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Groupe Arcelor

INP Grenoble

Application of Thermodynamics calculations to LG3 and EN10 Alloys

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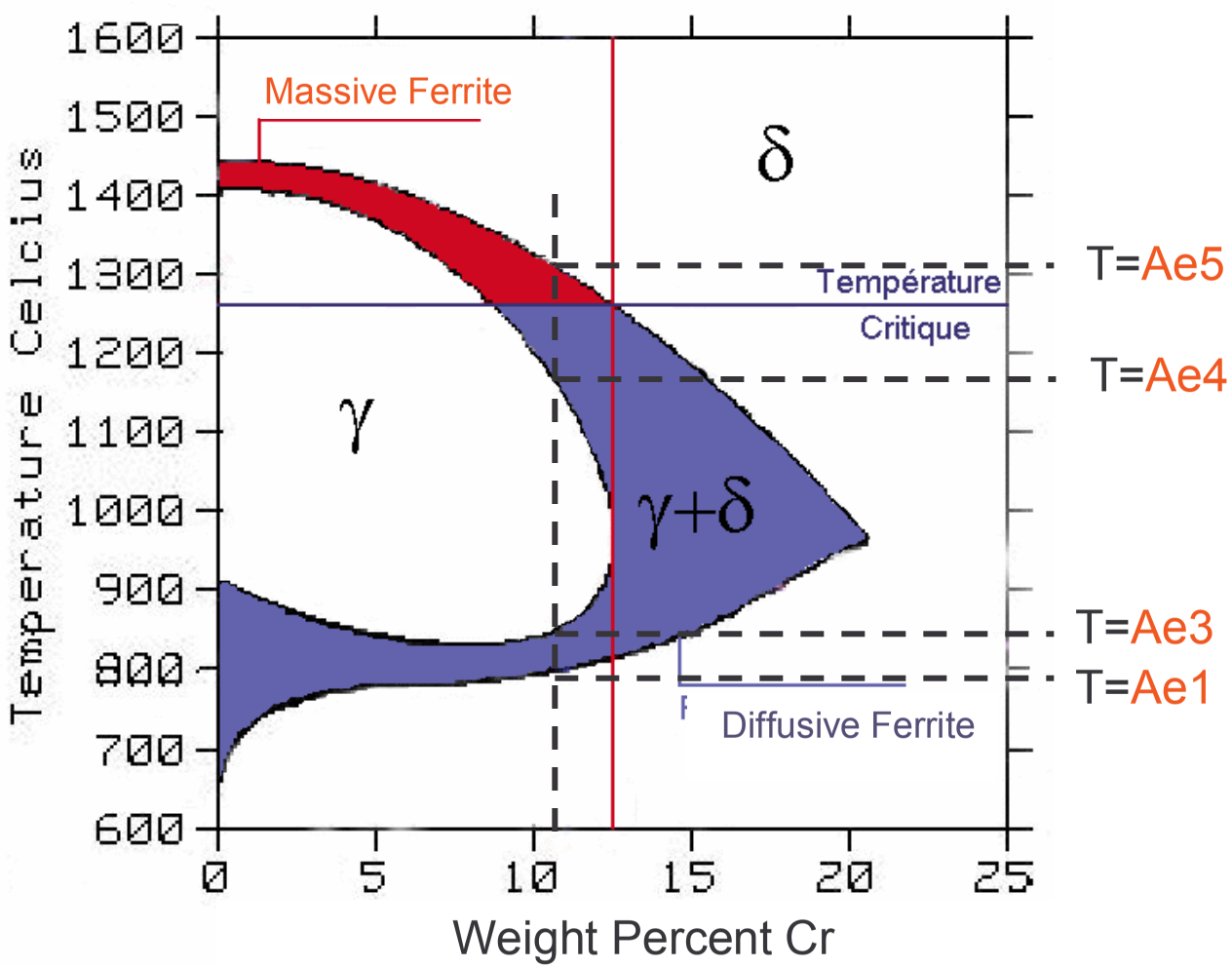
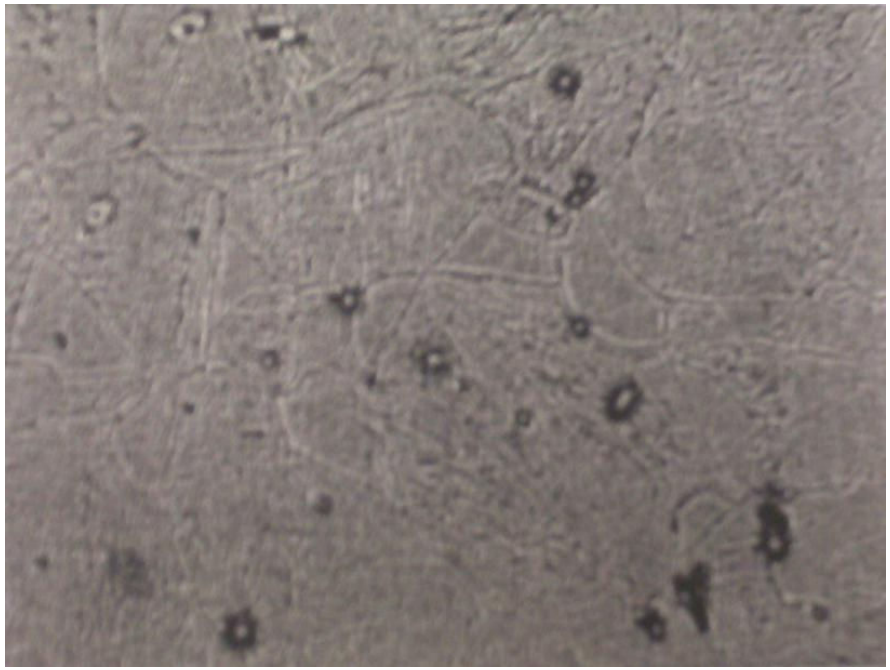
Presentation of Lacoude and Goux Model



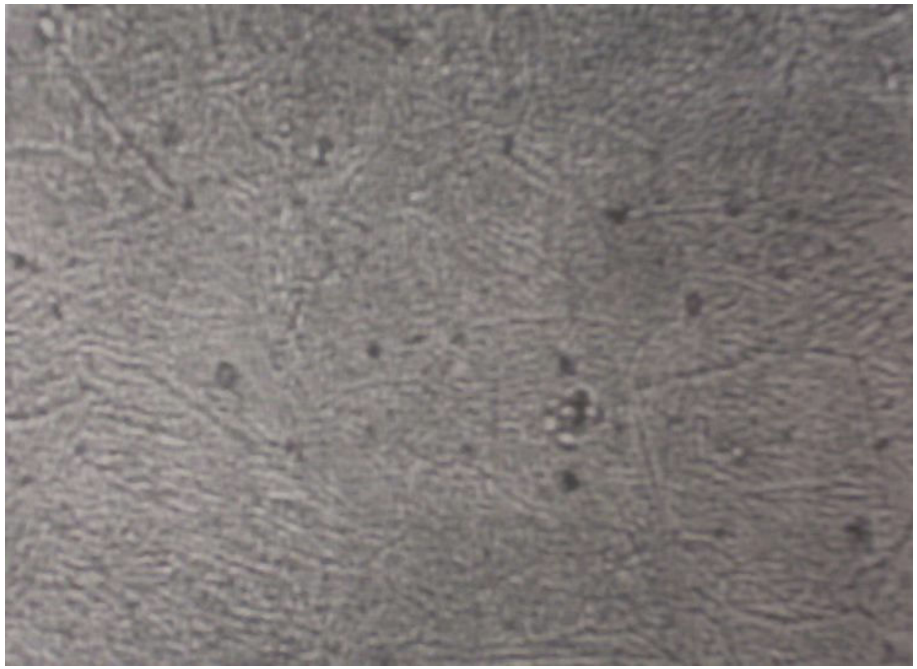
Isopleths of equilibrium phase diagram for Fe-Cr-0.010C-0.024 alloys.
Diagram calculated with ThermoCalc and TFCE3 database.

