Critical Evaluation and Optimization of the Fe-Nb-N System

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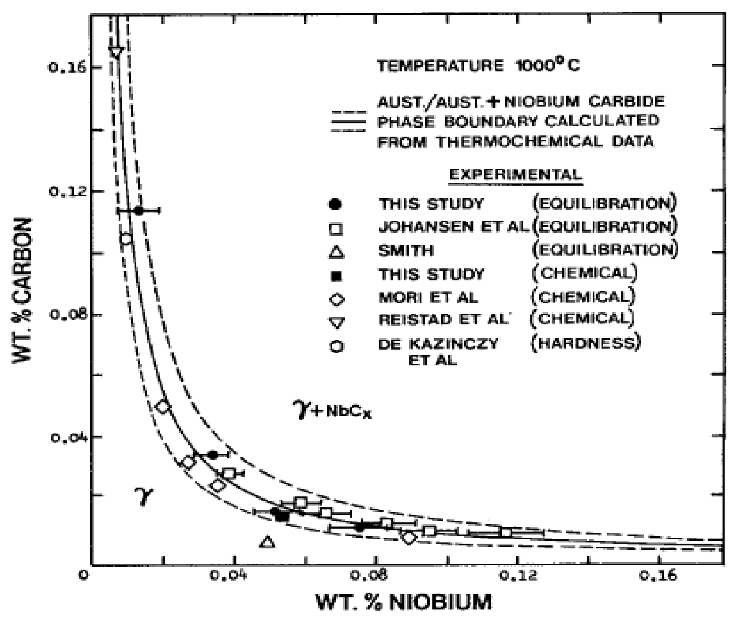
Introduction

Niobium Nitride

- Main strengthening element for commercial steel & hard coating materials
- Enables High strength Low Alloy steel(HSLA) to be resistant to corrosion



Model

- Solid solution (Compound Energy Formalism)

$[A]_p[C]_q + [B]_p[D]_q \rightarrow [A,B]_p[C,D]_q$

$$G_M = y_A y_C g^o_{AC} + y_A y_D g^o_{AD} + y_B y_C g^o_{BC} + y_B y_D g^o_{BD} + pRT(y_A \ln y_A + y_B \ln y_B) + qRT(y_C \ln y_C + y_D \ln y_D) + G^{XS}$$

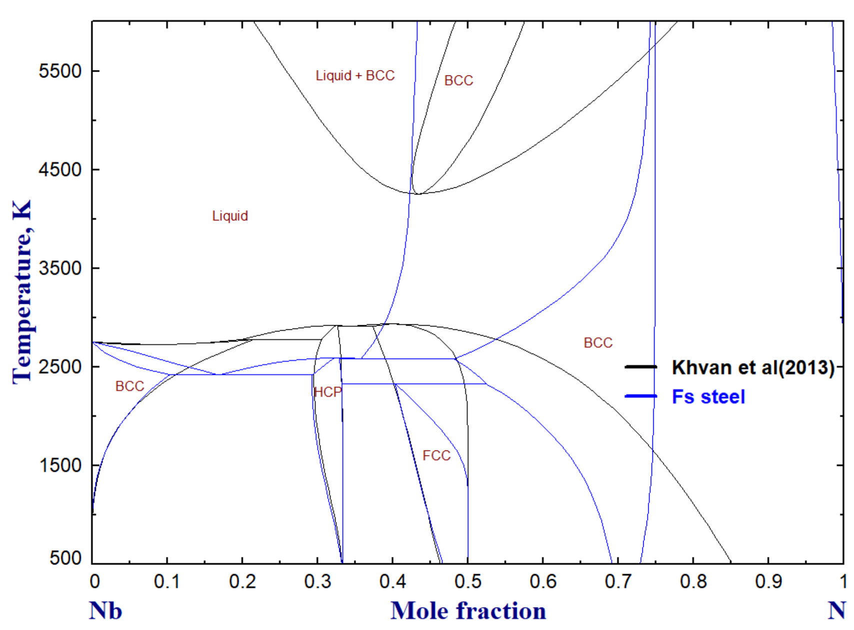
- Liquid solution (Modified Quasichemical Model)

$$G^m = (n_i g^o_i + n_j g^o_j) - RT\Delta S^{config} + \left(\frac{n_{i-j}}{2}\right)\Delta g_{i-j}$$

