

Fe-Nb-Ni (Iron-Niobium-Nickel)

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The early review of this ternary system by [1992Rag] presented a tentative isothermal section at 1000 °C from the studies of [1989Sav]. The updates by [2004Rag] and [2007Rag] presented an isothermal section at 1200 °C from [2001Tak] and [2005Tak]. Recently, [2009Mat] carried out a Calphad-type assessment of this ternary system and calculated a number of isothermal sections. This work will be reviewed briefly in this update.

Binary Systems

The Fe-Nb phase diagram [2000Tof] depicts two intermediate phases: Fe_2Nb (*C14*, MgZn_2 -type hexagonal) and Fe_7Nb_6 (*D8₅*, Fe_7W_6 -type rhombohedral). In the Fe-Ni phase diagram [1991Swa], a continuous face-centered cubic solid solution (denoted γ) forms between γFe and Ni and is stable over a wide range of temperature. At 517 °C, an ordered phase FeNi_3 (*L1₂*, AuCu_3 -type cubic) forms congruently from γ . The Nb-Ni phase diagram [2006Che, 1996Bol], has the following intermediate phases: Nb_7Ni_6 (*D8₅*, Fe_7W_6 -type rhombohedral), NbNi_3 (*D0₁₉*, Cu_3Ti -type orthorhombic) and NbNi_8 (tetragonal). Computed phase diagrams of the above systems were given by [2009Mat].

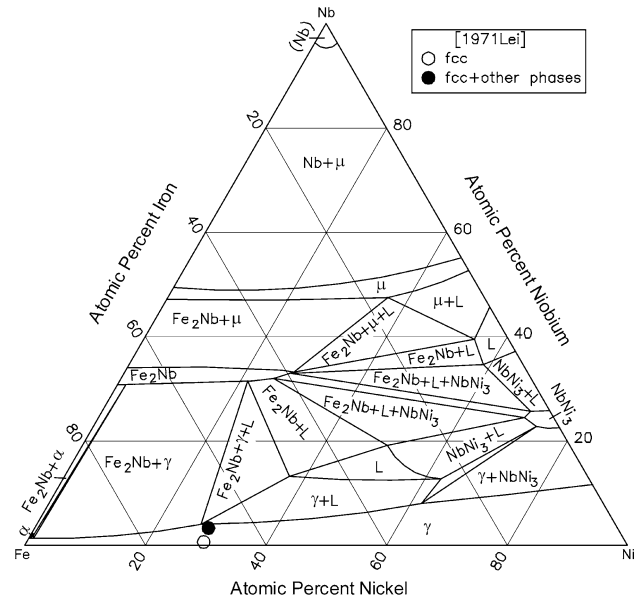


Fig. 2 Fe-Nb-Ni computed isothermal section at 1250 °C [2009Mat]

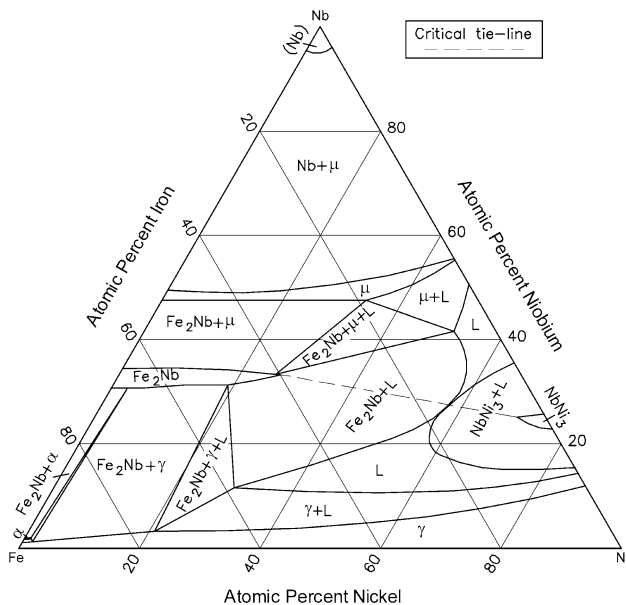


Fig. 1 Fe-Nb-Ni computed isothermal section at 1291 °C [2009Mat]

