Ref.State 📐
AS GA	7,0000E-01 3,0000E-01	7,1488E-01 2,8512E-01	1,2211E-03 1,2244E-06	-6,6929E+04 -1,3582E+05	SER SER
Number of moles 0 Mass fractions: AS 1,00000E+00 Constitution:	AS 1,00000E+00 GA 8,46591E-11 Constitution:				
AS4 9,8021E-01 AS2 1,7782E-02 AS3 2,0077E-03 AS1 2,3051E-07 GA1 3,5519E-10 AS1GA1 5,2777E-1 FCC_B3#1 STATUS ENTERED Driving force 0,0000E+00 Number of moles 4,9425E-01, Mass 3,5745E+01 Mass fractions: AS 5,17972E-01 GA 4,82028E-01 Constitution: Sublattice 1 Number of sites 0,5 GA 1,0000E+00 Sublattice 2 Number of sites 0,5 AS 1,0000E+00					
LIQUID#1STATUS ENTERED Driving force 0,0000E+00 Number of moles 5,0575E-01, Mass 3,7617E+01 Mass fractions: AS 9,01993E-01 GA 9,80068E-02 Constitution: AS 8,9545E-01 GA 1,0455E-01					
<		III.		J	

6. To map the phase diagram set X(GA) with range 0 to 1 and T with range 300 to 2000 (step length 25) as axis variables. Click *Next* to map.

MAP/STEP DEFINITION	
Axis 1 Variable X(GA)	Axis 2 Variable T
Min No of steps Max 0 50 1	Min (K) Step length ▼ Max (K) 300 25 2000
✓ Overwrite Previous Calculation ✓ Step Sepa ✓ Generate Automatic Start Points	irate
Back Script Management	Next Cancel <u>H</u> elp

7. Accept the default diagram axes. Click *Next* to plot the As-Ga phase diagram.

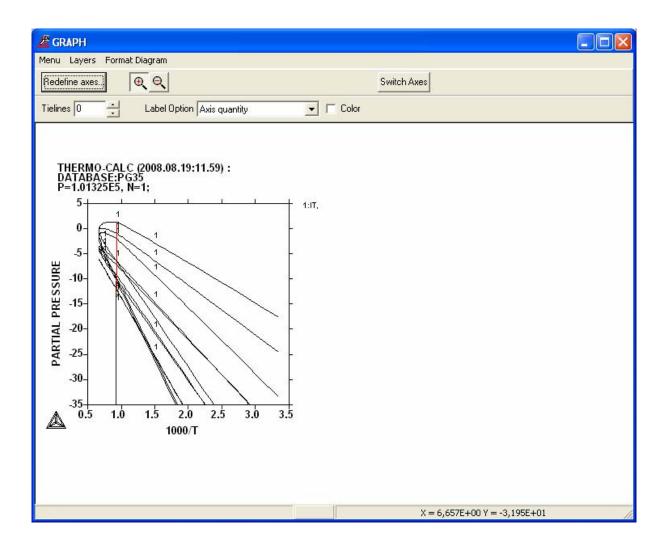


8. Now, one may be interested to know the partial pressures of the different gas species along the solubility lines. Click *Redefine* to return to the DIAGRAM DEFINITION window. Click the *User Symbols* tab and enter a number of functions and collect these in a table (see below).

Z DIAGRAM DEFINITION			
Diagram Axes Scaling User Symbols Advanced Diagra	All Defined Symbols PAS3=.4343*LNACR(AS3,GAS) PAS1=.4343*LNACR(AS1,GAS) PAS2=.4343*LNACR(AS1,GAS) PAS4=.4343*LNACR(AS4,GAS) PAS64=.4343*LNACR(GA1,GAS) PGA1=.4343*LNACR(GA1,GAS) IT=1000/T PP=PAS1,PAS2,PAS3,PAS4,PASGA	.PGA1	
X-Axis Text ✓ Autor MOLE_FRACTION GA		Y-Axis Text TEMPERATURE_KELVIN	Automatic
Back	New Graph Window		Next Cancel <u>H</u> elp

9. Go to the *Advanced Diagram Axes* tab and set *IT* on the X-axis and table *PP* on the Y-axis. Click *Next* to plot. In the GRAPH window select *Axis quantity* in the *Label Option* menu.

Z DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	
-X-Axis	Y-Axis
Temperature and Pressure Potential and Activity	Temperature and Pressure Potential and Activity
Compositional Variables Phase Variables	Compositional Variables Phase Variables
T T	_
Energy Variables Additional Quantities	Energy Variables Additional Quantities
Partial Derivatives	Partial Derivatives
	_
User Symbols	User Symbols
⊥ X-Axis Text	Y-Axis Text Cutomatic
FUNCTION IT	TABLE PP
Back 🔽 New Graph Window	Next Cancel <u>H</u> elp



14 Scheil-Gulliver Simulation of Solidification for an Al-Based Alloy

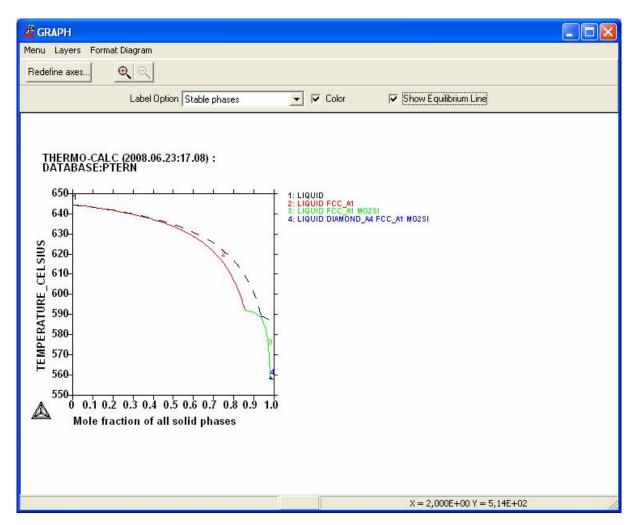
Click in the MAIN window.