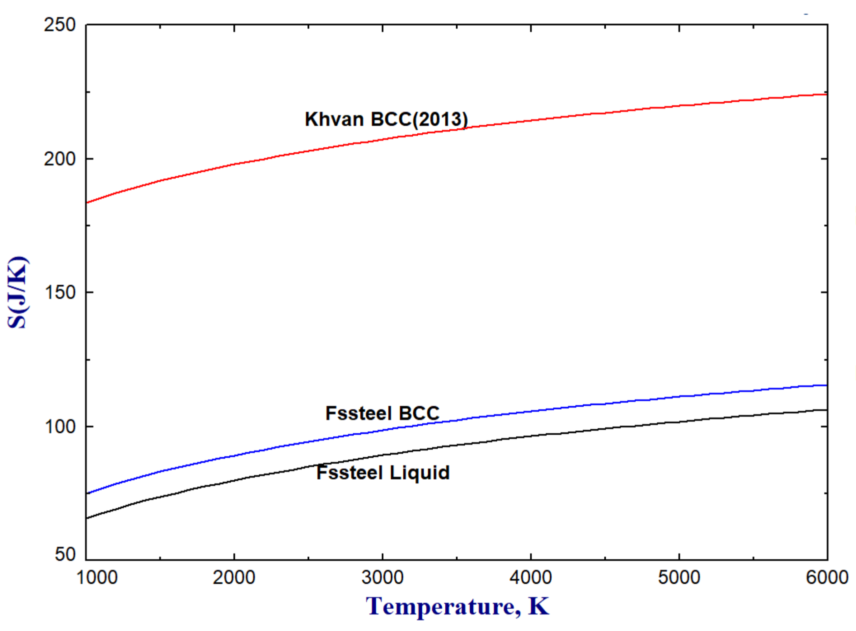
$$\Delta g_{i-j} = \Delta g^{00}_{i-j} + \sum q^{mn}_{i,j} X^m_{ii} X^n_{jj}$$

