

Fe-Ni-S (Iron-Nickel-Sulfur)

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At about the same time as a comprehensive update was presented recently by [2004Rag], a new thermodynamic assessment of this system was published by [2004Wal]. The update included a liquidus projection, isothermal sections at 1350, 1200, 1100, 1000, 900, 725, 600, 500 and 400 °C, and a vertical section along the $\text{Fe}_{0.96}\text{S}-\text{Ni}_{0.96}\text{S}$ join. The thermodynamic description of [2004Wal] presented seven computed isothermal sections between 1350 and 600 °C and five vertical sections. The computed isothermal sections are generally in good agreement with the experimental sections in the update.

Computed Phase Equilibria

For the nomenclature and brief descriptions of the binary and ternary compounds and solid solutions based on them, see [2004Rag]. In their thermodynamic modeling, [2004Wal] applied the quasichemical model for short-range ordering for the ternary sulfide liquid, using their own descriptions of the Fe-S and Ni-S subsystems. Two-sublattice models were used for solid solutions based on pyrrhotite (po) [or monosulfide solid solution (mss)], pentlandite (pn),

pyrite (py), vaesite (vs) and the high-temperature form of heazlewoodite. Recent experimental results on thermodynamic properties and phase equilibrium data were used in the optimization. The optimized interaction parameters were listed. As in the reviewed experimental data of [2004Rag], [2004Wal] discounted the existence of a high-temperature form of pentlandite and of two phases within the homogeneity range of the high-temperature Ni_3S_2 .

Computed isothermal sections at 1350, 1300, 1200, 900, 725, 700, and 600 °C were given by [2004Wal]. The computed sections at 1350, 1200, 900, 725, and 600 °C are in agreement with the corresponding experimental sections reviewed by [2004Rag]. As supplements to the data reviewed by [2004Rag], two computed isothermal sections of [2004Wal] at 1300 and 700 °C are redrawn in Fig. 1 and 2, where $(S)_l$ denotes the S-rich liquid.

[2004Wal] presented five computed vertical sections at Fe/Ni atom ratios of 0.6722 and 1.0, at a constant S content of 47.1 at.%, along the $\text{FeS}-\text{Ni}_3\text{S}_2$ and $\text{FeS}_2-\text{NiS}_2$ joins, respectively. The vertical section along the $\text{FeS}_2-\text{NiS}_2$ join is redrawn in Fig. 3. The following U-type transition reaction occurs at 1002 °C: $L + (S)_l \leftrightarrow po + vs$. One of the product three-phase fields, $po + vs + (S)_l$, reacts with the

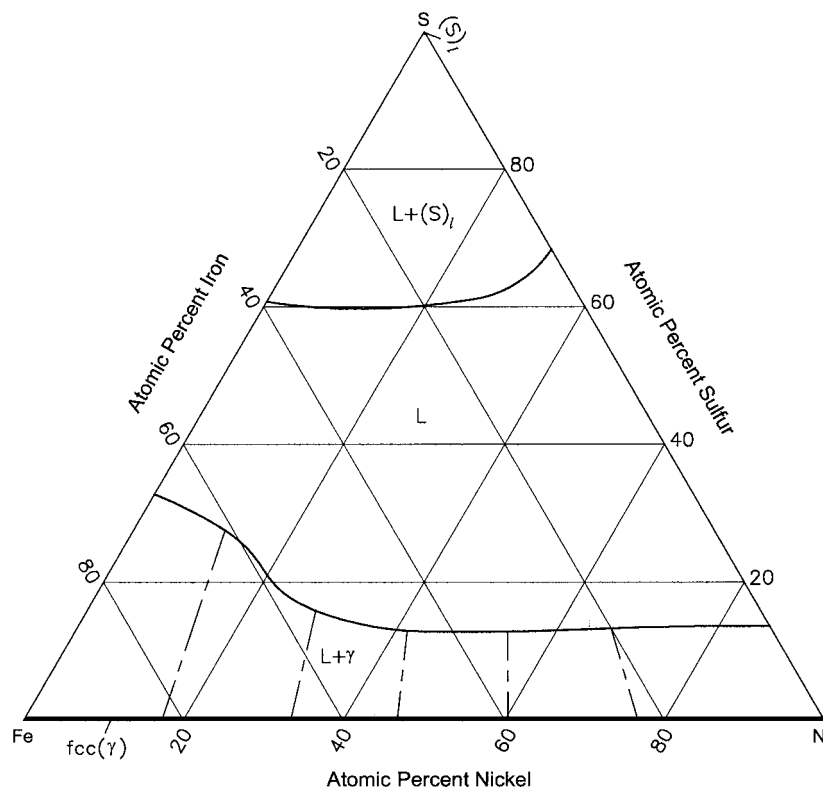


Fig. 1 Fe-Ni-S computed isothermal section at 1300 °C [2004Wal]