Select *PTERN* from the *Database* list and then click alloy elements *Al*, *Mg*, and *Si* in the periodic table. Click *Next*.

Specify the concentrations of Mg and Si as 2 and 1 mass-percent, respectively. Click Next.

Number of Missing Conditions 0 Start Temperature 2273,15 K Temperature Step 1 K	Composition Unit Mass-percent Allow BCC -> FCC Fast Component Value AL KG 2 %
All Defined Conditions in SI Units T=2273,15 W(MG)=0,02 W(SI)=0,01	SI 1 % F
Delete	Next Cancel <u>H</u> elp

1. Accept the default X and Y –Axis variables by clicking *Next*. The solidification range diagram is plotted.

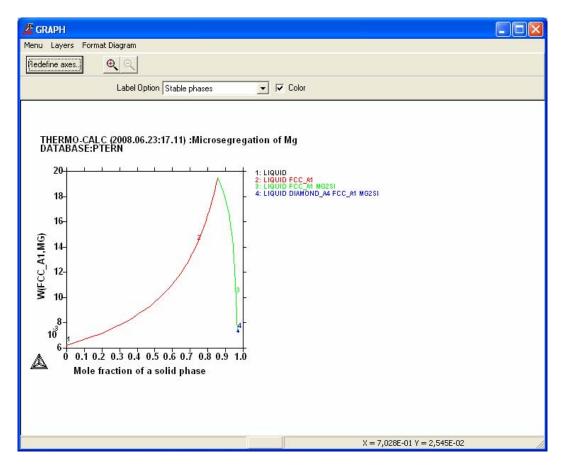


2. Check the *Show Equilibrium Line* box to add the equilibrium solidification curve.

3. Click *Redefine* and the SCHEIL DIAGRAM window reappears. In the *X-axis* panel, change the *Phase* option to *FCC_A1*. In the *Y-axis* panel, choose *Mass fraction*, *MG*, and *FCC_A1* under the *Variable*, *For Component*, and *Phase* options, respectively. Enter *Microsegregation of Mg* for the *Diagram Title*. Click *Next*

Z SCHEIL DIAGRAM	
Diagram Axis Scaling	
Diagram Title Microsegregation of Mg	
X-Axis	Y-Axis
Variable	Variable
NS	Mass fraction
For Component Phase	For Component Phase
NONE FCC_A1	MG V FCC_A1 V
Avia Text 🔽 Automatic	Avia Text 🔽 Automatic
Axis Text Automatic Mole fraction of a solid phase	Axis Text Automatic W(FCC_A1,MG)
Back 🔽 New Graph Window	Next Cancel <u>H</u> elp

4. The diagram for the microsegregation of Mg in this alloy is plotted.

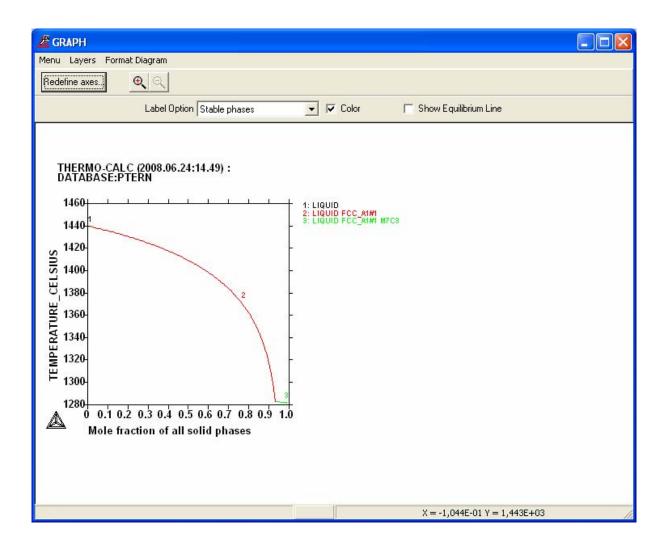


15 Scheil-Gulliver Simulation of Solidification for a Steel with Back Diffusion of Carbon in Solid Phases

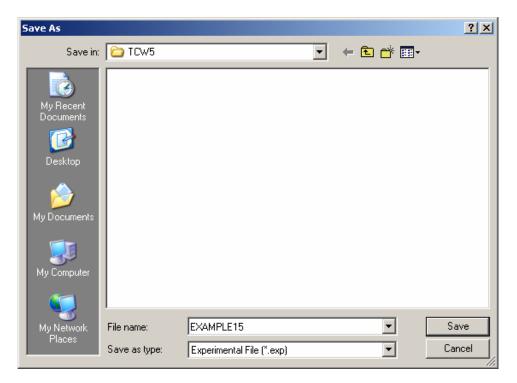
- 1. Click in the MAIN window.
- 2. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *Cr*, and *C* in the periodic table. Click *Next*.
- **3.** Specify the concentrations of C and Cr as *1* and *10 mass-percent*, respectively and check the *Fast Diffuser* box after C. Click *Next*.

