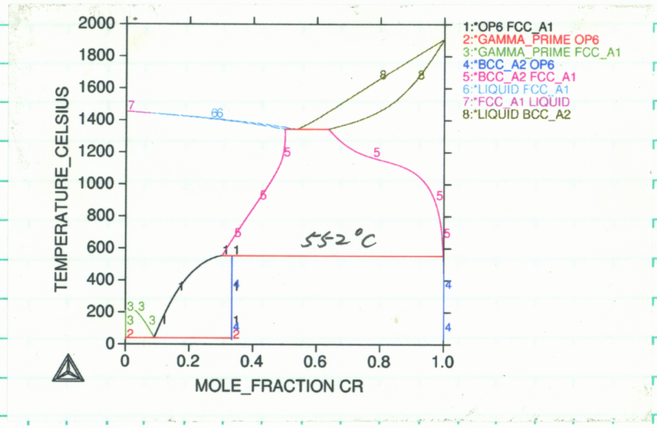
From Page No.

Case 9 - Replace with $\Delta E_{form}(Ni_2Cr) = -12000$ J/mol and exclude the $G(Cr_2Ni)$ term

```
CASE 9 with Ni-Data Database
 PARAM G(OP6,NI:CR;0) 298.15 +2*GHSERNI +GHSERCR -12000; 6000 N!
$ PARAM G(OP6,CR:NI;0) 298.15 +2*GHSERCR +GHSERNI +16443; 6000 N!
 PARAM G(OP6,NI,CR:CR;0) 298.15 +GHSERNI +2*GHSERCR +11690; 6000 N!
 PARAM G(OP6,NI,CR:NI;0) 298.15 +2*GHSERNI +GHSERCR -2703; 6000 N!
 PARAM G(OP6,NI:CR,NI;0) 298.15 +2.5*GHSERNI +0.5*GHSERCR -4171; 6000 N!
 PARAM G(OP6,CR:CR,NI;0) 298.15 +2.5*GHSERCR +0.5*GHSERNI +25506; 6000 N!
 PARAM G(OP6,NI,CR:CR,NI;0) 298.15 +1.5*GHSERNI +1.5*GHSERCR +8759; 6000 N!

 PARAM L(OP6,NI,CR:CR;0) 298.15 +62482;  6000 N!
 PARAM L(OP6,NI,CR:NI;0)  298.15 -43698;  6000 N!
 PARAM L(OP6,CR:CR,NI;0) 298.15 +69138;  6000 N!
 PARAM L(OP6,NI:CR,NI;0) 298.15 -2757;  6000 N!
 PARAM L(OP6,NI,CR:CR,NI;0) 298.15 -57782;  6000 N!
```



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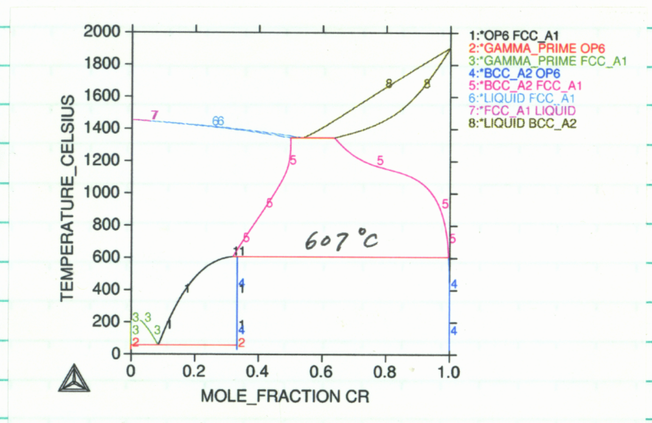
Case 10 - Replace with $\Delta E_{form}(Ni_2Cr) = -13000$ J/mol and exclude the $G(Cr_2Ni)$ term

```
CASE 10 with Ni-Data Database
 PARAM G(OP6,NI:CR;0) 298.15 +2*GHSERNI +GHSERCR -13000; 6000 N!
$ PARAM G(OP6,CR:NI;0) 298.15 +2*GHSERCR +GHSERNI +16443; 6000 N!
 PARAM G(OP6,NI,CR:CR;0) 298.15 +GHSERNI +2*GHSERCR +11690; 6000 N!
 PARAM G(OP6,NI,CR:NI;0) 298.15 +2*GHSERNI +GHSERCR -2703; 6000 N!
 PARAM G(OP6,NI:CR,NI;0) 298.15 +2.5*GHSERNI +0.5*GHSERCR -4171; 6000 N!
 PARAM G(OP6,CR:CR,NI;0) 298.15 +2.5*GHSERCR +0.5*GHSERNI +25506; 6000 N!
 PARAM G(OP6,NI,CR:CR,NI;0) 298.15 +1.5*GHSERNI +1.5*GHSERCR +8759; 6000 N!

 PARAM L(OP6,NI,CR:CR;0) 298.15 +62482;  6000 N!
 PARAM L(OP6,NI,CR:NI;0)  298.15 -43698;  6000 N!
 PARAM L(OP6,CR:CR,NI;0) 298.15 +69138;  6000 N!
 PARAM L(OP6,NI:CR,NI;0) 298.15 -2757;  6000 N!
 PARAM L(OP6,NI,CR:CR,NI;0) 298.15 -57782;  6000 N!
```