LG3 Alloy– Microstructural characterization

LG3: Fe-9.8Cr-0.010C-0.024N



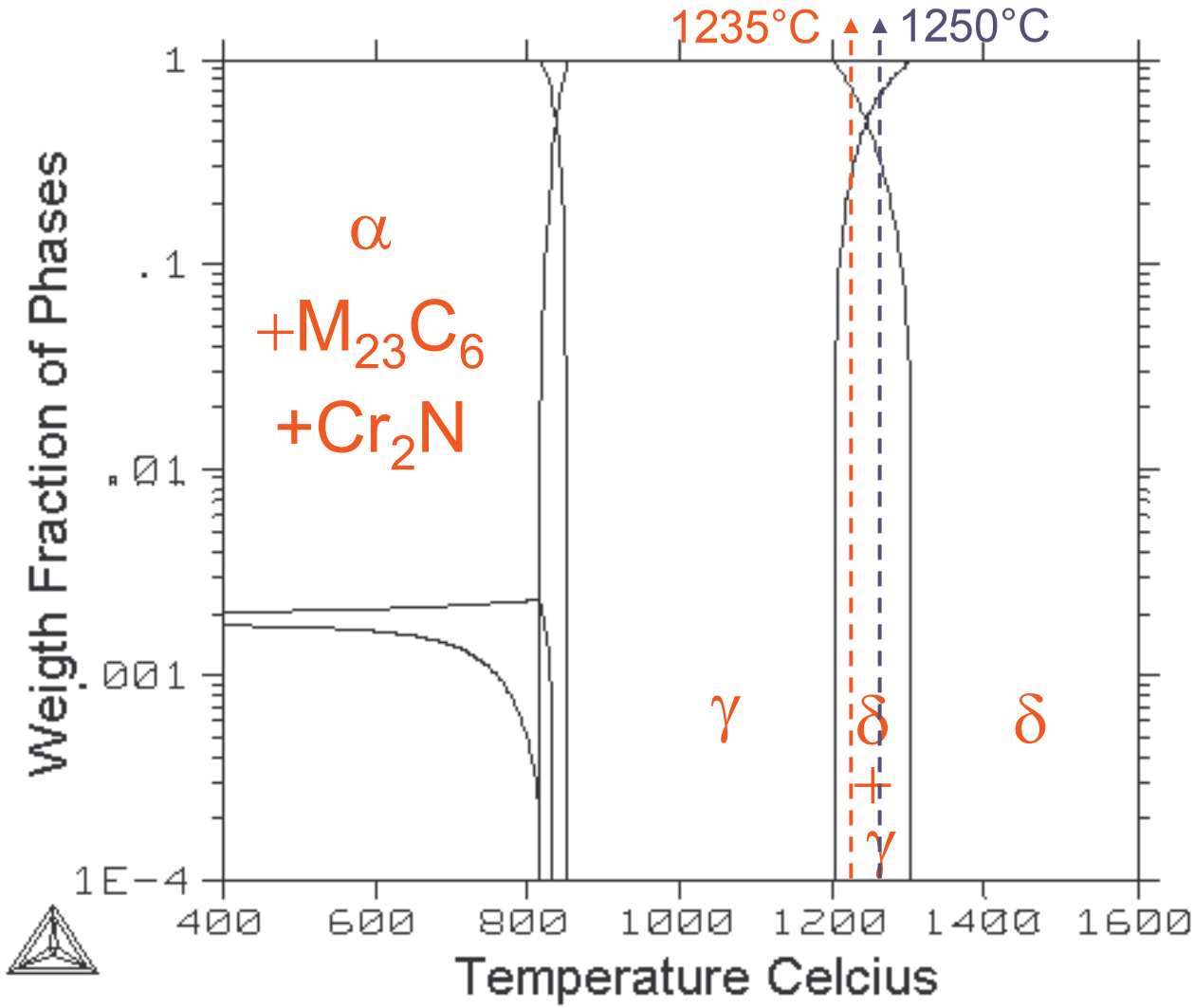
LG3 Alloy: Quenched in water after isothermal treatment at 1235°C.
2 phases: martensite + ferrite.
400x → Type II



LG3 Alloy: Quenched in water after isothermal treatment at 1250°C.
2 phases structure: 2 martensites.
400x → Type I

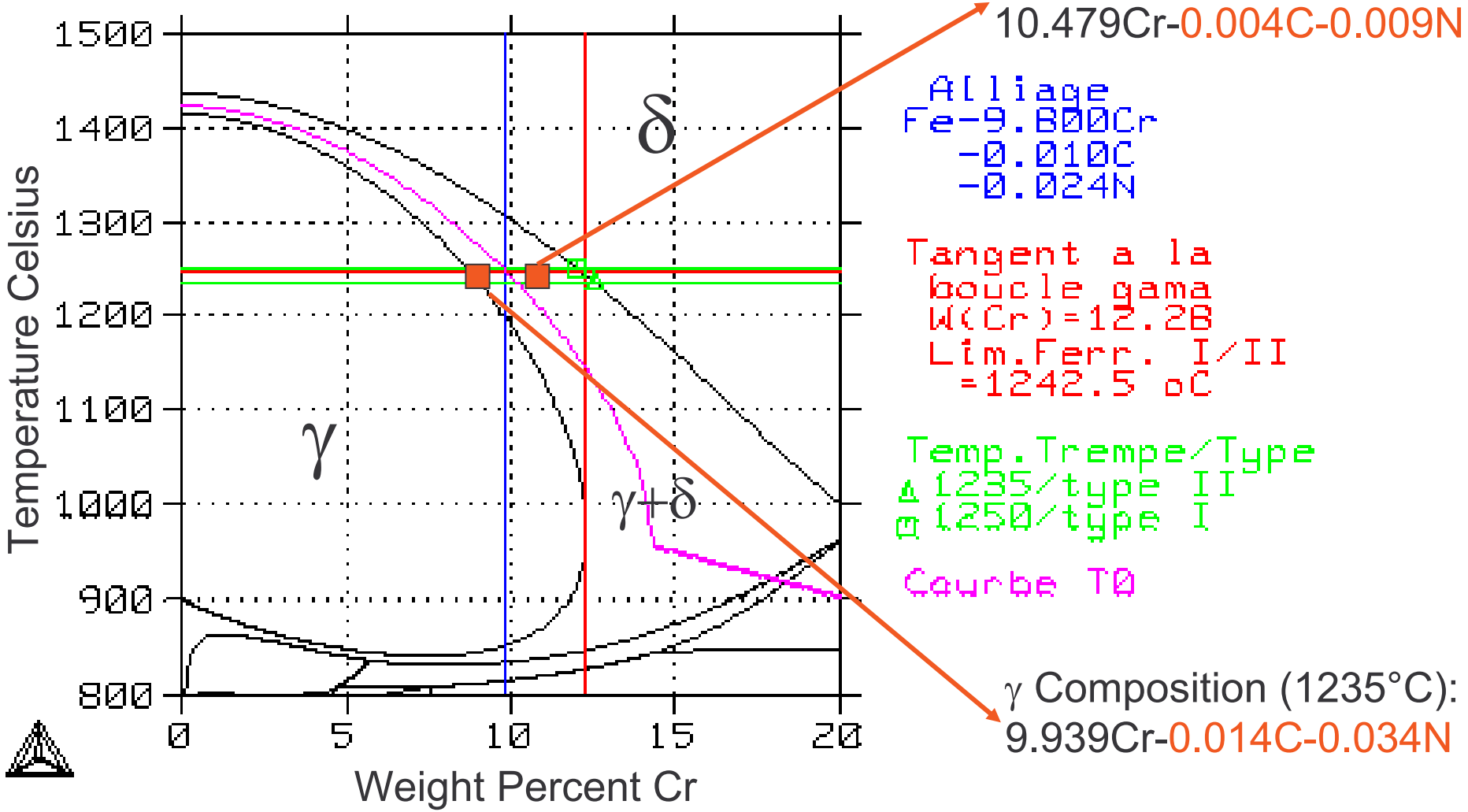
M. Lacoude, C. Goux. *"La transformation de la ferrite delta au cours d'un traitement de trempe".* Mem. Rev. Scient. Metall. LXIII, n°10, Oct. 1986, pp. 805-834

LG3 Alloy– Equilibrium diagram



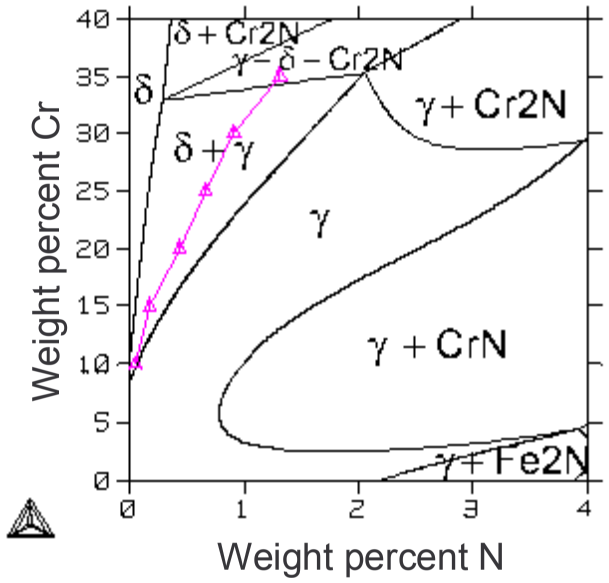
Equilibrium phase diagram for the Fe-9.8Cr-0.010C-0.024 alloy.
Diagram calculated with ThermoCalc and TCFE3 database.