Main Issue

Bcc Intrusion issue

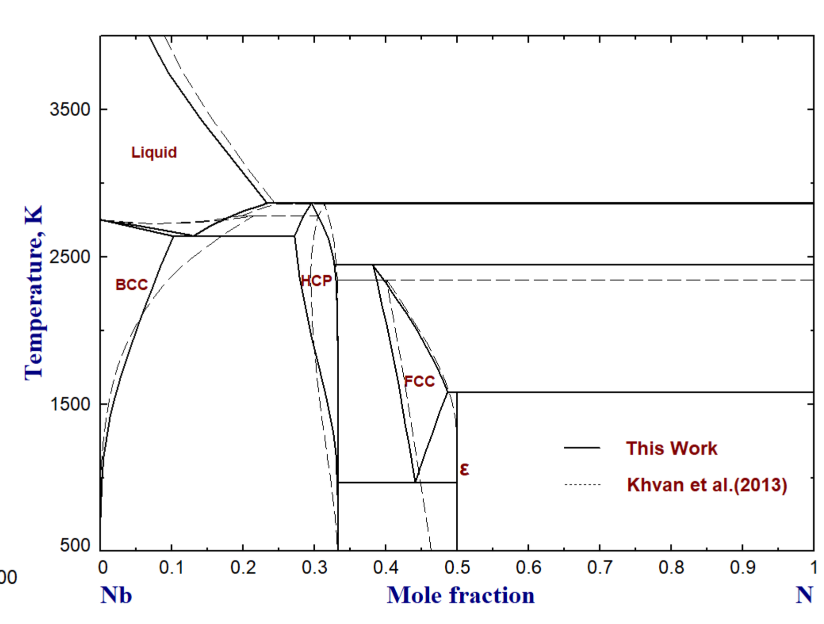


Gas suppressed condition

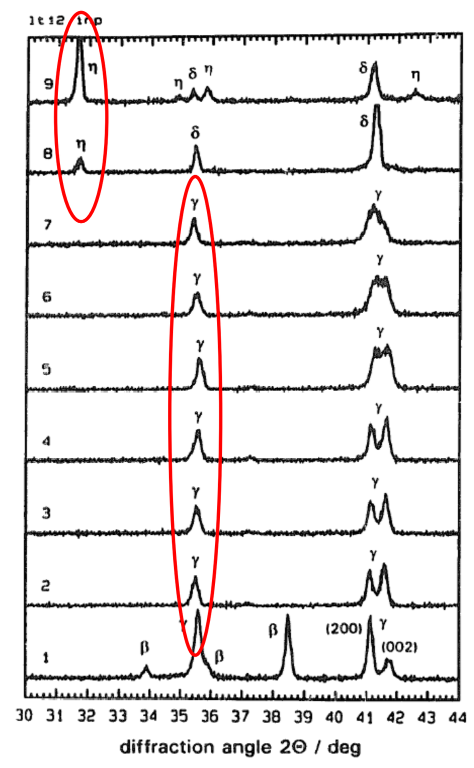


Entropy of Bcc and Liquid phase

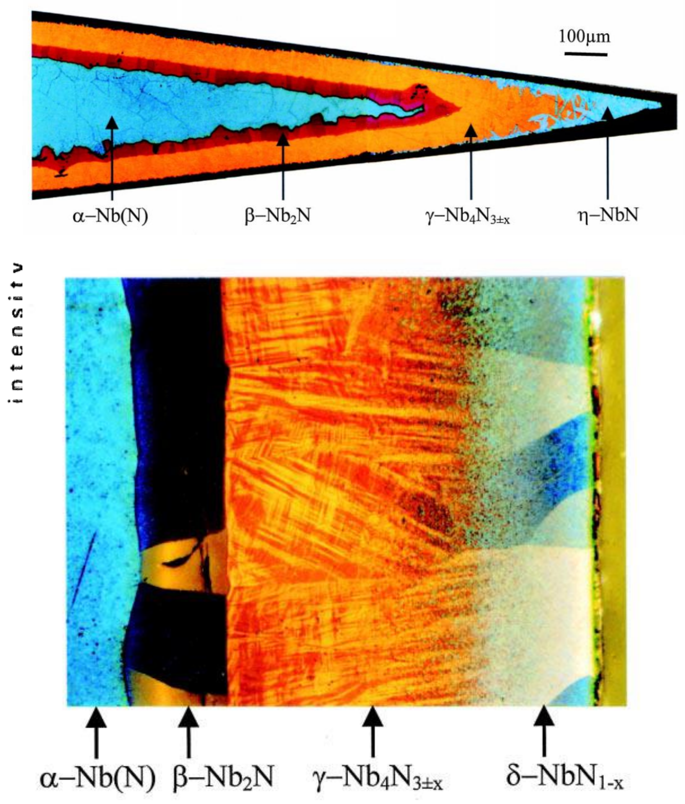
Stable phase issue



Stable phase modification



HTXRD



α–Nb(N) β–Nb_2N γ–$Nb_4N_{3\pm x}$ δ–NbN_{1-x}

Model Parameters

End members

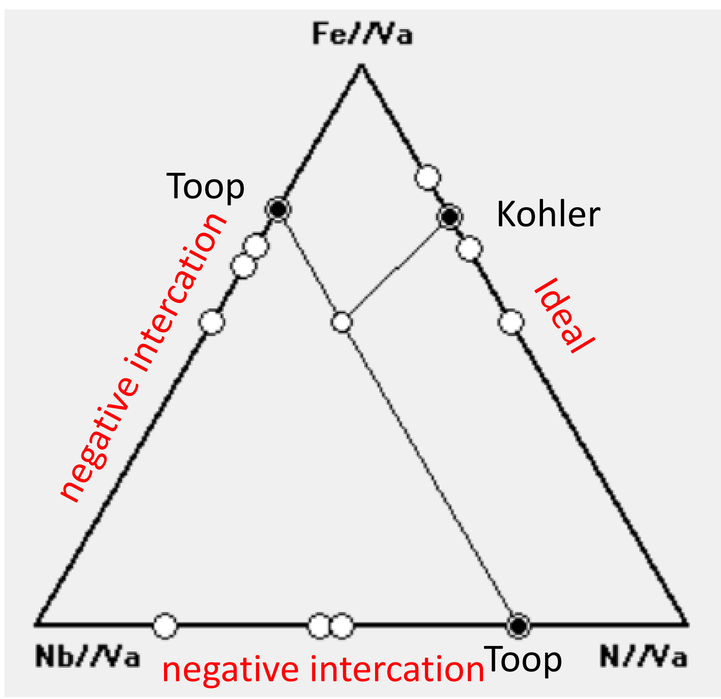
- **Liquid (Modified Quasichemical Model)**