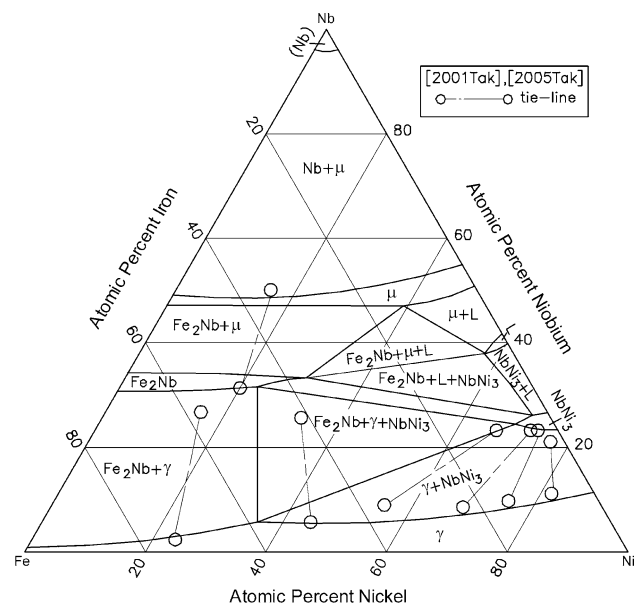


Fig. 3 Fe-Nb-Ni computed isothermal section at 1200 °C [2009Mat]

Computed Isothermal Sections

The liquid, disordered fcc and disordered bcc phases were modeled as substitutional solutions by [2009Mat]. The magnetic contribution to the Gibbs energy of the bcc and fcc phases was taken into account. The binary phases $C14$, $D8_5$, $D0_a$ and $L1_2$ were described by appropriate sublattice

models, providing for ternary solubility. In addition, the modeling included metastable phases $L1_0$, $D0_{22}$ and $C15$, to facilitate the future extension of the thermodynamic description to higher order systems. Ab-initio calculations were done by [2009Mat] to estimate the enthalpies of formation of the elements and the compounds on the basis of the Density Functional Theory, using the Generalized

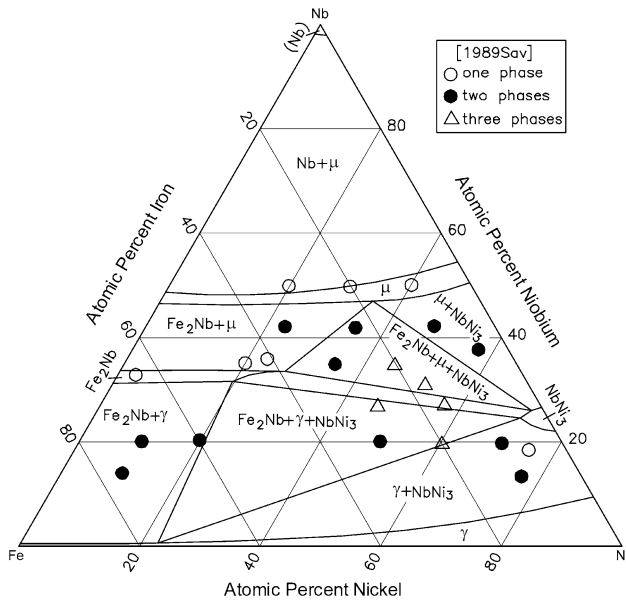


Fig. 4 Fe-Nb-Ni computed isothermal section at 1000 °C [2009Mat]

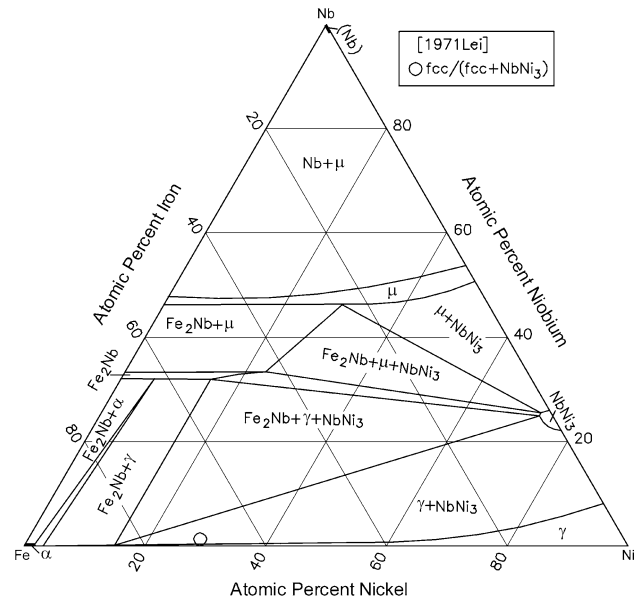


Fig. 6 Fe-Nb-Ni computed isothermal section at 800 °C [2009Mat]

