JPEDAV (2010) 31:455–458
DOI: 10.1007/s11669-010-9745-1
1547-7037 ©ASM International

Al-Fe-Ni (Aluminum-Iron-Nickel)

V. Raghavan

This technologically important system has been investigated experimentally, assessed thermodynamically, reviewed and updated a number of times. Table 1 gives the details of selected, more-recent studies. Very recently, [2009Zha] carried out a revised thermodynamic analysis, combining new calorimetric measurements of thermodynamic properties, first-principles calculations and the CALPHAD approach. This work will be reviewed briefly here.

Binary Systems

The Al-Fe phase diagram [1993Kat] shows that the face-centered cubic (fcc) solid solution based on Fe is restricted by a γ loop. The body-centered cubic (bcc) solid solution exists in the disordered *A*2 form, as well as the ordered *B*2 and $D0_3$ forms. Apart from the high temperature phase ε ($D8_2$, Cu_5Zn_8-type cubic; stable between 1232 and 1102 °C), there are three other intermediate phases in this system: $FeAl_2$ (triclinic), Fe_2Al_5(70-73 at.% Al, orthorhombic), and Fe_4Al_{13} (74.5-76.6 at.% Al, monoclinic). The Al-Ni phase diagram [1993Oka] shows five intermediate phases: $NiAl_3$ ($D0_{11}$, Fe_3C-type orthorhombic), Ni_2Al_3 ($D5_{13}$-type hexagonal), NiAl (*B*2, CsCl-type cubic, denoted β), Ni_5Al_3 (Ga_3Pt_5-type orthorhombic), and Ni_3Al ($L1_2$, $AuCu_3$-type cubic, denoted γ). The Fe-Ni phase diagram is characterized by a very narrow solidification range with a peritectic reaction at 1514 °C, that yields the Fe-based fcc solid solution. A continuous fcc solid solution γ is stable over a wide range of temperature. At 517 °C, an ordered phase $FeNi_3$ forms congruently from γ.

Ternary Phases

Three ternary phases are known in this system. $(Fe,Ni)_2Al_9$ (also written as $FeNiAl_9$) has the Co_2Al_9-type of monoclinic structure, with lattice parameters of a = 0.62406, b = 0.62993, c = 0.85992 nm, and β = 95.129° at $Fe_{0.7}Ni_{1.3}Al_9$ [2007Chu1]. Fe_3NiAl_{10} has the Co_2Al_5-type of hexagonal structure, with a = 0.770937 nm and c = 0.767947 nm at $Fe_{2.67}Ni_{1.43}Al_{9.9}$ [2007Chu1]. $(Fe,Ni)_2Al_9$ was denoted as τ_2 by [2007Chu1], [2008Rag], [2009Rag1], and [2009Rag2] and as τ_1 by [2005Cac], [2007Zha], and [2009Zha]. Fe_3NiAl_{10} was denoted as τ_1 by [2007Chu1], [2008Rag], [2009Rag1], and [2009Rag2] and as τ_2 by [2005Cac], [2007Zha], and [2009Zha]. This mix-up of terminology is unfortunate. Since this update is primarily based on the work of [2009Zha], the nomenclature adopted by [2009Zha] for τ_1 and τ_2 will be used, i.e., $FeNiAl_9 = \tau_1$ and $Fe_3NiAl_{10} = \tau_2$. The third ternary phase is a decagonal, quasicrystalline phase with a periodicity of ~0.4 nm. It is stable between 930 and 847 °C and occurs at the approximate composition $Fe_5Ni_{24}Al_{71}$ [2007Chu1]. It will be denoted as D here (denoted q by [2007Chu1] and τ_3 by [2009Zha]).