Non default Quadruplet

$Z^{Fe}_{Fe} = 6, Z^{Nb}_{Nb} = 4, Z^{Nb}_{Fe} = 4, Z^{Fe}_{Nb} = 6$

Kohler/Toop interpolation – Nb assymetric

Δg^{00}_{FeNb} :-15100+4.9624T
q^{10}_{FeNb} : 4100 – 4.6878T
q^{01}_{FeNb} :-14900 +5.4378T
Δg^{00}_{NbN} :-46247 -1.203T
q^{10}_{NbN} : -27625+10.9375T
q^{04}_{NbN} : -62041+17T



- **BCC : $(Fe,Nb)_1(N,Va)_3$**

$G^{BCC}_{Fe;Va} = G^0_{Fe(BCC)}$
$G^{BCC}_{Nb;Va} = G^0_{Nb(BCC)}$
$G^{BCC}_{Fe;N} = G^0_{Fe(BCC)} + 3G^0_{N(BCC)} + 61418$
$G^{BCC}_{Nb;N} = G^0_{Nb(BCC)} + 3G^0_{N(BCC)} + 29028 - 31.75$
$L^{BCC}_{0Fe;Nb,Va} = -5950 + 9.4T$
$L^{BCC}_{1Fe;Nb,Va} = 14000 - 13.96T$
$L^{BCC}_{0Nb,N;Va} = -660784 + 120T$
TCFe:Va = 1043, $\beta_{Fe:Va} = 2.22$

- **FCC : $(Fe,Nb)_1(N,Va)_1$**

$G^{FCC}_{Fe;Va} = G^0_{Fe(FCC)}$
$G^{FCC}_{Nb;Va} = G^0_{Nb(Bcc)} + 13500 + 1.7T$
$G^{FCC}_{Fe;N} = G^0_{Fe(FCC)} + G^0_{N(FCC)} - 22361 + 30T$
$G^{FCC}_{Nb;N} = G^0_{Nb(BCC)} + G^0_{N(FCC)} - 229190 + 30T$
$L^{FCC}_{0Fe;Nb,Va} = 7740 - 11.4T$
$L^{FCC}_{0Fe,N;Va} = -7041.7 - 15.3553T$
$L^{FCC}_{0Nb;N,Va} = -67500$
$T_{cFe;Va}$ = -201, $\beta_{Fe:Va} = 2.22$
$T_{cFe;N}$ = -201, $\beta_{Fe:N} = 2.22$

- **Mu : $(Fe)_1(Fe,Nb)_2 (Nb)_4 (Fe,Nb)_6$**

$G^{Mu}_{Fe;Fe;Nb;Fe} = 9G^0_{Fe(BCC)} + 4G^0_{Nb(BCC)} - 138800$
$G^{Mu}_{Fe;Fe;Nb;Nb} = 3G^0_{Fe(BCC)} + 10G^0_{Nb(BCC)} + 850000$
$G^{Mu}_{Fe;Nb;Nb;Fe} = 7G^0_{Fe(BCC)} + 6G^0_{Nb(BCC)} - 248480 + 60.9T$
$G^{Mu}_{Fe;Nb;Nb;Nb} = G^0_{Fe(BCC)} + 12G^0_{Nb(BCC)} + 150000$

- **Hcp : $(Fe,Nb)_1(N,Va)_{0.5}$**

$G^{HCP}_{Fe;Va} = G^0_{Fe(HCP)}$
$G^{HCP}_{Nb;Va} = G^0_{Nb(Bcc)} + 10000 + 2.4T$
$G^{HCP}_{Fe;N} = G^0_{Fe(HCP)} + 0.5G^0_{N(HCP)} - 17865 + 8.71T$
$G^{HCP}_{Nb;N} = G^0_{Nb(BCC)} + 0.5G^0_{N(HCP)} - 134800 + 12T$
$L^{HCP}_{0Fe,N;Va} = 15255 - 26.359T$
$L^{HCP}_{1Fe,N;Va} = -16840 + 16.8824T$
$L^{BCC}_{0Nb;N,Va} = 18600 - 10T$