Isopleths Pseudo Binary

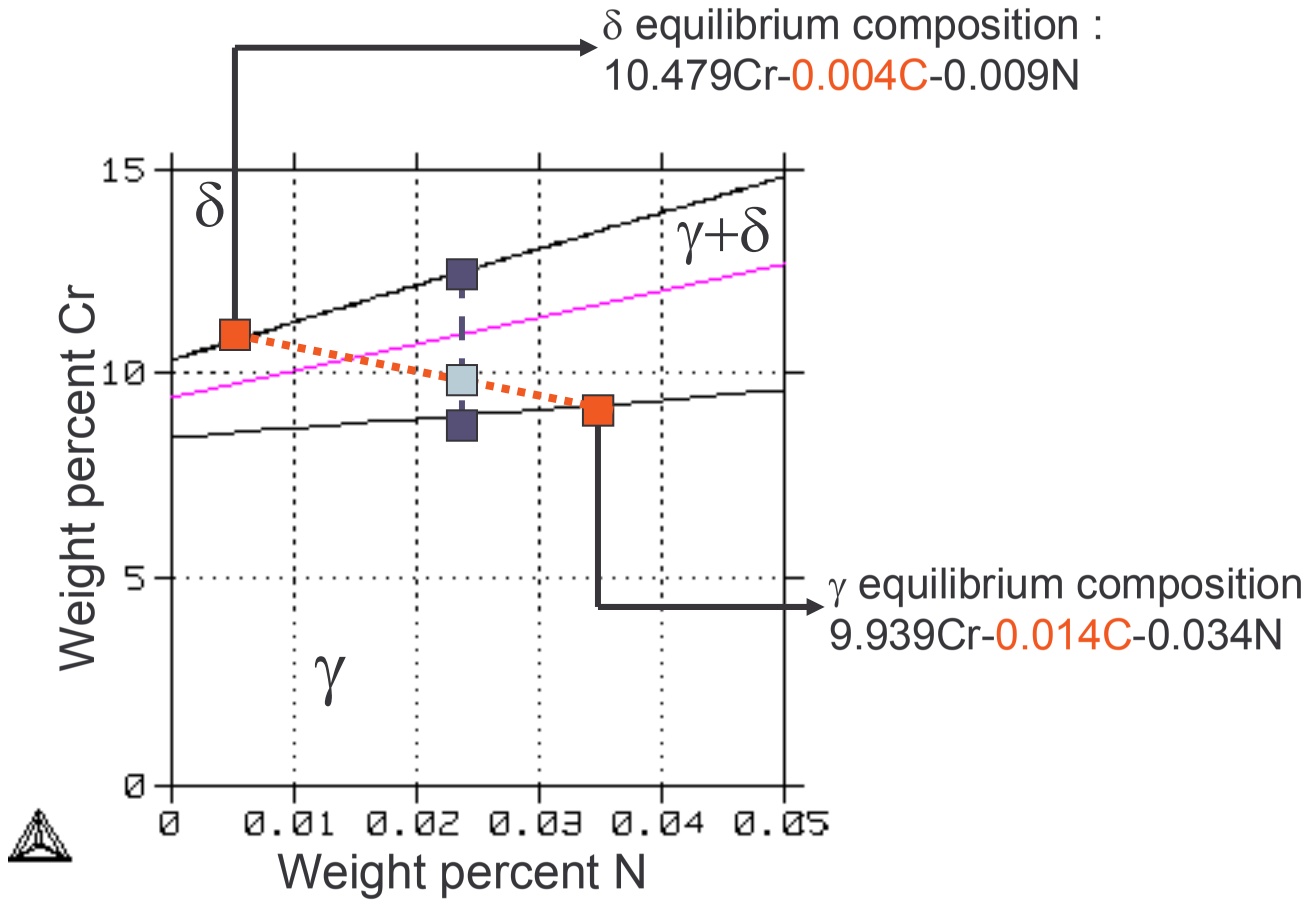


Isopleths of the equilibrium phase diagram for Fe-Cr-0.010C-0.024 alloys.
Diagram calculated with ThermoCalc and TCFE3 database.

Pseudo Ternary Isotherm – 1235°C



T_0 Curves

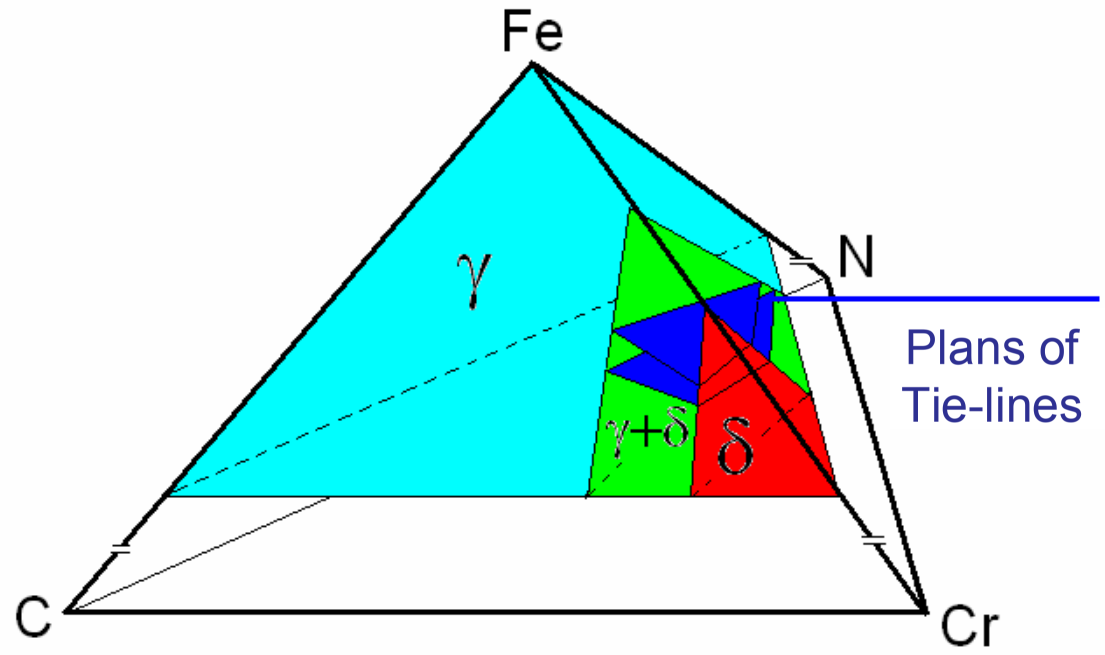


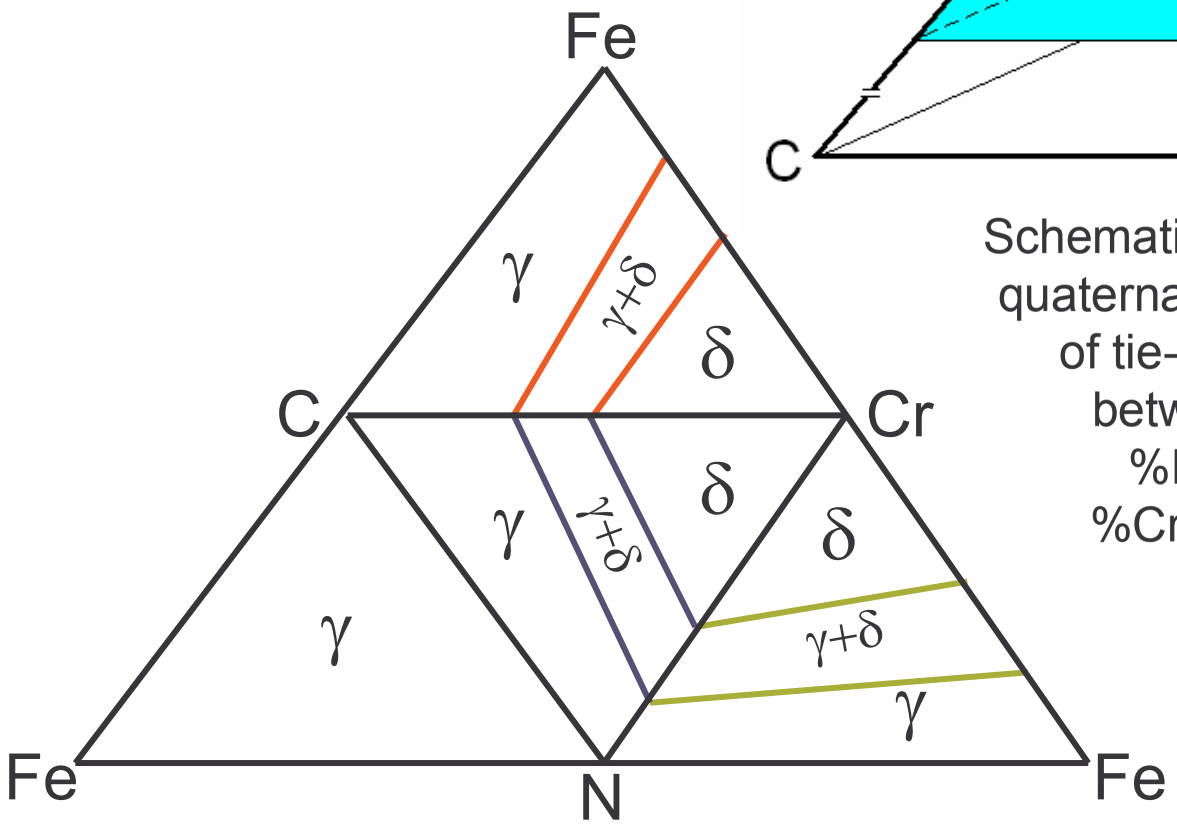
Pseudo ternary isotherms of the equilibrium phase diagram for Fe-Cr-0.010C-N alloys.
Diagram calculated with ThermoCalc and TFCE3 database.