Table 1 Details of selected previous studies of the Al-Fe-Ni system

Reference	Nature of study	Evaluated data presented
[1988Ray]	Review	Liquidus and solidus projections, isothermal sections at 1250, 950, 850, 750, and 600 °C, reaction sequence
[1994Rag]	Update	Isothermal sections at 1050 and 950 °C, vertical section along Ni_3Fe-Ni_3Al join
[2005Cac]	Review	Partial liquidus projections, isothermal sections at 1350, 1250, 1150, 950, 850, 750, and 620 °C, four vertical sections, reaction sequence
[2005Rag]	Update	Isothermal sections at 1127 and 1100 °C
[2006Ele]	Review	Liquiuds projection, isothermal sections at 1350, 1250, 1150, 1050, 950, 850, and 750 °C, vertical sections along Ni_3Al-Ni_3Fe and FeAl-NiAl joins
[2006Rag]	Update	Isothermal sections at 1300, 1100, and 900 °C, vertical section along Ni_3Fe-Ni_3Al join
[2007Chu1]	Experimental	Liquidus projection, isothermal sections at 850 °C, vertical sections at 80, 75, 71.5, 67, and 60 at.% Al
[2007Chu2]	Experimental	Vertical sections along the Ni_3Al-Ni_3Fe join
[2007Zha]	Thermodynamic analysis, experimental	Computed liquidus projection, computed isothermal sections at 1250, 1050, 950, and 850 °C, three computed vertical sections at 1 mass% Ni, 1 mass% Fe, and along Ni_3Fe-Ni_3Al join, respectively
[2008Chu]	Experimental	Isothermal sections in the Al-lean region at 1200, 1100, 1000, and 900 °C
[2008Rag]	Update	Liquidus projection, isothermal sections at 850 °C, Vertical sections at 71.5 and 60 at.% Al, reaction sequence
[2008Zha]	Experimental	Isothermal sections at 850 and 627 °C
[2009Rag1]	Update	Isothermal sections at 1200, 1100, 1000, 900, 850, and 627 °C, vertical section along Ni_3Fe-Ni_3Al join
[2009Rag2]	Update	Isothermal sections at 1250, 1050, 950, and 850 °C, a vertical section along the Ni_3Fe-Ni_3Al join

Computed Ternary Phase Equilibria

A thermodynamic assessment of this system was reported recently by [2007Zha] and reviewed by [2009Rag2]. [2009Zha] made a revised assessment of the system. New experimental results on the phase equilibria by [2007Chu1], [2007Chu2], [2008Chu], and [2008Zha] were included in the optimization, in addition to those used by [2007Zha]. Using high temperature reaction calorimetry, the enthalpies of formation of $FeNiAl_9$ and Fe_3NiAl_{10} were determined by [2009Zha]. With starting metal powders of 99.97% Al, 99.99% Fe, and 99.996% Ni, pellets of the above ternary compositions were prepared for the calorimetric experiments. First-principles calculations were performed to obtain the enthalpies of formation of the end-members of the ternary phases $(Fe,Ni)_2Al_9$ and $(Fe,Ni)_2Al_5$, varying the composition of the sublattice housing Fe and Ni. Calculations were done also to estimate

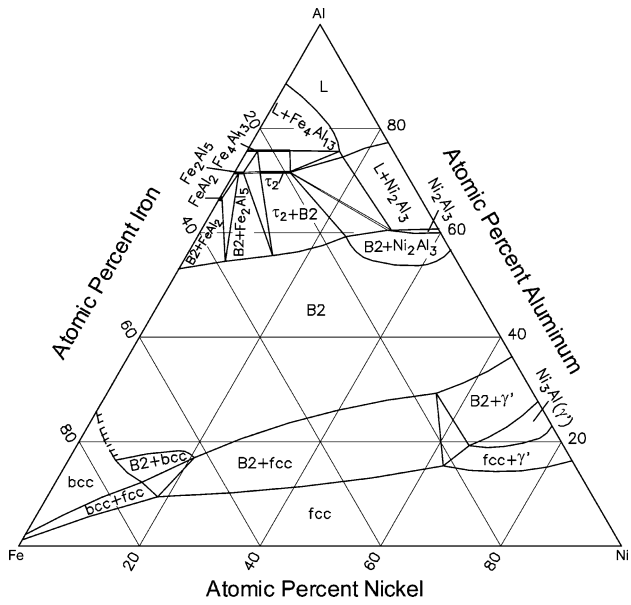

Fig. 1 Al-Fe-Ni computed isothermal section at 1050 °C [2009Zha]