Number of Missing Conditions 0	1	Composition Unit	
Start Temperature 2273,15	К	Component Value	Fast Diffuser
Temperature Step 1	К	FE CR 10	* * *
Redefine Components			
All Defined Conditions in SI Units			
T=2273,15 W(CR)=0,1 W(C)=0,01			
Delete			
		Next Cancel	Help

4. Accept the default X and Y -Axis variables by clicking *Next*. The solidification range diagram is plotted.



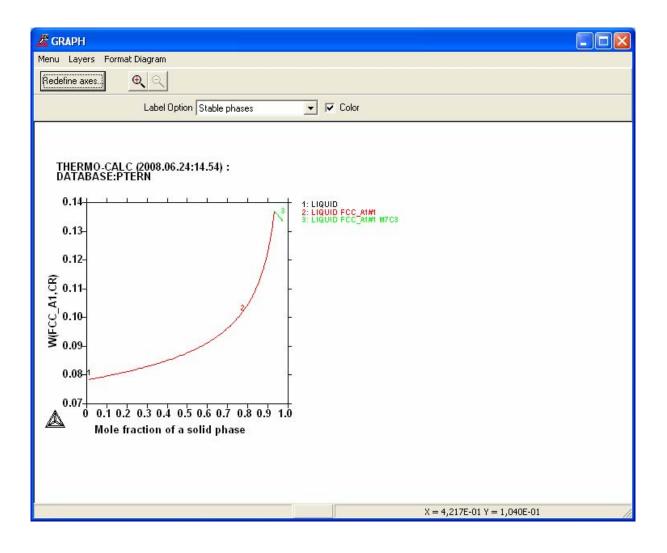
5. Click $Menu \rightarrow Save$. Specify file type as Experimental File (*.exp) and file name as EXAMPLE15. Click *Save*.



6. Click *Redefine*. In the *X-axis* panel, change the *Variable* option to *NS* and *Phase* option to *FCC_A1*. In the *Y-axis* panel, choose *Mass fraction*, *CR*, and *FCC_A1* under the *Variable*, *For Component*, and *Phase* options, respectively. Click *Next*.

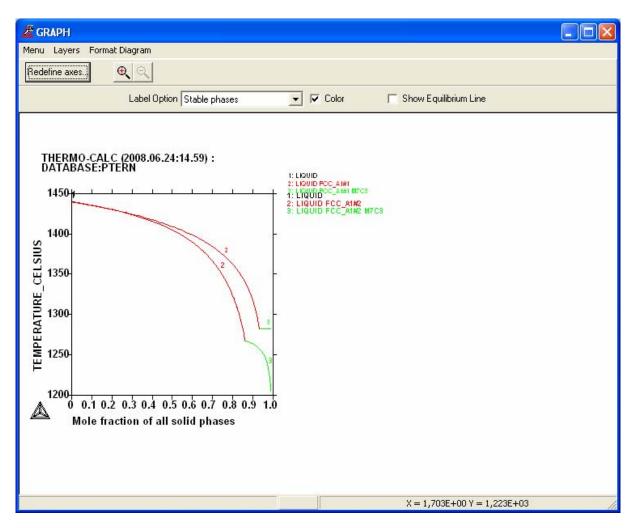
SCHEIL DIAGRAM	
Diagram Axis Scaling	
Diagram Title	
X-Axis	Y-Axis
Variable	Variable
NS	Mass fraction
,	
For Component Phase	For Component Phase
NONE FCC_A1	CR FCC_A1 -
Axis Text 🔽 Automatic	Axis Text Cutomatic
Mole fraction of a solid phase	W(FCC_A1,CR)
Back 📃 🔽 New Graph Window	Next Cancel <u>H</u> elp

7. The diagram for the microsegregation of Cr in this alloy is plotted.

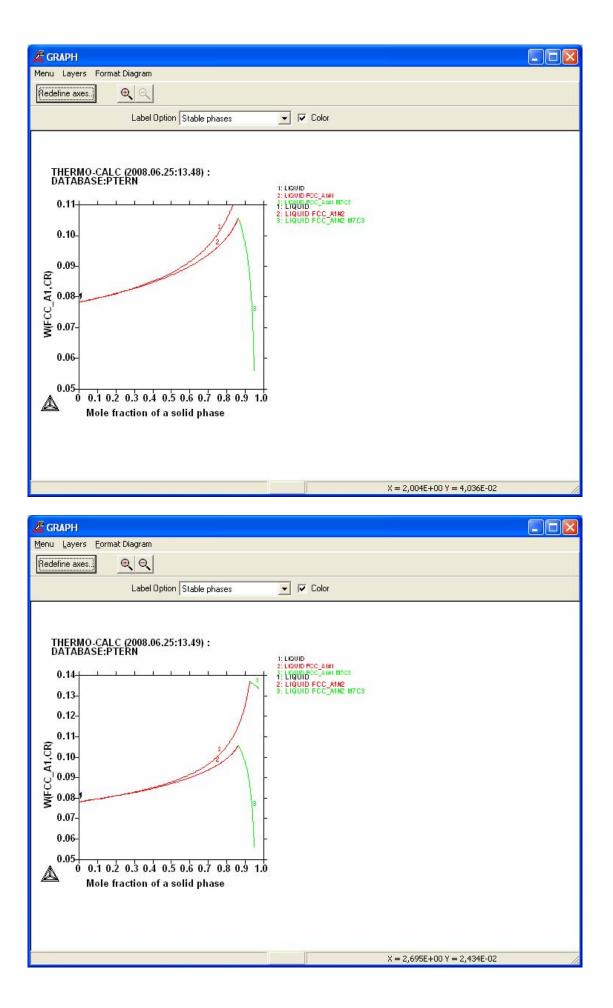


- 8. Click <u>Menu</u> \rightarrow Save. Specify file type as Experimental File (*.exp) and file name as EXAMPLE15_2. Click <u>Save</u>.
- **9.** Activate the MAIN window. Click \square . We are going to do a simple Scheil simulation without considering C back diffusion and compare the results.
- **10.** Click *Next*. The previously selected database and elements has been kept and no need to change.
- **11.** Click *Next*. Enter the same conditions as before (10 mass-percent Cr, 1 mass-percent C and T=2273.15) but keep the interstitial box for C unchecked.
- 12. Click *Next* to accept default X and Y-axis variables to plot the solidification curve.
- **13.** Click *Menu* \rightarrow *Append* and then *Add*. Select file *EXAMPLE15.exp* and click *Open* followed by *OK* (*make sure the file has the box checked*).