- **C14 : $(Fe,Nb)_2(Fe,Nb)_1$**

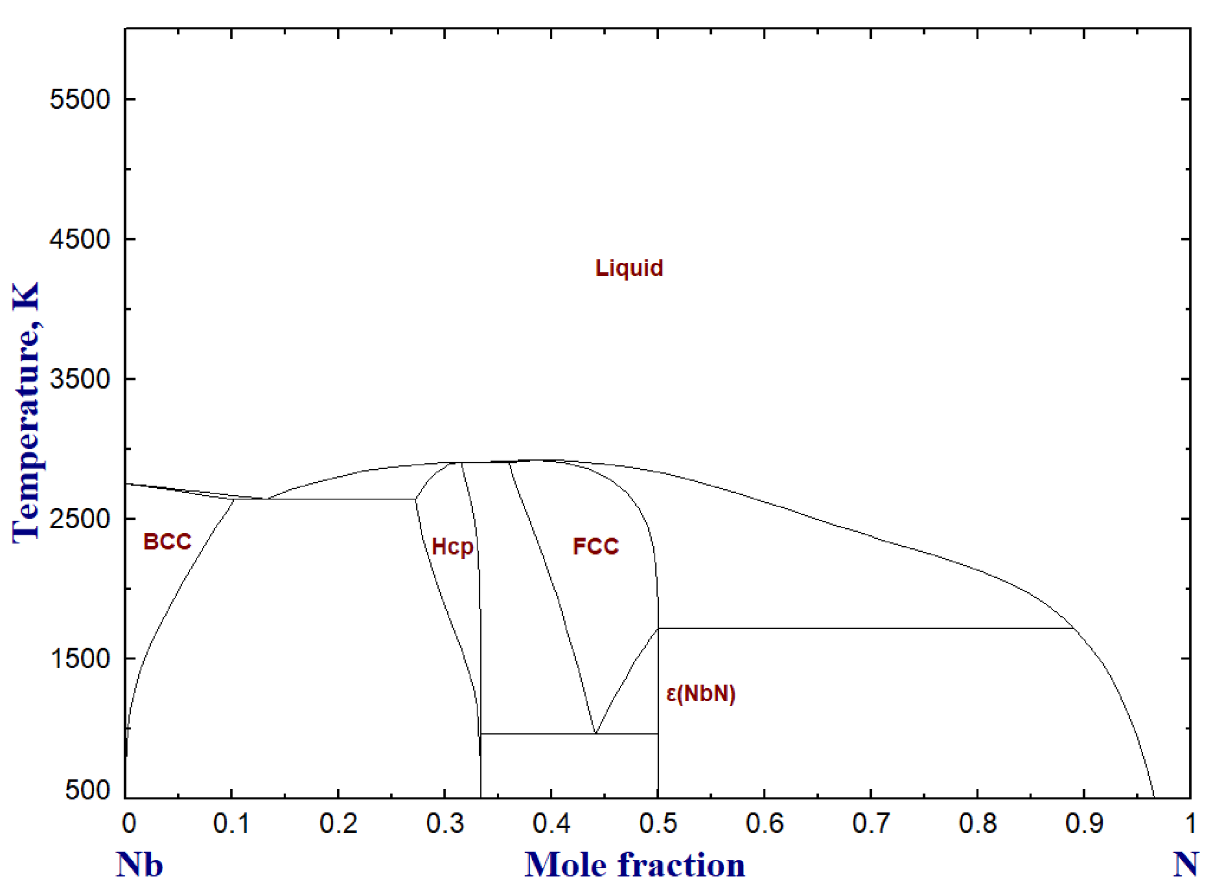
$G^{C14}_{Fe;Fe} = 3G^0_{Fe(BCC)} + 51292 - 5T$
$G^{C14}_{Fe;Nb} = 2G^0_{Fe(Bcc)} + G^0_{Nb(Bcc)} - 61732 + 12.9T$
$G^{C14}_{Nb;Fe} = G^0_{Fe(BCC)} + 2G^0_{Nb(BCC)} + 90000$
$G^{C14}_{Nb;Nb} = 3G^0_{Nb(BCC)} + 46110$
$L^{C14}_{0Fe,Fe;Nb} = -59320 + 13T$
$L^{C14}_{0Fe;Nb,Nb} = 32000$