Isotherm Quaternary - Tetrahedron

Ternary systems:
Fe-Cr-N, Fe-C-N Fe-C-Cr

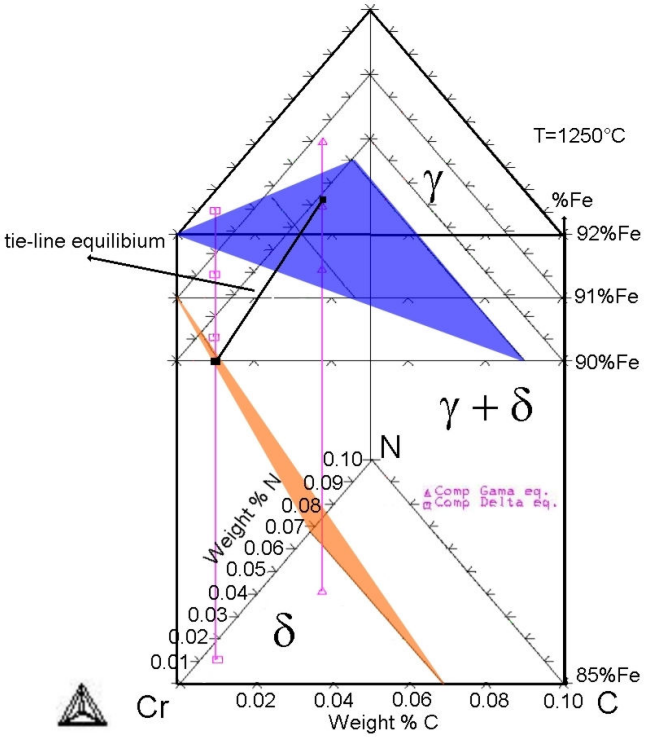
Pseudo-ternary system:
C-Cr-N-85.00Fe

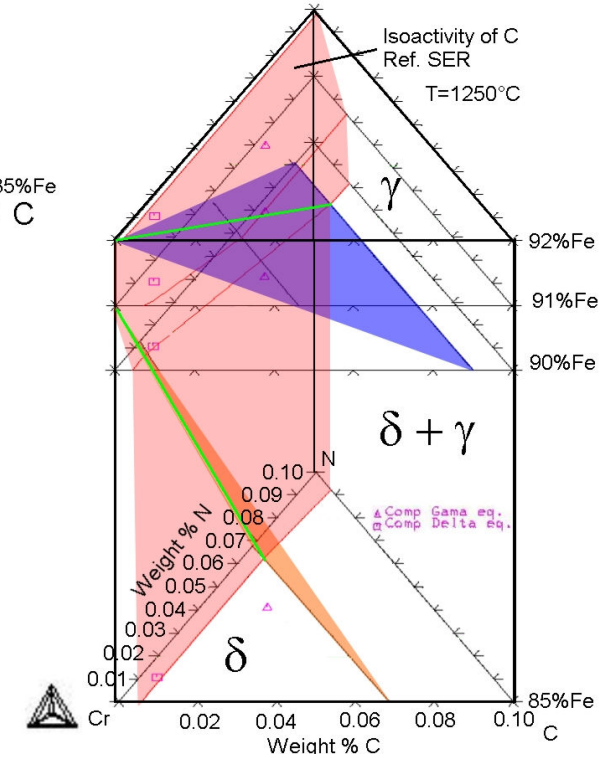


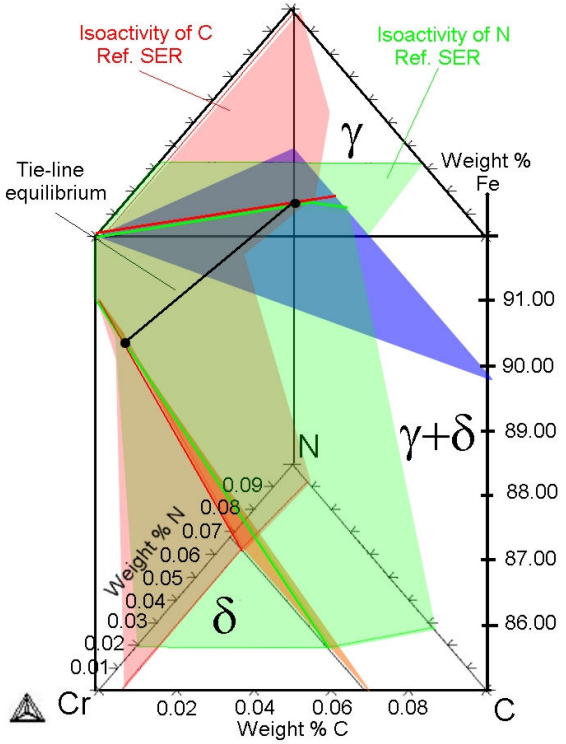


Schematic isothermal equilibrium for the quaternary system Fe-Cr-N-C, with the of tie-lines planes (Temperatures between 1000°C and 1450°C, %N, %C less than 1% and %Cr less than 20% in weight.)

Isotherms Quaternaries – Prisms







Pseudo ternary isotherms of the equilibrium phase diagram for %Fe-Cr-C-N alloys. Diagrams calculated with ThermoCalc and TFCE3 database.

Transposition of Lacoude and Goux Hypothesis for the quaternary system Fe-Cr-C-N

LG3 Alloy (type I at 1250°C / type II at 1235°C)

1) Calculation of equilibrium composition of delta ferrite at T_M
   → (Cr, C, N) at 1250°
   → (Cr, C, N) at 1235°

2) May those compositions exist for the one-phase field of austenite?
   → Calculation of solubility limits of Cr, C and N for the austenite
   → Verification of delta ferrite compositions with these solubility limits

3) Conclusions about the validity of Lacoude and Goux hypothesis for quaternary system.

Transposition of Lacoude and Goux Hypothesis for the quaternary system Fe-Cr-C-N

1) Calculation of equilibriums compositions of delta ferrite at T_M
   → (%Cr, %C, %N) at 1250°
   → (%Cr, %C, %N) at 1235°

Equilibriums compositions of delta ferrite for LG3 alloy: Fe-9.8Cr-0.010C-0.024N

Temperature	%Cr	%C	%N
1235°C	10.479	0.004	0.009
1250°C	10.266	0.004	0.011

Transposition of Lacoude and Goux Hypothesis for the quaternary system Fe-Cr-C-N

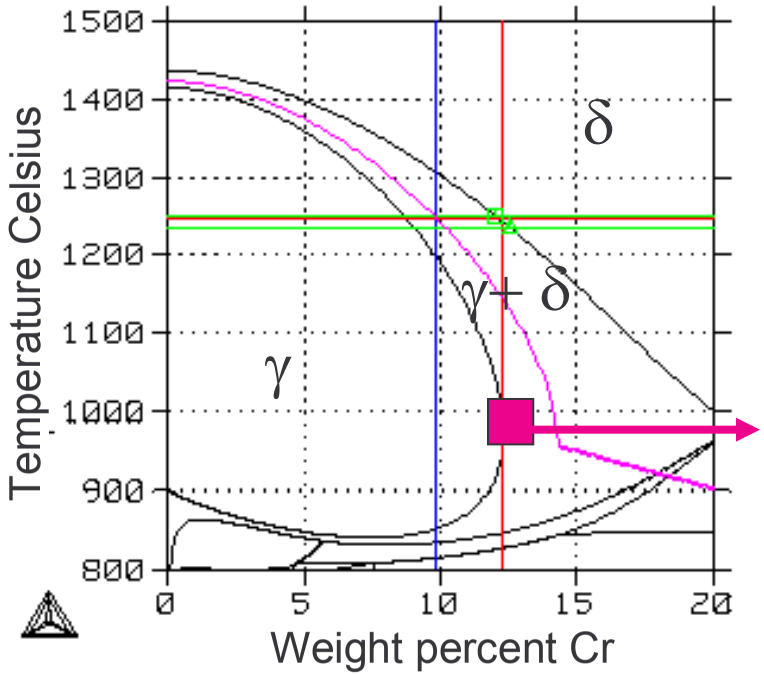
2) May those compositions exist for the mono-phase fields of austenite?
→ Calculation of solubility limits of Cr, C and N for austenite

Diagram	Positive Point	Negative Point
Isopleths Fe-Cr-C-N	Simple diagram in function of the temperature	Two compositions are fixed. They can not describe correctly the thermodynamics of the system.
Pseudo ternaries Fe-Cr-C-N	They are the correct variation for three elements.	Temperature and one composition are fixed.
Quaternary	They are the correct description for the system.	Hard to see and to draw the diagram (3D). Temperature is fixed.

Transposition of Lacoude and Goux Hypothesis for the quaternary system Fe-Cr-C-N

2) May those compositions exist for the mono-phase fields of austenite?