14. The solidification curve from the modified Scheil simulation is now superimposed on the result of the simple Scheil simulation.



- **15.** Do the same as Steps 9, 10, 11 and 6. Append file *EXAMPLE15_2.exp* in a way similar as in Step 13. One gets a comparison of solute segregation result from the two simulation models.
- **16.** Choose *Scaling...* from the *Format Diagram* menu. Specify the minimum as 0.05 and maximum as 0.11 for the *Y-axis*. Click *Next*. A better scaled diagram is drawn.



16 Calculation of Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel

- 1. Click *Elements* in the MAIN window.
- 2. Select *TCFE6* under the Database option and then click alloy elements *Fe*, *Cr*, *Ni*, *Mo*, *C*, *N*, *Si*, and *Mn* in the periodic table. Select the *Phases* tab. Click dots to reject all phases first, and then mark the phases *FCC_A1*, *BCC_A2*, *HCP_A3*, *M23C6*, and *SIGMA* and click dots to restore only these phases.

Z DATA		
Alphabetic List Periodic Table	Phases Constituents	
Rejected Phases:	Selected Phases:	
B2_BCC B2_VACANCY L12_FCC HIGH_SIGMA GAS:G LIQUID:L DIAMOND_FCC_A4 GRAPHITE CEMENTITE M7C3 M6C M5C2 M3C2 MC_ETA MC_SHP KSI_CARBIDE A1_KAPPA Z_PHASE FE4N_LP1 FECN_CHI C:	 FCC_A1 BCC_A2 HCP_A3 M23C6 SIGMA >>> 	
Material	Next Cancel	<u>H</u> elp

3. Click *Next*. Specify the concentrations of CR, NI, MO, C, N, SI, and MN as 25, 7, 4, 0.002, 0.27, 0.3, and 0.3, mass-percent respectively. Set start temperature to 1323 K. The default temperature unit can be changed by selecting *Output* in the *Options* menu in the MAIN window.

Number of Missing Conditions	0		Set Reference State Components	User Symbols Advanced Condition	1.1	Start Values Phases
Temperature Pressure System Size Moles	1323 101325 1	K Pa moles	Redefine Componer FE CR NI		* C * C	s-percent Condition Composition Composition Composition
-All Defined Conditions in SI Units T=1000 P=1.01325E5 N=1 W(CR)=0.25 W(NI)=7E-2 W(M0)=4E-2 W(C)=2E-5 W(N)=2.7E-3 W(SI)=3E-3 W(M)=2E-3			MŪ C N SI MN	4 0,002 0,27 0,3 0,3	% (% (% (Composition V Composition V Composition V Composition V Composition V
Fixed Phases						
Back Script Managemen	t Show Value		Compute	Next	Cancel	Help

4. Click *Compute*. The phase equilibrium is calculated and the result is shown in a text window.

🖉 MAIN	
File Edit Applications Script Options Window Help	
Constant Con	
🖉 Eq. 1	
BCC_A2#1 STATUS ENTERED Driving force 0,0000E+00 Number of moles 4,4223E-01, Mass 2,4671E+01 Mass fractions: FE 6,24173E-01 MO 5,01575E-02 N 3,38915E-04 CR 2,68972E-01 SI 3,51472E-03 C 5,25959E-06	
NI 5,03822E-02 MN 2,45631E-03 Constitution: Sublattice 1 Number of sites 1 FE 6,2437E-01 CR 2,8898E-01 NI 4,7957E-02 MO 2,9206E-02 SI 6,9909E-03 MN 2,4977E-03 Sublattice 2 Number of sites 3 VA 9,9954E-01 N 4,5057E-04 C 8,1543E-06	
FCC_A1#1 STATUS ENTERED Driving force 0,0000E+00 Number of moles 5,5777E-01, Mass 3,0647E+01 Mass fractions: FE 6,37001E-01 MO 3,18233E-02 SI 2,58565E-03 CR 2,34728E-01 N 4,60067E-03 C 3,18660E-05 NI 8,57922E-02 MN 3,43767E-03	
Constitution: Sublattice 1 Number of sites 1 FE 6,3834E-01 CR 2,5264E-01 NI 8,1807E-02 MO 1,8563E-02 SI 5,1522E-03 MN 3,5019E-03 Sublattice 2 Number of sites 1 VA 9,8147E-01 N 1,8382E-02 C 1,4848E-04 Constitution: Sublattice 1 Number of sites 1	H
Sublatice 1 Number of Sites 1 FE 6,3834E-01 CR 2,5264E-01 NI 8,1807E-02 MO 1,8563E-02 SI 5,1522E-03 MN 3,5019E-03 Sublatice 2 Number of Sites 1 VA 9,8147E-01 N 1,8382E-02 C 1,4848E-04	~
	>

5. Select the *Phases* tab on the CONDITIONS window. Choose *BCC_A2* and change the *Phase Status* option to *FIXED* with an amount of 0.5 moles. In a similar way, change the phase status of *FCC_A1#2* to *SUSPENDED* in order to avoid possible trouble with this suppose-to-be MC carbide phase during calculation. The system is over-conditioned now and the Degree of Freedom becomes -1. Release the Temperature condition by either removing 1323 in the Temperature box or marking the T=1323 condition in the list of defined conditions and then clicking *Delete*.