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Project No.
Book No.
TITLE Phase Diagram Calculations for Nominal Alloy 22 Composition

From Page No.

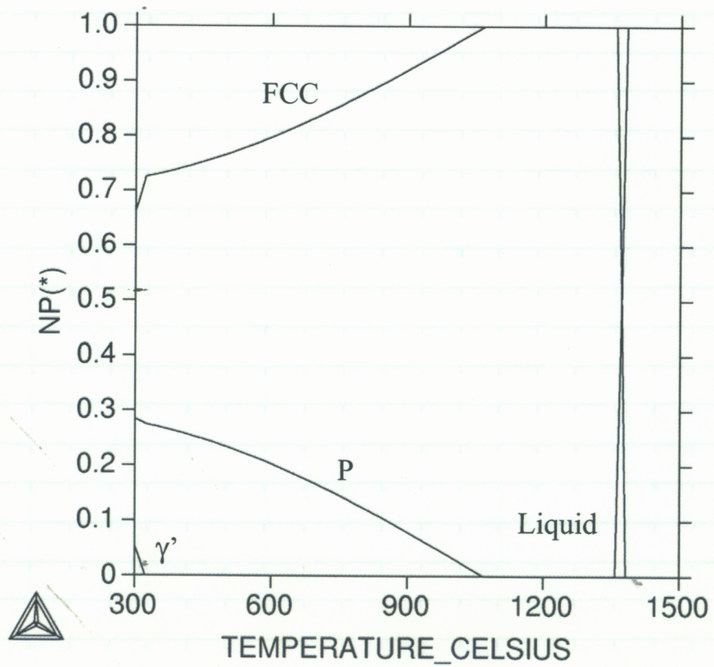
obj.: To extend the phase diagram calculations for multicomponent alloy systems such as Alloy 22

Software: THERMOCALC Version N
Database: Thermotech Ni-DATA Version 5 with the addition of the first-principles thermodynamic data set Case 7 (see page 35) for OP6 phase.

Nominal Composition: Ni-21.2 Cr-13.5 Mo-4 Fe-3 W in wt%

Results: Plots of phase fractions as a function of temperature

a. without first-principles thermodynamic data



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TITLE

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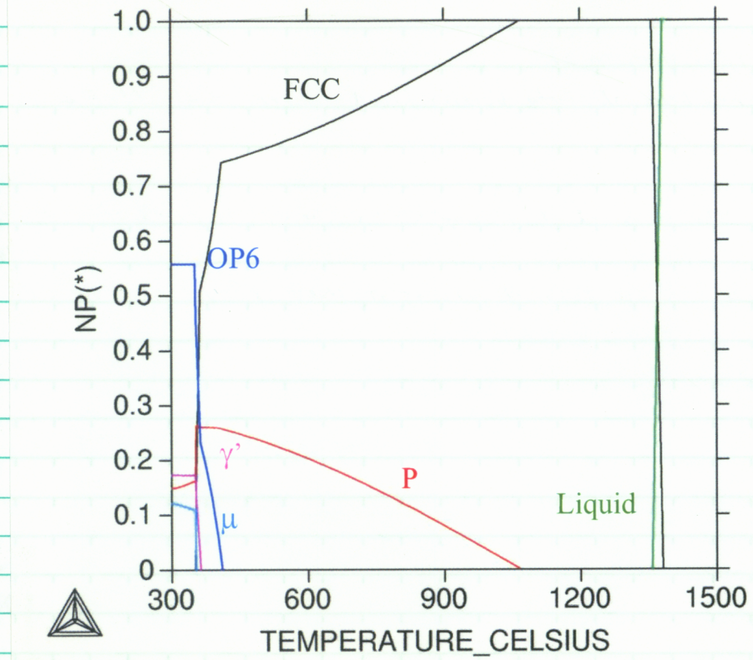
b. With first-principles thermodynamic data