- **Gamma : $(Fe)_4(N,Va)_1$**

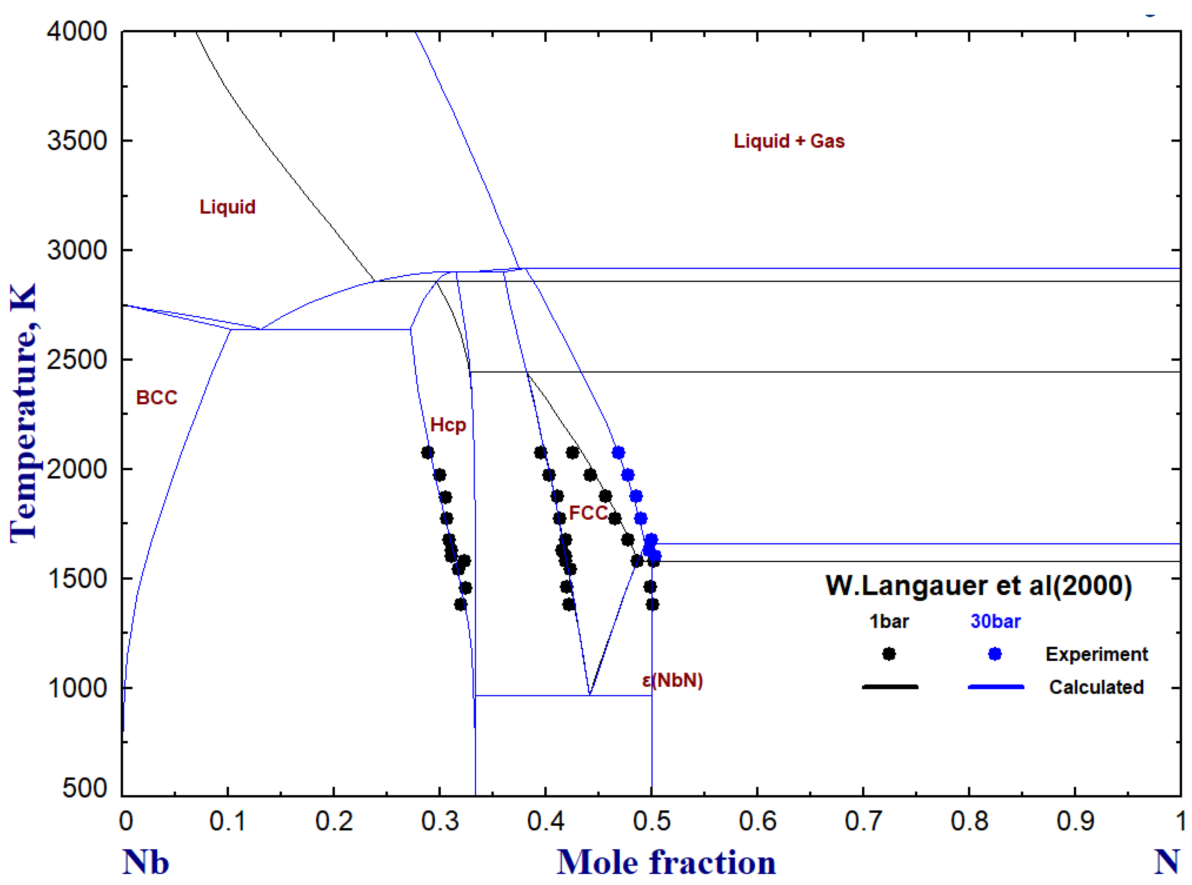
$G^{Gamma}_{Fe;N} = 4G^0_{Fe(FCC)} + G^0_{N(Gamma)} - 44439 + 14.3T$
$G^{Gamma}_{Fe;Va} = 4G^0_{Fe(FCC)} + 200$
$L^{Gamma}_{0Fe,N;Va} = 50446.5 = 23.6396T$
$L1^{Gamma}_{Fe,N;Va} = -13388.8$