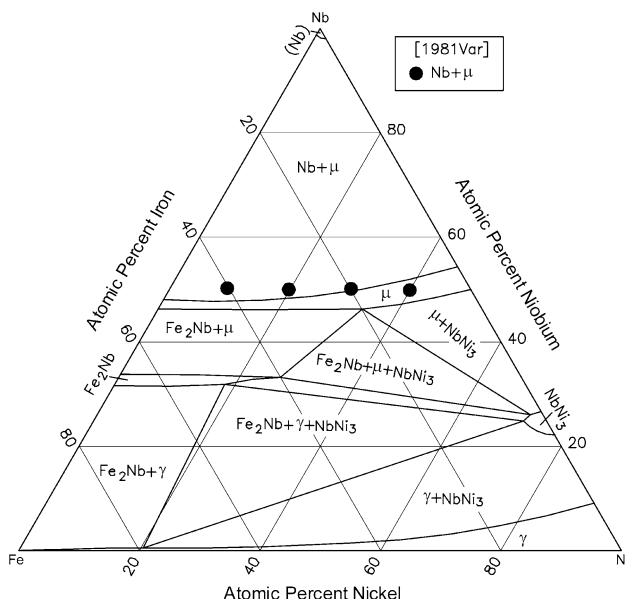


Fig. 5 Fe-Nb-Ni computed isothermal section at 950 °C [2009Mat]

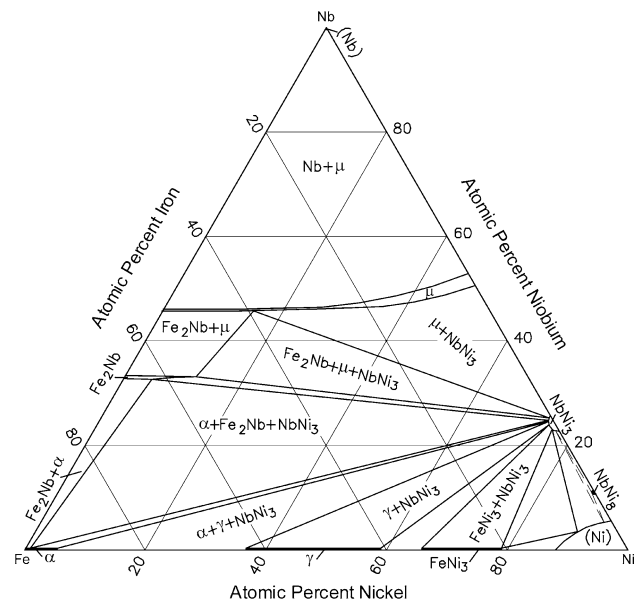


Fig. 7 Fe-Nb-Ni computed isothermal section at 450 °C [2009Mat]