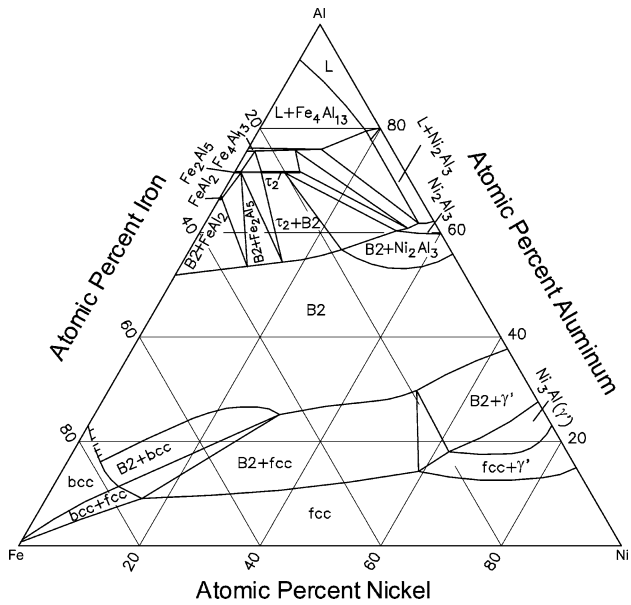

Fig. 2 Al-Fe-Ni computed isothermal section at 950 °C [2009Zha]

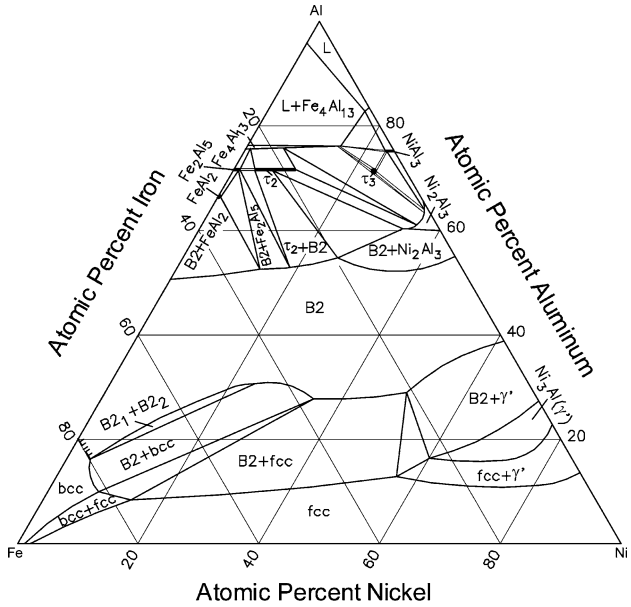

Fig. 3 Al-Fe-Ni computed isothermal section at 850 °C [2009Zha]

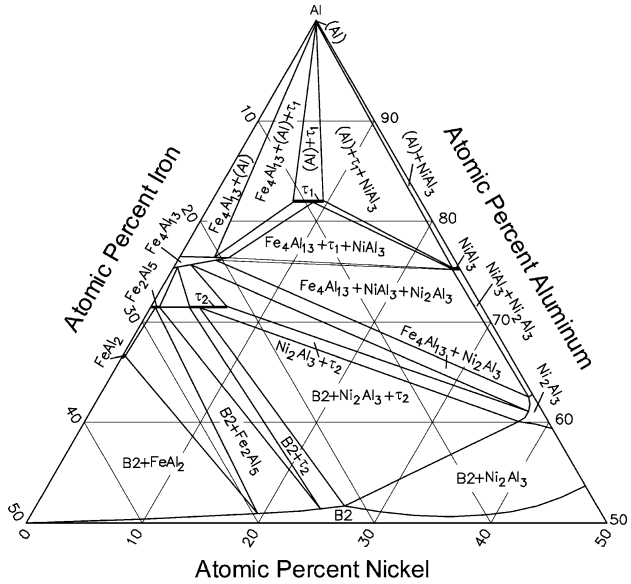

Fig. 4 Al-Fe-Ni computed isothermal section at 627 °C for Al-rich alloys [2009Zha]