Results & Discussion

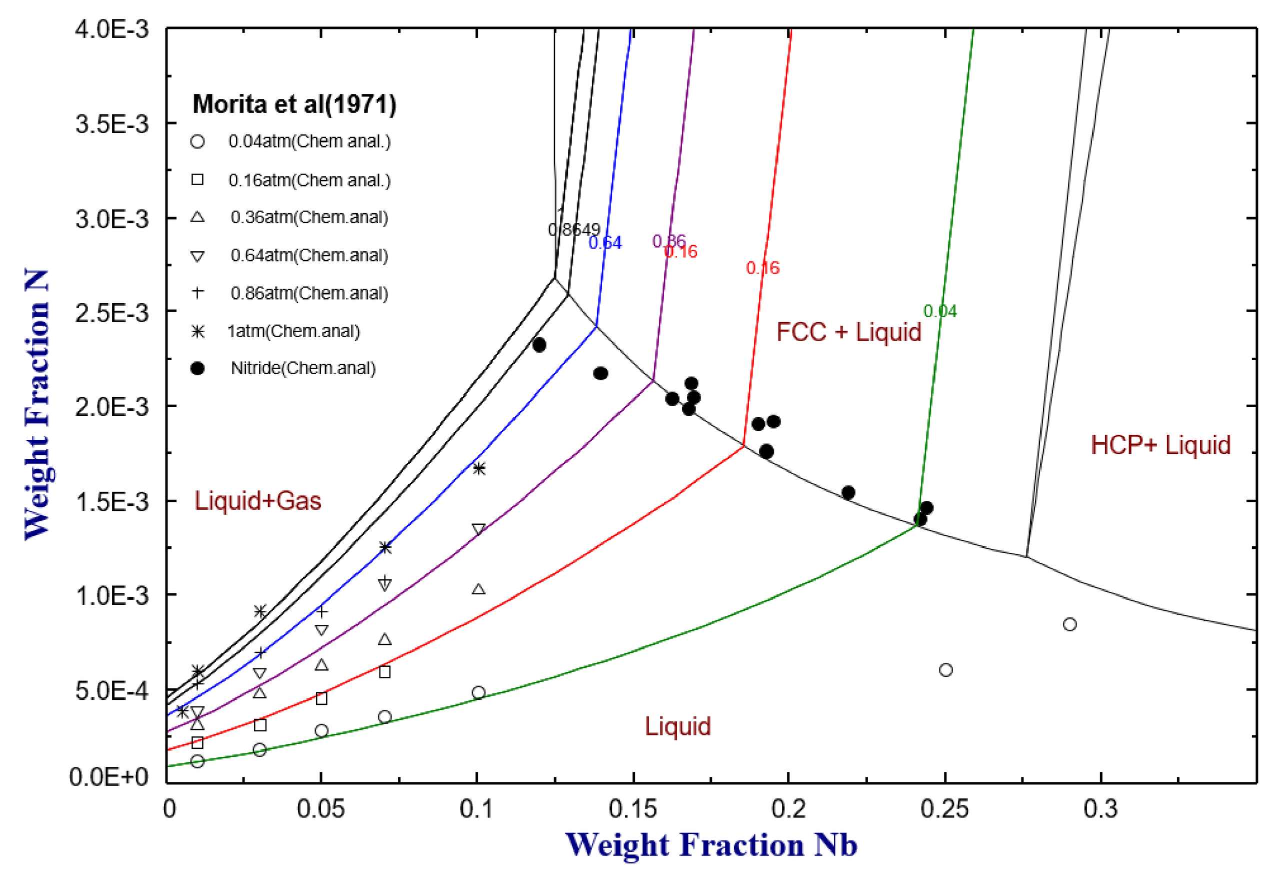
- **Fe-Nb-N phase diagram**
  - **Gas suppressed condition**



- **Binary phase boundary**



- **Ternary phase boundary (1923K)**



Conclusion

- Fe-Nb-N system was optimized
- Stable phase issue was addressed to determine γ, ε phase as stable phases
- Bcc phase inclusion issue was addressed and solved using specific reference energy for each nitrogen phase
- Fe-rich ternary phase boundary could be properly expressed using Nb assymetric Toop interpolation

Future work

- Expand to Fe-Nb-C-N system to successfully express property of Carbonitrides in austentie steel

HYUNDAI STEEL POSCO TATA STEEL RHI NIPPON STEEL & SUMITOMO METAL voestalpine JFE DOOSAN Doosan Heavy Industries & Construction NUCOR RioTinto SeAH Besteel SCHOTT glass made of ideas