Critical Evaluation and Optimization of the Fe-Nb-N System
JiHo Bang¹, In-Ho Jung¹
1) Department of Materials Science and Engineering, Seoul National University, South Korea

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)
  \[ \Delta G_m = \Delta G_m^{\text{sol}} + \Delta G_m^{\text{liq}} + (\frac{\Delta C_{\text{sol}}^0}{2}) \Delta G_{\text{sol}} \]
- Liquid solution (Modified Quasichemical Model)
  \[ \Delta G_m = \Delta G_m^{\text{sol}} + \Delta G_m^{\text{liq}} + (\frac{\Delta C_{\text{sol}}^0}{2}) \Delta G_{\text{sol}} \]

Main Issue

Bcc Invasion Issue

Stable phase issue

Model Parameters

End members

- Liquid (Modified Quasichemical Model)
  Non default Quadruplet
  \[ Z_{\text{N}} = 6, Z_{\text{Fe}} = 4, Z_{\text{Nb}} = 6 \]
  Kohler/Toop interpolation – Nb asymetric
  \[ \Delta G_{\text{N}}^{\text{sol}} = -11500 + 86247 \]
  \[ \Delta G_{\text{Fe}}^{\text{sol}} = -41000 + 81737 \]
  \[ \Delta G_{\text{Nb}}^{\text{sol}} = -6347 + 1.23 \%

Results & Discussion

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

Conclusion

- Fe-Nb-N system was optimized
- Stable phase issue was addressed to determine \( \gamma, \epsilon \) 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 asymmetric Toop interpolation

Future work

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