Section II: Phase Diagram Evaluations

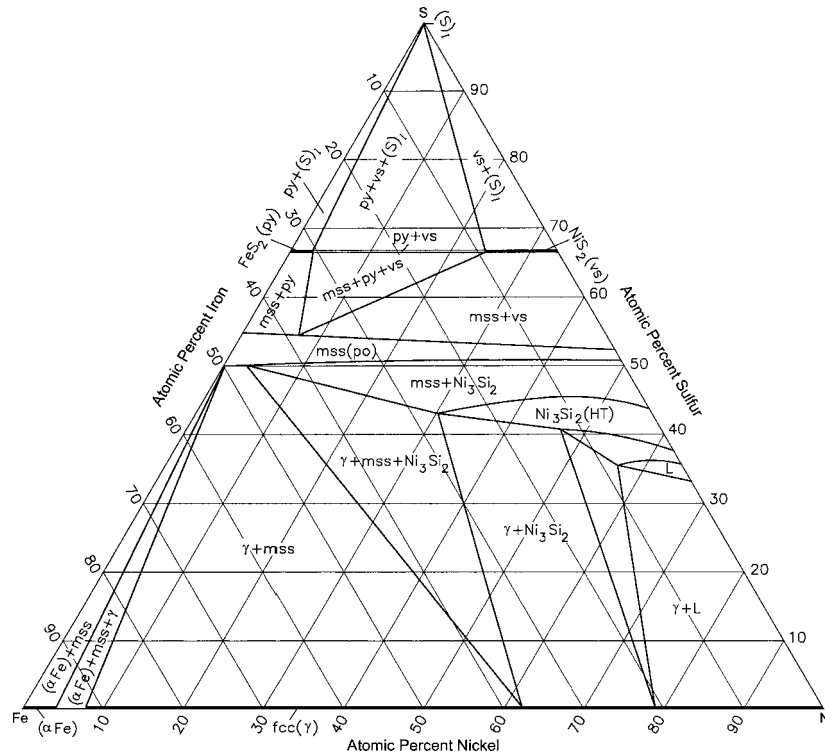


Fig. 2 Fe-Ni-S computed isothermal section at 700 °C [2004Wal]

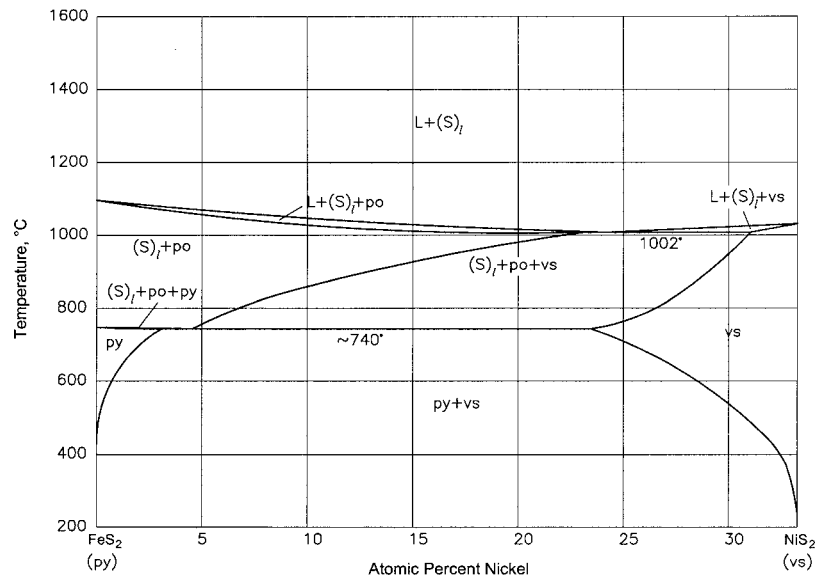


Fig. 3 Fe-Ni-S computed vertical section along the FeS₂-NiS₂ join [2004Wal]

three-phase field originating from the Fe-S peritectic reaction $po + (S)_1 \leftrightarrow py$ to yield another transition reaction at about 740 °C, $po + (S)_1 \leftrightarrow vs + py$. Neither of the three-phase fields resulting from this second reaction lies on the FeS₂-NiS₂ join, which becomes pseudobinary below this temperature (refer to the isothermal section at 725 °C in Fig. 7 of [2004Rag] or Fig. 10 of [2004Wal]).

[2004Wal] computed the equilibrium sulfur pressures over various alloy compositions and temperatures and compared them with the experimental data from the literature.

The solubility of nickel in po (mss) was redetermined by [1996Ebe] at 1100 °C, using the sealed tube technique and electron probe microanalysis. The measured compositions of the coexisting mss and the liquid were listed. These re-

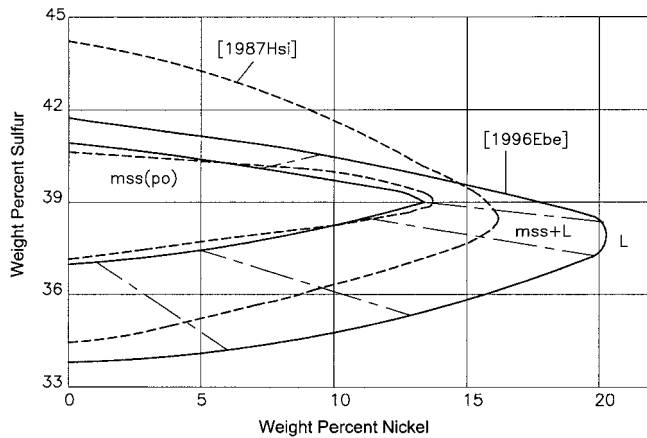


Fig. 4 Fe-Ni-S homogeneity region of *mss* at 1100 °C [1996Ebe]

sults were not included in the optimization by [2004Wal]. In Fig. 4, the phase boundaries of *mss* determined by [1996Ebe] are compared with the computed boundaries of

[1987Hsi]. There is good agreement regarding the maximum solubility of Ni in *mss*, but the new results indicate that the composition of the coexisting liquid is significantly richer in Ni than in the earlier studies. The tie-lines in Fig. 4 show that Ni resides preferentially in the liquid phase. [1996Ebe] also found that the addition of small amounts of copper (less than 3 wt.%) shrinks the *mss* field, which becomes less Ni-rich at constant temperature.

References

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