Number of Missing Conditions	0		Set Reference State Components	User Symb Advanced Cond		Start Values Phases
Temperature		к	Phases	Status	Moles	
Pressure	101325	Pa	BCC_A2 FCC_A1 FCC_A1#2	FIXED ENTERED SUSPENDED	0,50 0.56	_
System Size Moles	1	moles	HCP_A3 HCP_A3#2 M23C6 SIGMA SIGMA#2 SIGMA#3	ENTERED ENTERED ENTERED ENTERED SUSPENDED SUSPENDED	0.00 0.00 0.00 0.00	
P=1.01325E5 N=1 W(CR)=0.25 W(NI)=7E-2 W(M0)=4E-2 W(C)=2E-5 W(N)=2.7E-3 W(SI)=3E-3 W(MN)=3E-3			Phase Status:		moles	
Delete					mores	
Fixed Phases BCC_A2 = 0,50				Phase Condi		
Back Script Managemen	t Show Value		Compute	Next	Cancel	<u>H</u> elp

6. Click *Compute*. The equilibrium under the defined conditions is calculated. The temperature for developing the duplex structure in this steel is obtained and can be found in the equilibrium result window.

A MAIN					
File Edit Applications	Script Options Window	Help Elements Materi	ial		
🖉 Eq 2					
Number of moles o	K (1108C, 2027F), Pi f components 1,0000 -7,86534E+04, Enth	IOE+00, Mass 5,531	80E+01	6	^
Component	Moles	Mass-Fraction	Activity	Potential	Ref.State
C CR FE MN MO N N SI	9,2112E-05 2,6597E-01 6,2530E-01 3,0208E-03 2,3064E-02 1,0663E-02 6,5978E-02 5,9088E-03	2,0000E-05 2,5000E-01 6,3128E-01 3,0000E-03 4,0000E-02 2,7000E-03 7,0000E-02 3,0000E-03	2,7951E-05 2,0954E-03 1,3658E-03 2,3755E-06 4,7945E-04 6,6471E-07 1,0967E-04 4,7824E-09	-1,2043E+05 -7,0845E+04 -7,5761E+04 -1,4875E+05 -8,7785E+04 -1,6337E+05 -1,0473E+05 -2,2005E+05	SER SER SER SER SER SER SER SER SER
BCC_A2#1 STATUS FIXED Driving force 0,0000E+00 Number of moles 5,0095E-01, Mass 2,7933E+01 Mass fractions: FE 6,26660E-01 MO 4,86103E-02 N 4,70180E-04 CR 2,64435E-01 SI 3,46209E-03 C 5,96269E-06 NI 5,38048E-02 MN 2,55179E-03 Constitution: Sublattice 1 Number of sites 1 FE 6,2688E-01 CR 2,8412E-01 NI 5,1216E-02 MO 2,8306E-02 SI 6,8865E-03 MN 2,5949E-03 Sublattice 2 Number of sites 3 VA 9,9937E-01 N 6,2510E-04 C 9,2447E-06					
Mass fractions: FE 6,35993E-01	STATUS ENTERED ,9905E-01, Mass 2,73 MO 3,12173E-02 9 N 4,97447E-03 C MN 3,45719E-03	385E+01 6I 2,52865E-03	orce 0,0000E+00		
<					

7. Go back to the CONDITIONS window and select the User Symbols tab to define two PRE functions. In the Name box, input PREFCC. In the Expression box, input 100*W(FCC,CR)+300*W(FCC,MO)+1600*W(FCC,N). Click Add Symbol. Then, in a similar way, enter the PRE function for BCC_A2, i.e., enter the name PREBCC and the expression 100*W(BCC,CR)+300*W(BCC,MO)+1600*W(BCC,N).

Number of Missing Conditions	0	Components Advanced Conditions Phases Set Reference State User Symbols Start Values
Temperature Pressure System Size Moles	I01325 Pa 1 moles	All Defined Symbols PREFCC=100*W(FCC_A1#1,CR)+300*W(FCC_A1#1,M0)+1 PREBCC=100*W(BCC_A2,CR)+300*W(BCC_A2,M0)+1600*
All Defined Conditions in SI Units P=1.01325E5 N=1 W(CR)=0.25 W(NI)=7E-2 W(M0)=4E-2 W(C)=2E-5 W(N)=2.7E-3 W(SI)=3E-3 W(MN)=3E-3 W(MN)=3E-3		Type Name Function Expression
Fixed Phases BCC_A2 = 0,50		Add Symbol
Back Script Managemen	t Show Value	ComputeNextCancelHelp

8. Let's have a look of the PRE values now. Click *Show Value*. A window pops up. Choose the function *PREFCC* from the *User Symbols* list and click *Show*. Do same with PREBCC. Close the window by clicking *Close*.