→ Simplification



{ 972°C
12.61%Cr

Composition at equilibrium of δ

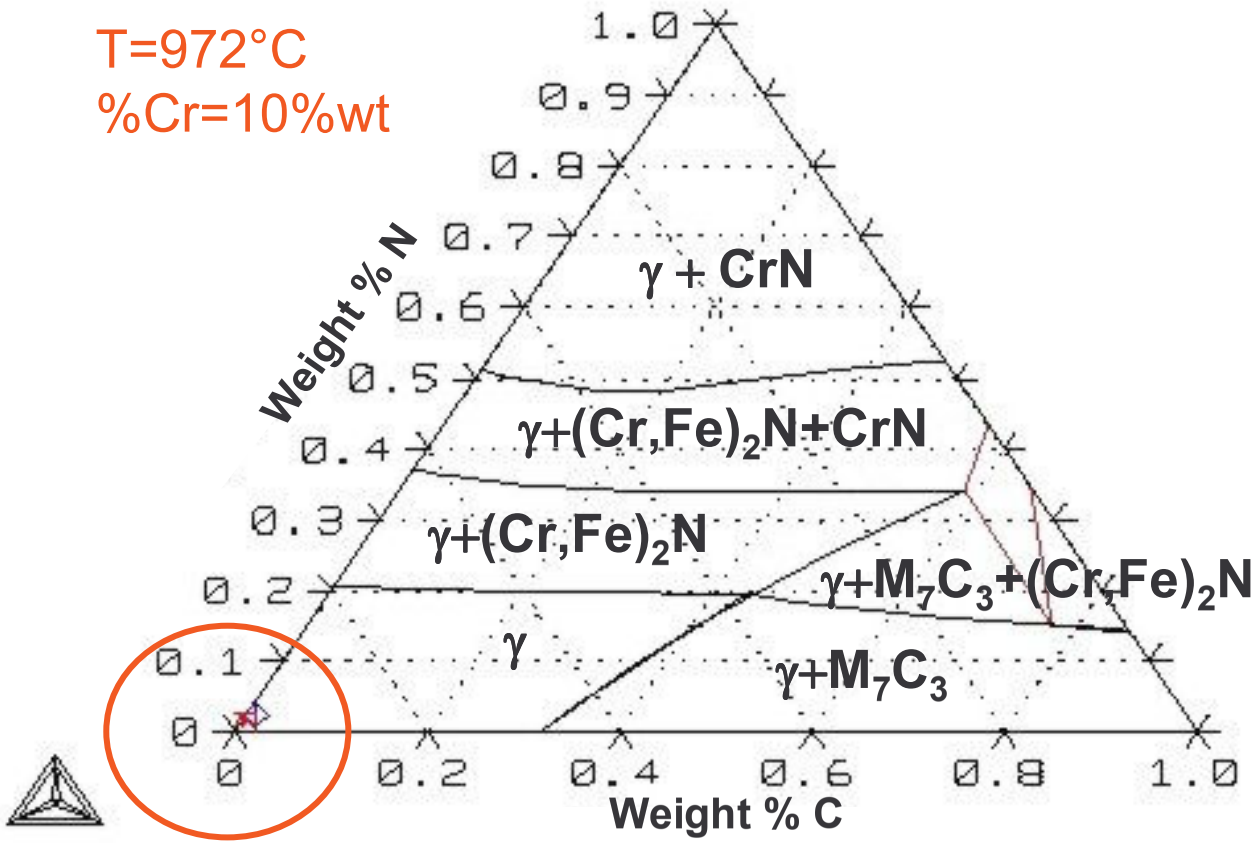
Temperature	%Cr
1235°C	10.479
1250°C	10.266

Solubility limit is superior to the $\%Cr_{eq}$

Isopleths of the equilibrium phase diagram for Fe-Cr-0.010C-0.024 alloys.
Diagram calculated with ThermoCalc and TCFE3 database.

Transposition of Lacoude and Goux Hypothesis for the quaternary system Fe-Cr-C-N

T=972°C
%Cr=10%wt



Temperature	%Cr
1235°C	10.479
1250°C	10.266
Average	10

Pseudo ternary isotherms of the equilibrium phase diagram for 90Fe-Cr-C-N alloys. Diagram calculated with ThermoCalc and TFCE3 database.

Transposition of Lacoude and Goux Hypothesis for the quaternary system Fe-Cr-C-N Alloy LG3

3) Conclusions:

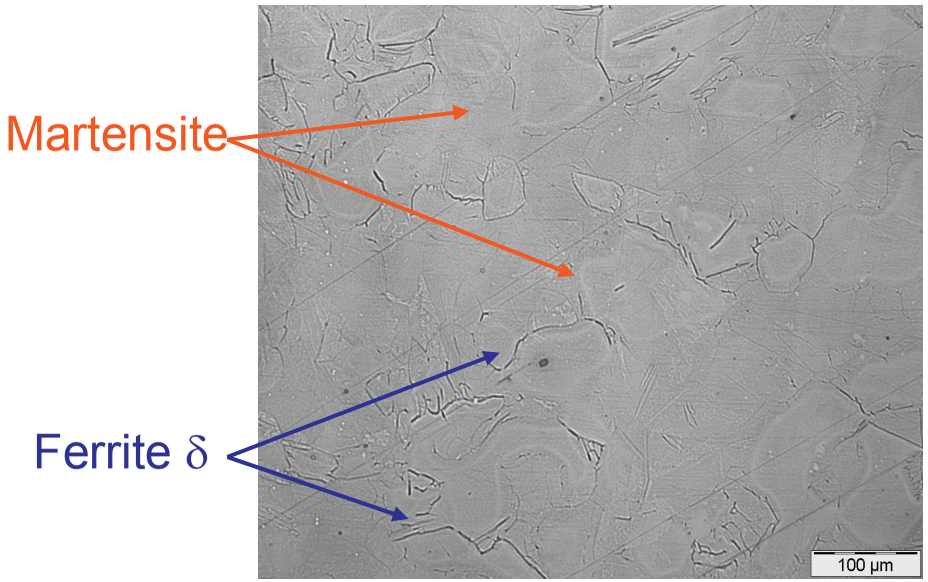
→ Can be verified that the compositions of delta ferrite at 1250°C and 1235°C exist between Ae3 and Ae4. So for the two temperatures there should be the massive transformation of delta ferrite.

$\gamma_1 + \delta \rightarrow M_1 + \delta$ ⟶ 1250°C

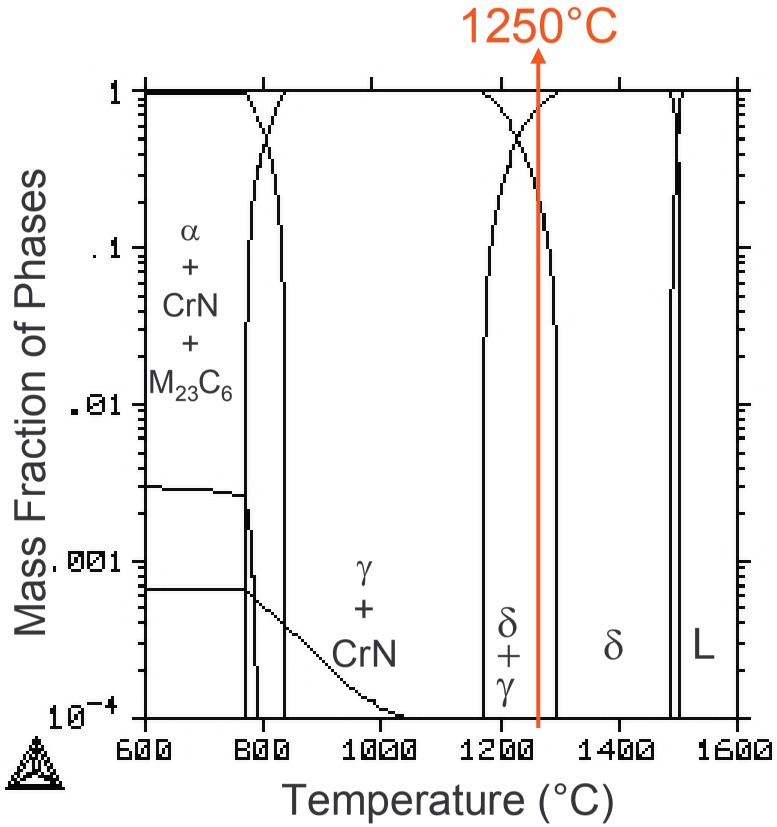
$\gamma_1 + \delta \rightarrow \gamma_1 + \gamma_{2,mass} \rightarrow M_1 + M_2$ ⟶ 1235°C