Section II: Phase Diagram Evaluations

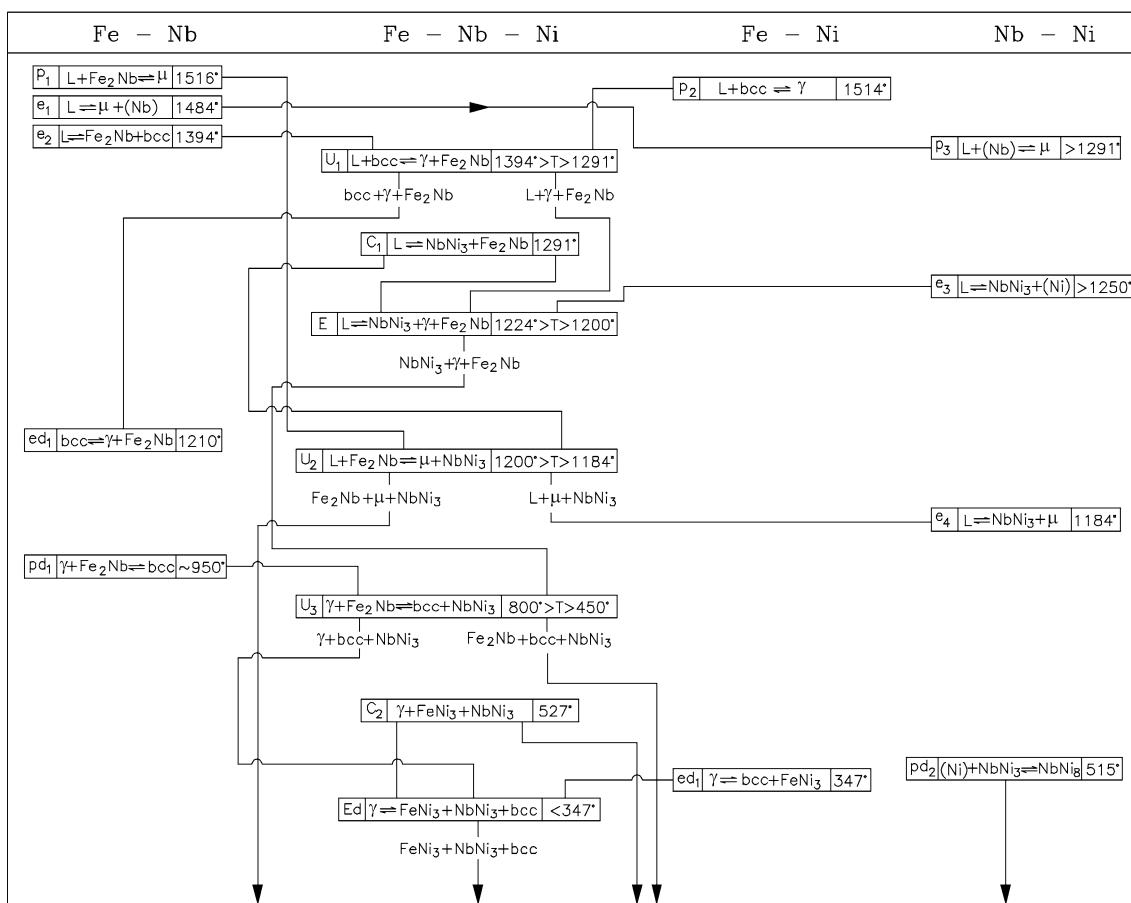


Fig. 8 Fe-Nb-Ni tentative reaction sequence

Gradient Approximation method. The ab-initio values were used in the optimization. Detailed discussion and comparison of the modeling, the magnetic contribution and the ab-initio calculations were presented by [2009Mat]. The available experimental phase diagram data, with the exception of one or two results, were used in the optimization. The optimized parameters were listed.

[2009Mat] computed seven isothermal sections at 1291, 1250, 1200, 1000, 950, 800 and 450 °C and compared them with the available experimental data. The overall agreement was found to be satisfactory. These sections are shown in Fig. 1-7. At 1291 °C (Fig. 1), the critical line of the three-phase equilibrium of (L + NbNi₃ + Fe₂Nb) is seen. This temperature is just 1 °C above the experimental pseudobinary eutectic temperature reported by [1975Pan] along the NbNi₃-Fe₂Nb join. The D₈₅ binary compounds with the nominal composition Fe₇Nb₆ and Nb₇Ni₆ form a continuous solid solution μ at this temperature as well as at lower temperatures down to at least 450 °C. At 1250 °C (Fig. 2), the liquid originating on the Ni-Nb side has split into two parts and is separated by a three-phase field of (NbNi₃ + Fe₂Nb + L). At 1200 °C (Fig. 3), that part of the liquid which lies within the ternary region has solidified, probably through a ternary eutectic reaction E, see the reaction sequence in Fig. 8. At 1000 °C (Fig. 4), no liquid phase is

present in the system. Solid-state transition reactions occur below 950 °C (Fig. 5), to yield the phase distribution seen at 800 and 450 °C (Fig. 6 and 7). Based on the computed isothermal sections of [2009Mat] and the binary systems, a tentative reaction sequence is shown in Fig. 8.

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