K SHOW VALUE		
Temperature and Pressure	Potential and Activity	
_	•	
Compositional Variables	Phase Variables	
•	•	
Energy Variables	Additional Quantities	
•	•	
Partial Derivatives		
	•	
User Symbols		
PREBCC		(Show)
Show Value of: PREBCC		
Variable	Mnemonic	Value
	PREBCC	41,7789
	PREFCC	40,852
Calculate Equilibrium	Clear	Close

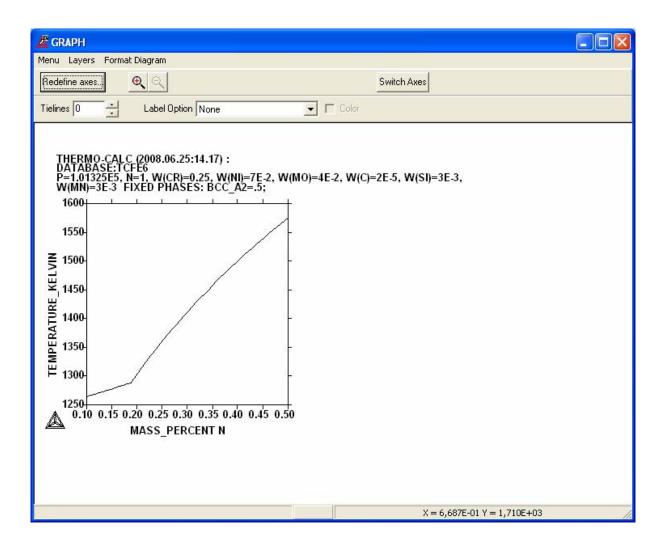
9. Calculate the PRE of duplex steel with different content of nitrogen. Click *Next* on the CONDITIONS window. The MAP/STEP DEFINITION window appears. Select *W(N)* for *Axis 1* and change Min value to 0.1 and Max value to 0.5. Click *Next*.

A MAP/STEP DEFINITION	
Axis 1 Variable W(N) ▼ Min (%) No of steps Max (%) 0.1 50 0.5	Axis 2 Variable NONE
Overwrite Previous Calculation Step Sepa Generate Automatic Start Points Back Script Management Script Management	nate Next Cancel <u>H</u> elp

10. The DIAGRAM DEFINITION window appears. First let's see how the temperature for the formation of duplex structure varies with nitrogen content. Select *Mass Percent* for the X-Axis and *Temperature Kelvin* for the Y-Axis. Click *Next*.

Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Temperature Unit C Celsius Kelvin C Fahrenheit	Composition Unit C Moles V Percent C Mass
Diagram Title	
X-Axis Variable Composition	Y-Axis Variable Temperature
For Component For Phase	For Component For Phase
X-Axis Text 🔽 Automatic MASS_PERCENT N	Y-Axis Text CAutomatic TEMPERATURE_KELVIN
Back	Next Cancel <u>H</u> elp

11. The dependence of temperature on nitrogen concentration is shown for the steel with duplex structure.



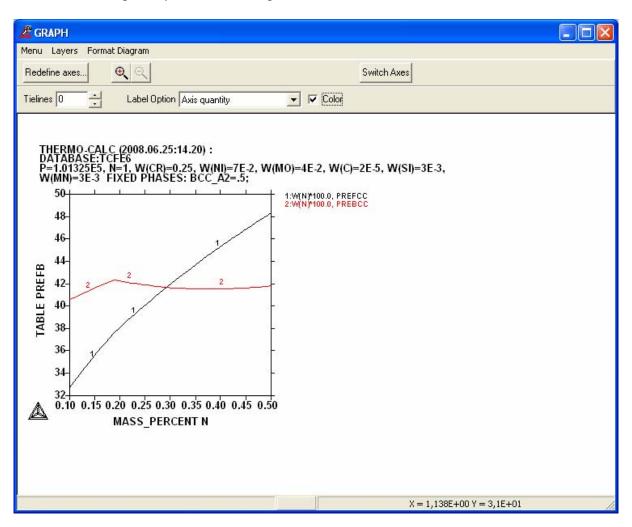
12. Click *Redefine*. Select the *User Symbols* tab. Change symbol *Type* to *Table*. Enter name *PREFB*. Enter expression *PREFCC*, *PREBCC*, click *Add Symbol*.

A DIAGRAM DEFINITION			
Diagram Axes Scaling User Symbols Advanced Diagra	m Axes All Defined Symbols PREFCC=100*W(FCC_A1#1,CR)+ PREBCC=100*W(BCC_A2,CR)+30 PREFB=PREFCC,PREBCC	300°W(FCC_A1#1,M0)+1 0°W(BCC_A2,M0)+1600°	
	Type Table	Name	
X.dvie Text V Auto	Add Symbol Delete Sym		Automatic
X-Axis Text Autor MASS_PERCENT N Back	matic	Y-Axis Text TEMPERATURE_KELVIN Next	Cancel

13. Select *Advanced Diagram Axes* tab. Select *PREFB* as Y-Axis *Variable*. Click *next* to plot.

A DIAGRAM DEFINITION	
Diagram Axes Scaling User Symbols Advanced Diagram Axes	
Diagram Title	
J.	
X-Axis	Y-Axis
Temperature and Pressure Potential and Activity	Temperature and Pressure Potential and Activity
For Component Compositional Variables Phase Variables N	Compositional Variables Phase Variables
Mass-percent 💌	
Energy Variables Additional Quantities	Energy Variables Additional Quantities
Partial Derivatives	Partial Derivatives
User Symbols	User Symbols
	PREFB
,	
X-Axis Text 🔽 Automatic	Y-Axis Text 🔽 Automatic
MASS_PERCENT N	TABLE PREFB
- New Creek Mindew	
Back New Graph Window	Next Cancel <u>H</u> elp

14. Choose Axis quantity in the Label Option menu and check the Color box.



17 Calculation of Speciation of a Gas

- 1. Click *Elements* in the MAIN window.
- 2. Select *SSUB4* from the Database list and then click elements *C*, *H*, *O*, and *S* in the periodic table. Click *Next*.
- **3.** Click *Redefine*. In the REDEFINE COMPONENTS window, change C to *C1O2*, H to *H2*, O to *O2S1*. Click *OK*.