Analysis of EN10 Alloy

Chemical Composition:
Fe-10.83Cr–0.0168C-0.0133N-0.465Ni-0.72Mn-0.47Si

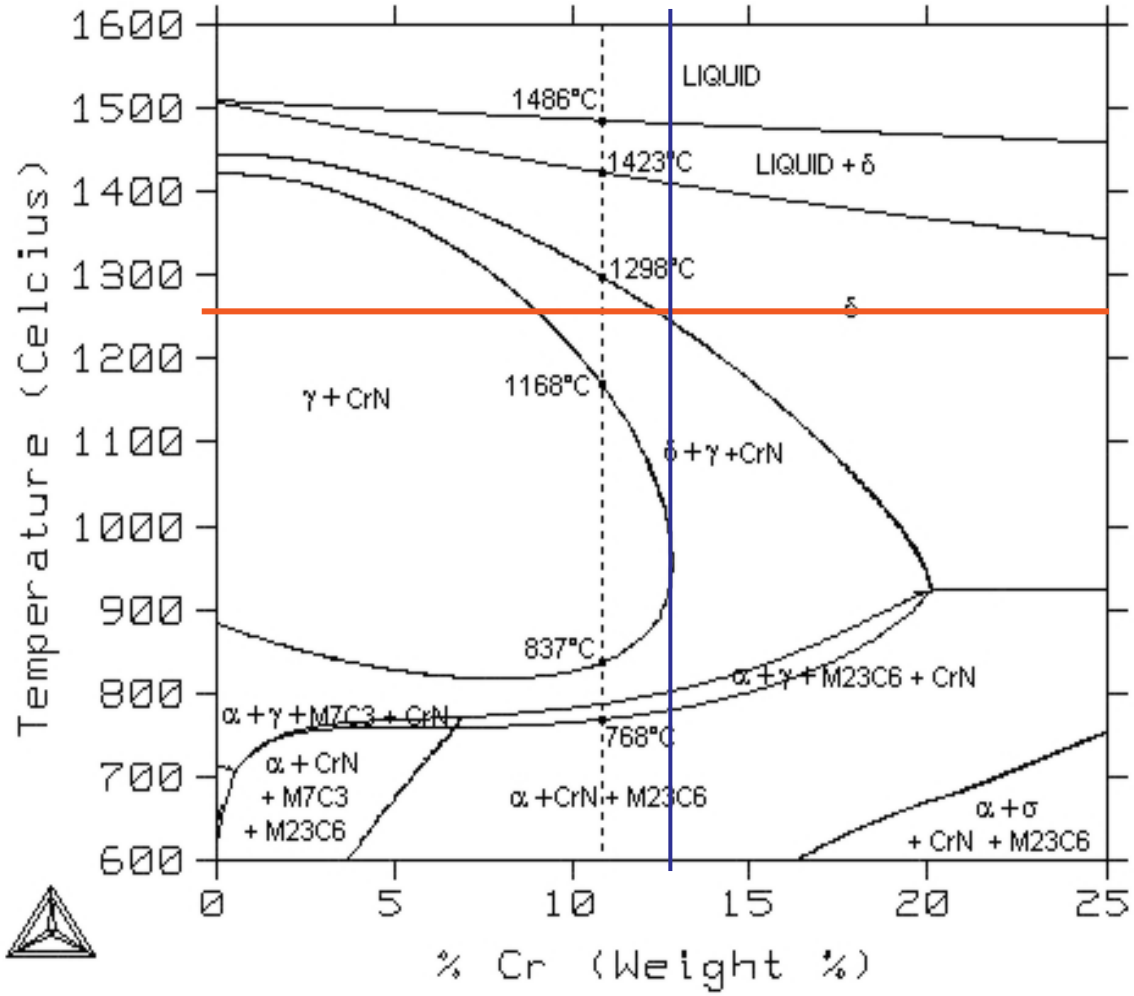


30min at 1250°C
+ water quenching



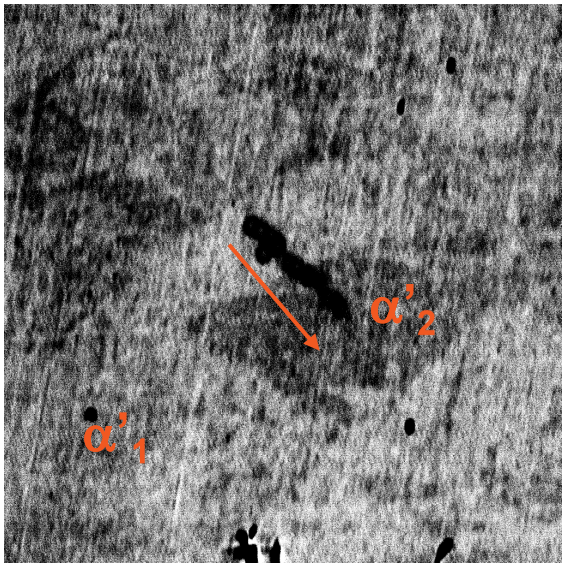
Equilibrium phase diagram for the Fe-10.83Cr–0.0168C-0.0133N-0.465Ni-0.72Mn-0.47Si alloy.
Diagram calculated with ThermoCalc and TCFE3 database.

Analysis of EN10 Alloy

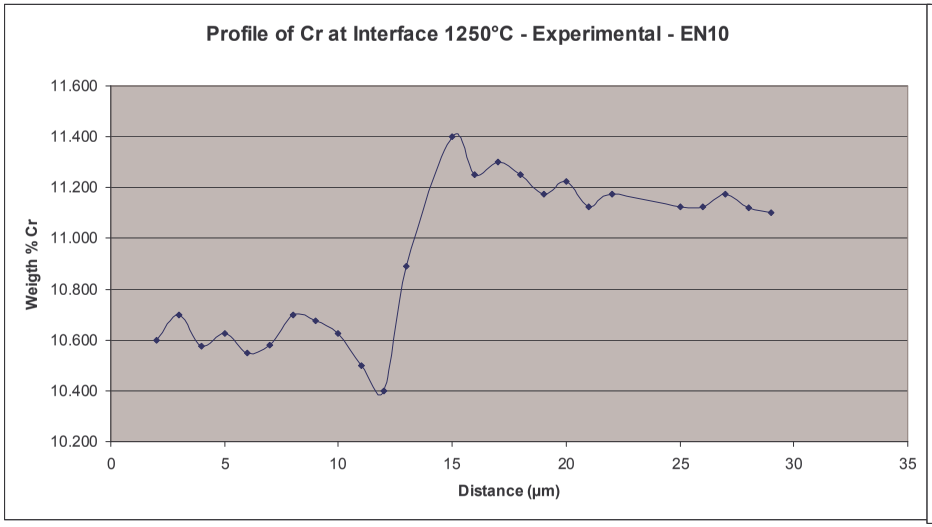


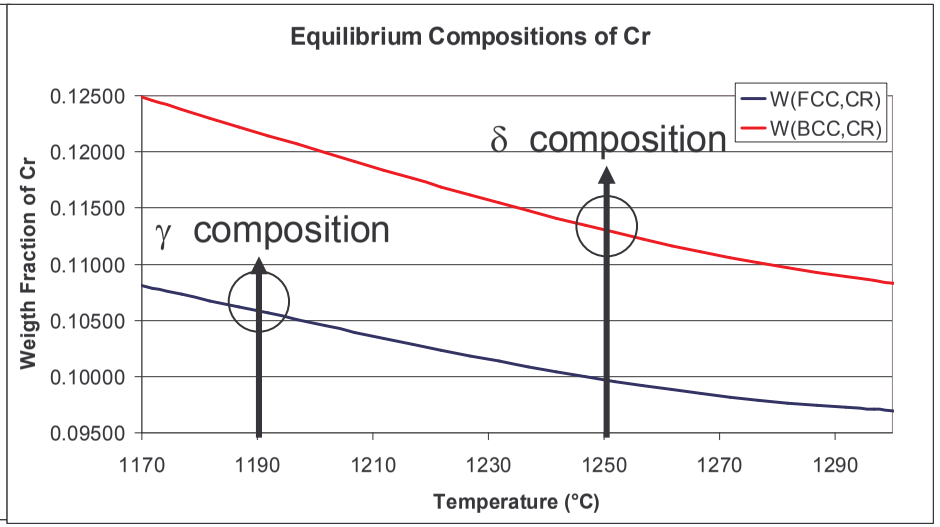
Isopleths of the phase diagram for Fe-Cr–0.0168C-0.0133N-0.465Ni-0.72Mn-0.47S alloys.
Diagram calculated with ThermoCalc and TCFE3 database.