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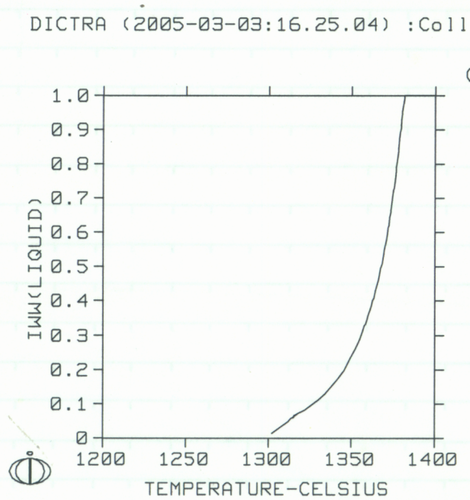
From Page No.

Obj.: To predict the solidification path of Alloy 22 by applying the moving boundary model incorporated with atomic mobility data in the DICTRA software package

Software: DICTRA Version 21
Database: Thermotech Ni-Data Version 5 and Thermo-Calc MOB2

1. Moving phase boundary simulations were conducted to predict the solidification path for Alloy 22. The nominal alloy composition, Ni-21.2Cr-13.5Mo-4Fe-3W in wt%, was used. Metastable calculation with suspension of σ-phase was assumed. The cooling rates in the DICTRA simulations were 1°C/s and 10°C/s. A cell size of 50 μm was used.

a. Cooling rate 1°C/s



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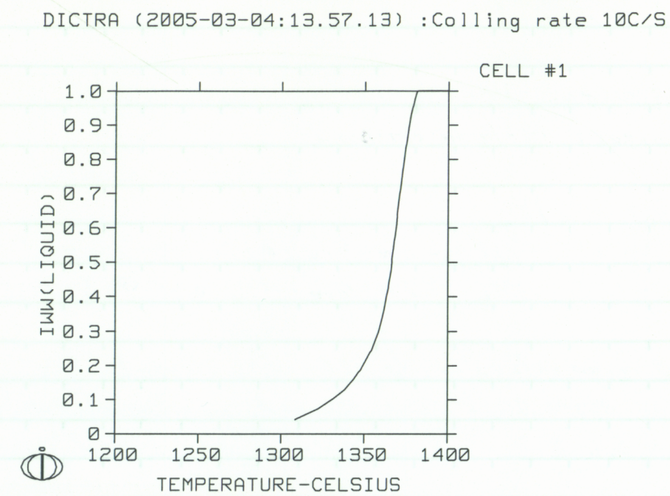
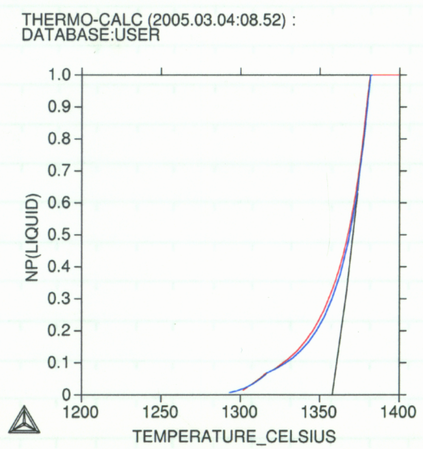
b. Cooling rate 10°C/s



2. Comparison was made with both equilibrium and Scheil simulations using THERMOCALC Version N (See #N 498, pages 86-91).



Red: DICTRA 1°C/s
Blue: THERMOCALC Scheil modulus
Black: THERMOCALC Equilibrium

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		Recorded by Mi Pan	3/8/05	copies sent to QA records Mi Pan 4/12/05