🖉 REDI	FINE COMPO	NENTS	
Comp	ponents:		
C102		H2 S	
		the components nditions will be lo	
]	ОК	Cancel	Help

4. Select *Moles* as *Default Unit*. Enter value 5 for C1O2, *10* for H2, *0.1* for O2S1, and *0* for S. Set the temperature to 750 °C and the pressure to *1E5*. Click *Next*.

Number of Missing Conditions Temperature	0 750 C	Set Reference State Components	User Symbols Advanced Conditions Composition Unit	Start Values Phases Moles
Pressure System Size Moles All Defined Conditions in SI Units N(H2)=10 N(C102)=5 N(02S1)=0.1 N(S)=0 T=1023.15	100000 Pa moles	Redefine Component C102 H2 02S1 S	Value 5 mol 10 mol 0.1 mol 0 mol	es Composition - composition -
P=1E5	L. Show Value	Compute	Next Can	sel Help

5. Keep the temperature variable for *Axis 2* and change the variable of *Axis 1* to *NONE*.

A MAP/STEP DEFINITION	
Axis 1 Variable NONE Min No of steps Max	Axis 2 Variable T Min (C) No of steps Max (C) 500 50 2000
Image: Constraint of the second se	ate
Back Script Management	Next Cancel <u>H</u> elp

6. Click *Next*. A stepping calculation is performed and the DIAGRAM DEFINITION window appears. The default axes are *Temperature Celsius* and *Phase Fraction* for *all* phases. Keep these axes and click *Next*.

Z DIAGRAM DEFINITION		
Diagram Axes Scaling User Symbols Advanced Diagram Axe	18	
Temperature Unit Celsius C Kelvin C Fahrenheit		Moles 🗖 Percent Mass
Diagram Title		
X-Axis Variable Temperature	Y-Axis Variable Phase Fraction For Component	▼ For Phase
		ALL
X-Axis Text Zet Automatic	Y-Axis Text NPM(*)	🔽 Automatic
Back	┌─ New Graph Window	Cancel <u>H</u> elp

7. Click *Next* to plot the diagram. Choose *Logarithmic Y-axis* in the *Format Diagram* menu. Select *Axis quantity* in the *Label Option* menu and check the *Color* box.

🔏 graph	
Menu Layers Format Diagram	
Redefine axes 🔍 🔍 Switch Axes	
Label Option Axis quantity	
THERMO-CALC (2008.08.18:15.51): DATABASE:SSUB4 N(C102)=5, N(H2)=10, N(02S1)=0.1, N(S)=0, P=1E5; 10 10 10 10 10 10 10 10 10 10 10 10 10	
unable to detect with logarithmic axis X = 1,054E+03 Y = 1,758E-29	1

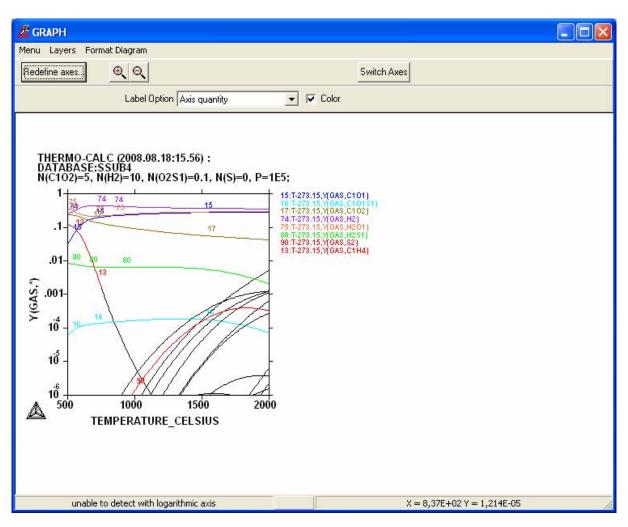
8. Click *Redefine*. Go to the *Advanced Diagram Axes* tab and select *Phase Constitution* for *all* species in the *GAS* phase as the Y-axis.

Z DIAGRAM DEFINITION		
Diagram Axes Scaling User Symbols Advanced Diagram Axes		
Diagram Title		
X-Axis	Y-Axis	
Temperature and Pressure Potential and Activity Temperature Celsius	Temperature and Pressure Potential and Activity	
Compositional Variables Phase Variables	For Species Compositional Variables Phase Variables ALL	•
	For Phase For Phase GAS	•
Energy Variables Additional Quantities	Energy Variables Additional Quantities	
Partial Derivatives	Partial Derivatives	
User Symbols	User Symbols	
X-Axis Text Automatic TEMPERATURE CELSIUS	Y-Axis Text IV Automatic	
Back	New Graph Window Next Cancel <u>H</u> elp	

9. Click *Next* to plot. Select *Axis quantity* in the *Label Option* menu, check the *Color* box and select *Logarithmic Y-axis* in the *Format Diagram* menu.