Analysis of EN10 Alloy



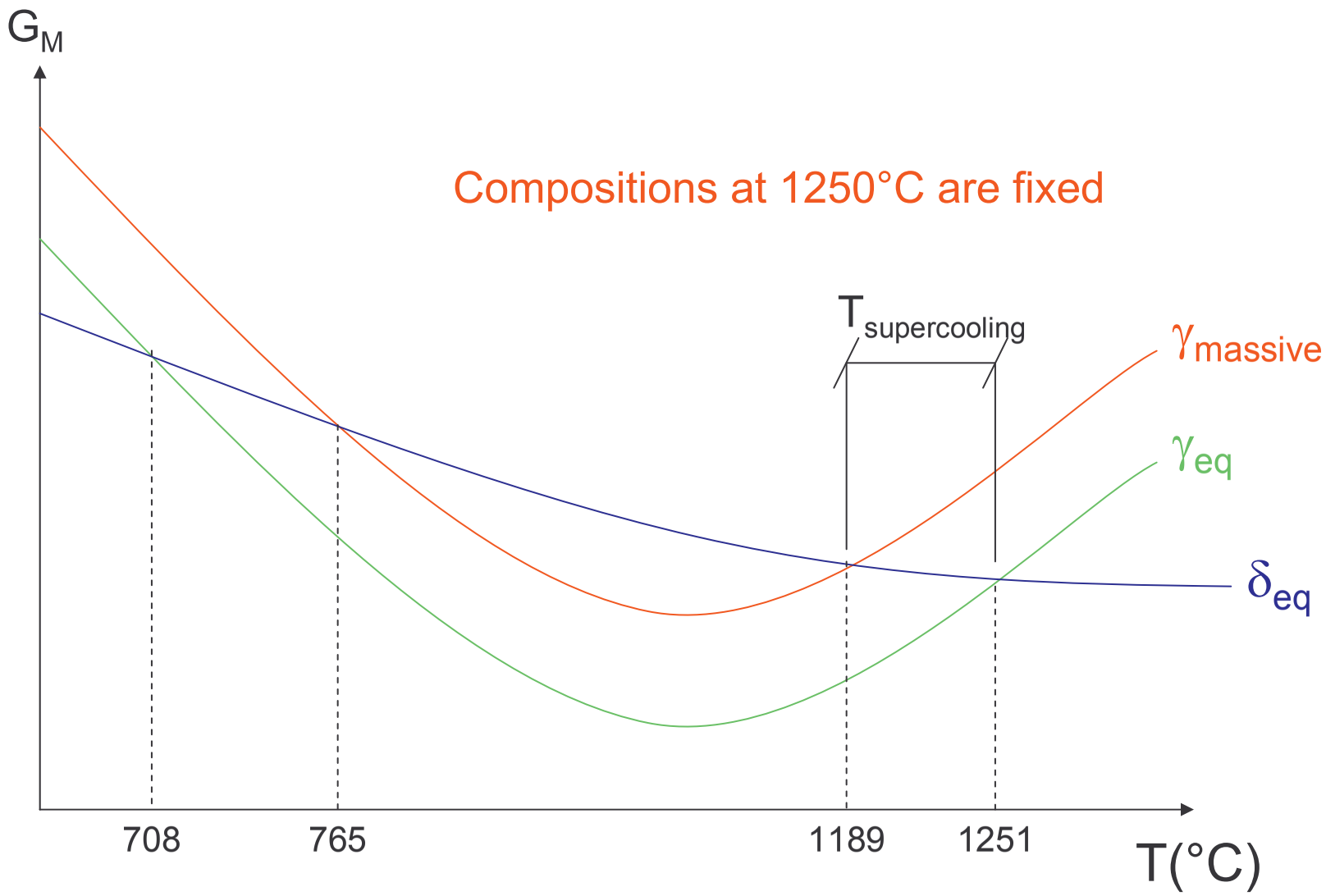
$$\gamma + \delta \rightarrow \gamma + \gamma_{mass} \rightarrow \alpha'_1 + \alpha'_2$$



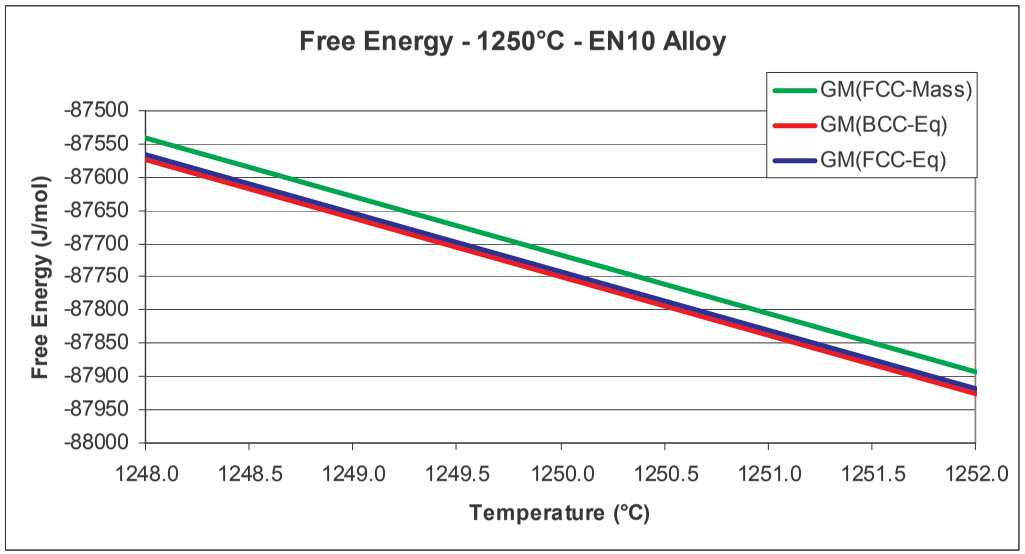


Equilibrium compositions for EN10 alloy calculated with ThermoCalc and TCFE3 database.

Analysis of EN10 Alloy



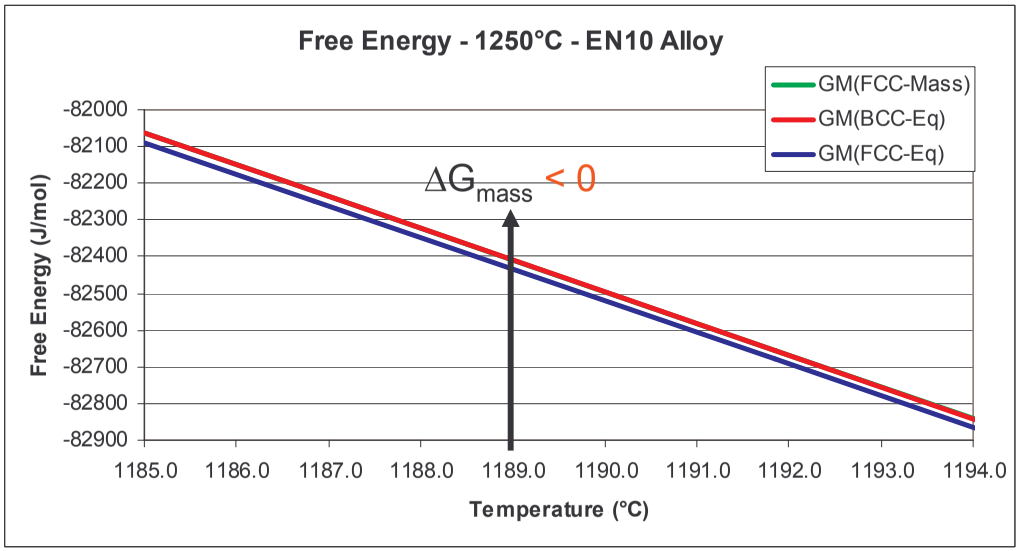
Analysis of EN10 Alloy



$$G_{\gamma\text{-mass}} = -0.01285T^2 - 55.581T + 1852.0$$

$$G_{\delta\text{-eq}} = -0.013840T^2 - 53.641T + 945.90$$

$$G_{\gamma\text{-eq}} = -0.012839T^2 - 55.603T + 1833.6$$



$$\Delta G_{mass} = G_{\gamma\text{-mass}} - G_{\delta\text{-eq}} < 0$$

$$\downarrow$$

$$\Delta T_{\text{super cooling}} > 61°C$$

Free Energy curves for EN10 alloy calculated with ThermoCalc and TCFE3 database.
Compositions of the phases were fixed with equilibrium compositions at 1250°C

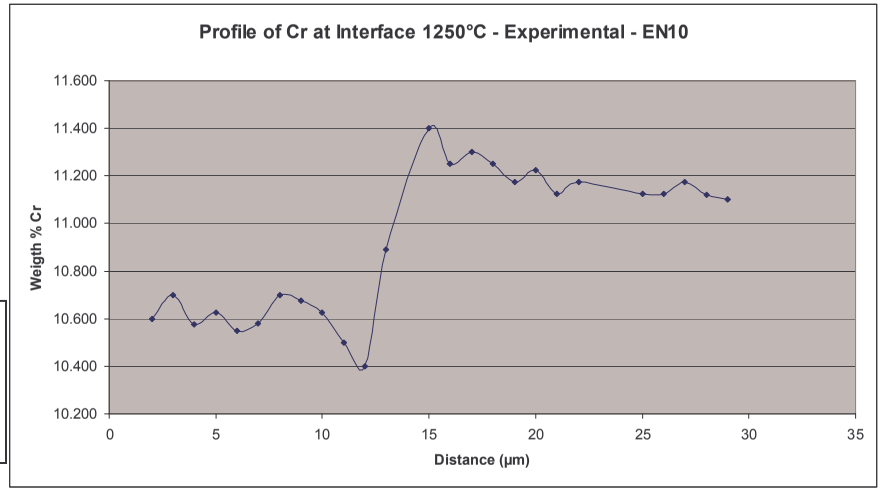
Analysis of EN10 Alloy

Murray-Landis Method

$$\Delta t < \left(\frac{(\Delta x_t)^2}{2 D_i^{\delta}} \right)$$

$$\upsilon = -\left(\frac{D_i^{\delta}}{C^t_{\delta eq - \gamma eq} - C^t_{\gamma mass}} \right) \left(\frac{-3C_1^t + 4C_2^t - C_3^t}{2\Delta x_t} \right)$$

$$C_i^{t+1} = \left[\left[\left(\frac{D_i^{\delta} \left(C_{i-1}^t - 2C_i^t + C_{i+1}^t \right)}{(\Delta x_t)^2} \right) + \upsilon \left(\frac{n-i}{n-1} \right) \left(\frac{C_{i+1}^t - C_{i-1}^t}{2\Delta x_t} \right) \right] \Delta t \right] + C_i^t$$



Conditions:

$D_{Cr}=10^{-14} m^2/s$

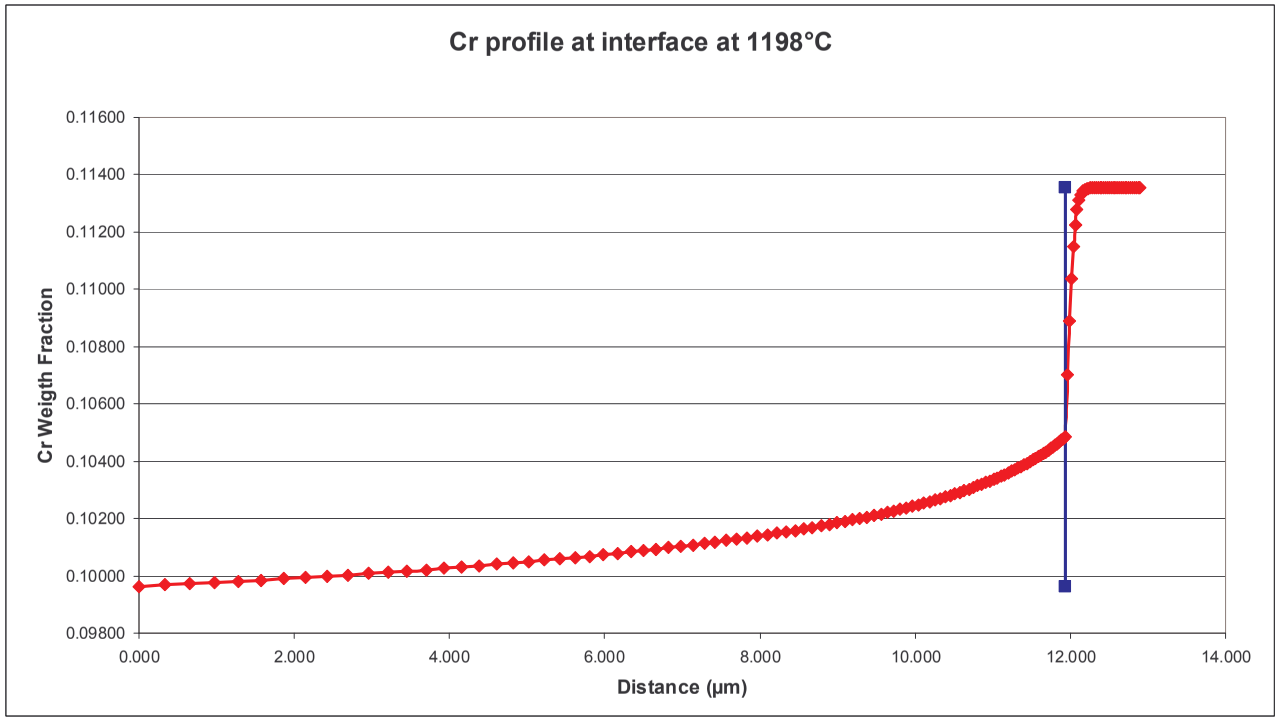
$\nu=50°C/s$

$W(\delta,Cr)=f(T)$

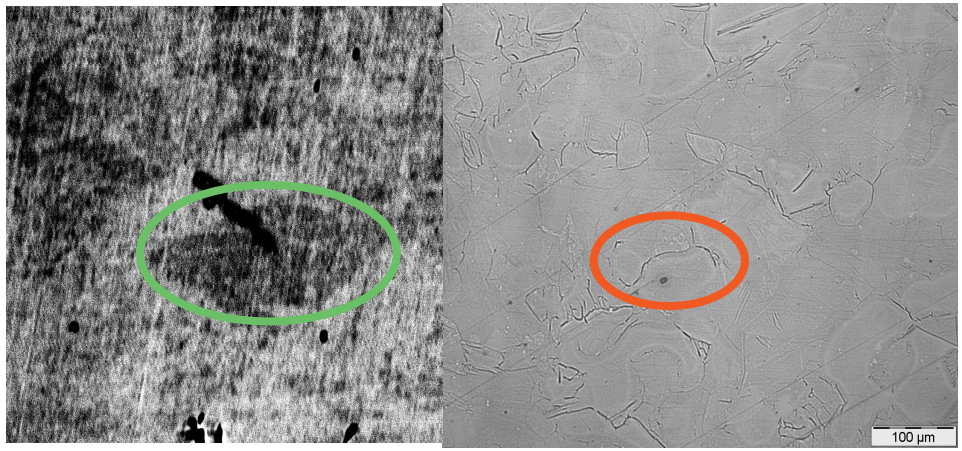
$W(\gamma,Cr)=f(T)$

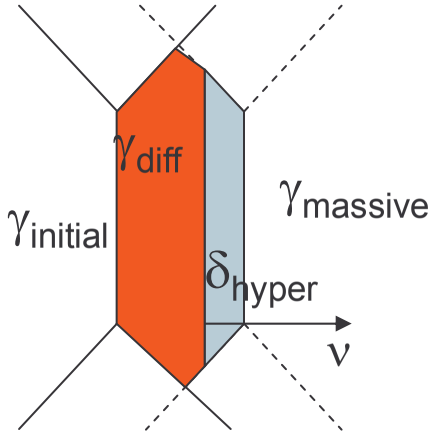
$T_{initial}=1250°C$

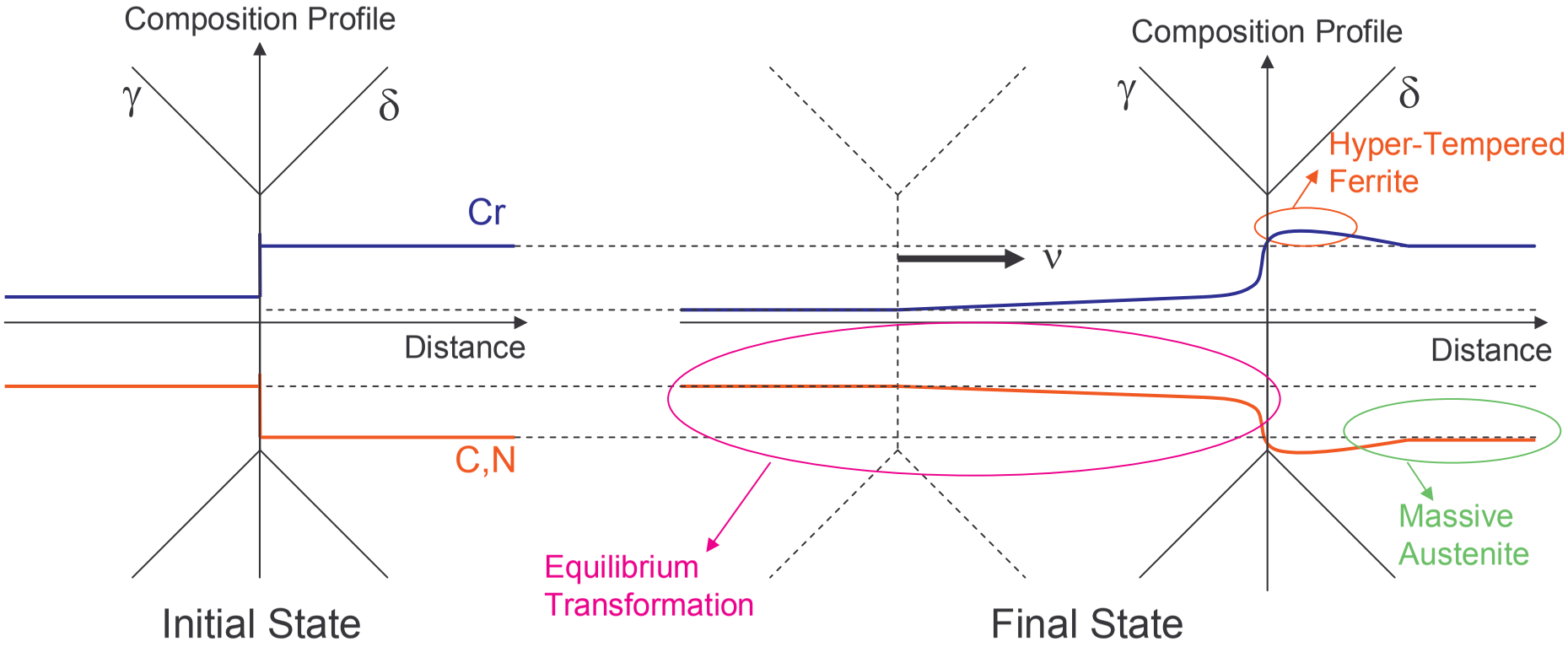
$\Delta t=0.0104s$



Analysis of EN10 Alloy







Thanks