CRAPH	
Menu Layers Format Diagram	
Redefine axes.]	Switch Axes
Label Option Axis quantity	💌 🔽 Color
THERMO-CAL C (2008.08.18:15.53) : DATABASE:SUB4 N(C102)=5, N(H2)=10, N(02S1)=0.1, N(S)=0, P=1	1:T-273 15:Y(GAS.C) 2:T-273 15:Y(GAS.C)H01 2:T-273 15:Y(GAS.C)H01 4:T-273 15:Y(GAS.C)H01 4:T-273 15:Y(GAS.C)H01 5:T-273 15:Y(GAS.C)H201 5:T-273 15:Y(GAS.C)H202 5:T-273 15:Y(GAS.C)H202 10:T-273 15:Y(GAS.C)H202 10:T-273 15:Y(GAS.C)H202 10:T-273 15:Y(GAS.C)H201 11:T-273 15:Y(GAS.C)H201 12:T-273 15:Y(GAS.C)H201 13:T-273 15:Y(GAS.C)H201 11:T-273

10. Choose *Scaling...* from the *Format Diagram* menu. Change the Min value to *1E-6* and Max to *1* on the *Y-Axis* panel. Click next to plot.

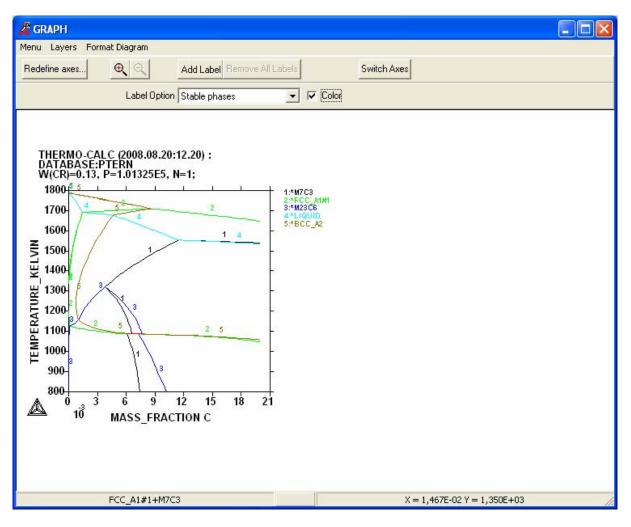


18 Calculation Using Script and how to Implement a Figure to a Word/PowerPoint file

- 1. Start TCW and select the *Script* tab in the MAIN window.
- 2. Choose *Run Script* under the *Script* tab and select the *Name* BENCH. Click *OK*.

🖉 RUN S	CRIPT
Name	BENCH
Database	PTERN
Elements	FE C CR
Initial Cond	litions W(C)=0.01 W(CR)=0.13 T=1200 P=101325 N=1 Axis 1: Condition W(C), Min 0, Step 0.0005, Max 0.02 Axis 2: Condition T, Min 800, Step 30, Max 2000
Amend	OK Cancel <u>H</u> elp

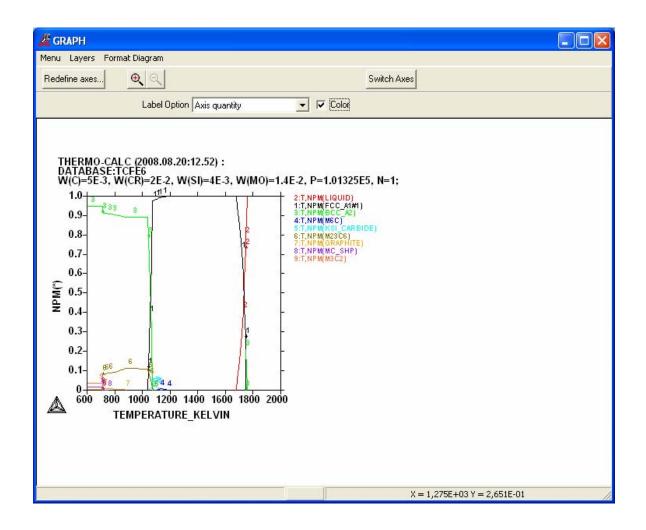
3. Select *Stable phases* in the *Label Option* menu and check the *Color* box.



- **4.** To create your own Script select *Script Management* under the *Script* tab in the MAIN window. Click on *New Script*.
- 5. Give the new Script the *Name* EXAMPLE18 and select e.g. the TCFE6 Database. Define Fe, C, Cr, Si, and Mo in the *Components* box and click the *Add* button. Enter T in the *Condition* box and give it the value 1200. Click the *Add* button. Repeat the last procedure to enter the composition of the defined system; W(C)=0.005, W(Cr)=0.02, W(Si)=0.004, W(Mo)=0.014. To fulfill all the degrees of freedom one must define the pressure, P=101325, and the size of the system, N=1.
- 6. Enter T as *Condition* for *Axis 1* with min 600 and max 2000 with a step length of 20. Click *Save*.

	т ма	NAGEMENT			
Name		EXAMPLE18	•	Ne	w Script
Databa	se	TCFE6	•	Del	ete Script
Components					
Condition Value					
Info Name: EXAMPLE18 Add Database: TCFE6 Components: FE C CR SI M0 Delete Conditions: T=1200 W(C)=0.005 W(CR)=0.02 W(SI)=0.004 W(M0)=0.014 P=101325 N=1 Axis1: Condition T, Min 600, Step 20, Max 2000					
Axis1 C	Conditio F	n	Min 600	Step 20	Max 2000
Axis2 C	onditio	n	Min	Step	Max
Axis3 C	onditio	n	Min	Step	Max
		[Save	Cancel	<u>H</u> elp

7. Choose *Run Script* under the *Script* tab in the MAIN window and select the *Name* EXAMPLE18. Click *OK* (the *Amend* button take you to the CONDITIONS window). Select *Axis quantity* in the *Label Option* menu and check the *Colo*r box.



8. Click *Menu* \rightarrow *Save*. Specify file type as e.g. Enhanced Meta File (*.emf) and file name as EXAMPLE18. Click *Save*.



9. Implement the figure into a Word/PowerPoint file using *Picture→From File* under the *Insert* tab (in Word or PowerPoint).