the enthalpies of formation of Al_2FeNi, $AlFe_2Ni$, and $AlFeNi_2$ with the $L1_2$ ordered structure. The calculations were based on the generalized gradient approximation method. For details, see [2009Zha]. In all the cases, the values obtained experimentally, by first-principles calculation and by CALPHAD optimization showed reasonable agreement.

For the binary systems, [2009Zha] used the published descriptions from the literature. For the binary compounds Fe_4Al_{13}, Fe_2Al_5, $FeAl_2$ and Ni_2Al_3 and $NiAl_3$, which exhibit ternary solubility, appropriate sublattice models were used. The ternary solubility in ε and Ni_5Al_3 was ignored. Sublattice models of the type $(Fe,Ni)_2Al_9$ and $(Fe,Ni)_2Al_5$ were used for the ternary compounds τ_1 and τ_2, respectively. The high-temperature, quasicrystalline phase D (τ_3 in [2009Zha]) was treated as a stoichiometric compound. The liquid, disordered fcc, and disordered bcc phases were treated as substitutional solutions. The magnetic contribution to the Gibbs energy was taken into account. An ordering term was added to the Gibbs energy term of the disordered bcc and fcc phases, in order to describe the *B*2 and $L1_2$ ordered phases, respectively. The calculated thermodynamic properties were used as inputs for the optimization. The optimized interaction parameters were listed.

The isothermal sections for the entire composition range at 1050, 950, and 850 °C computed by [2009Zha] are shown in Fig. 1-3. The agreement with the experimental results from various sources is satisfactory. To preserve clarity, the experimental data points are not included in the figures. The decagonal phase D, which forms peritectically at 928 °C and decomposes eutectoidally at 848 °C, is present only in Fig. 3. A miscibility gap is seen in the *B*2 phase at 850 °C. Figure 4 is the computed isothermal section at 627 °C for Al-rich alloys, which was compared with the experimental section of [2008Zha]. Figures 5 and 6 show the partial isothermal sections at 1200 and 900 °C for Al-lean alloys. Here again, the agreement with the experimental data from various sources (not shown) was found to be satisfactory.

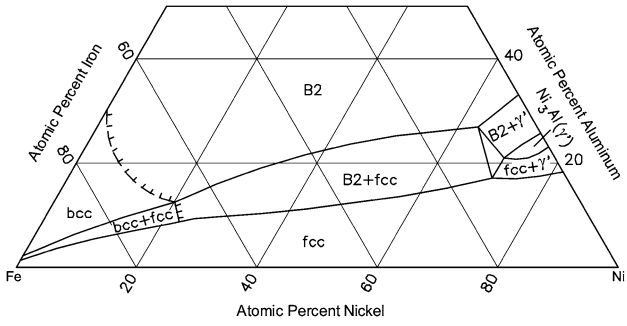

Fig. 5 Al-Fe-Ni computed isothermal section at 1200 °C for Al-lean alloys [2009Zha]

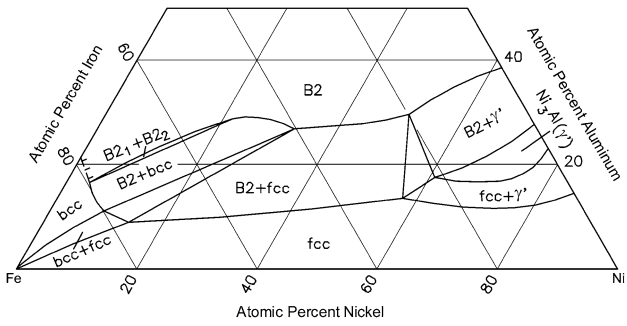

Fig. 6 Al-Fe-Ni computed isothermal section at 900 °C for Al-lean alloys [2009Zha]

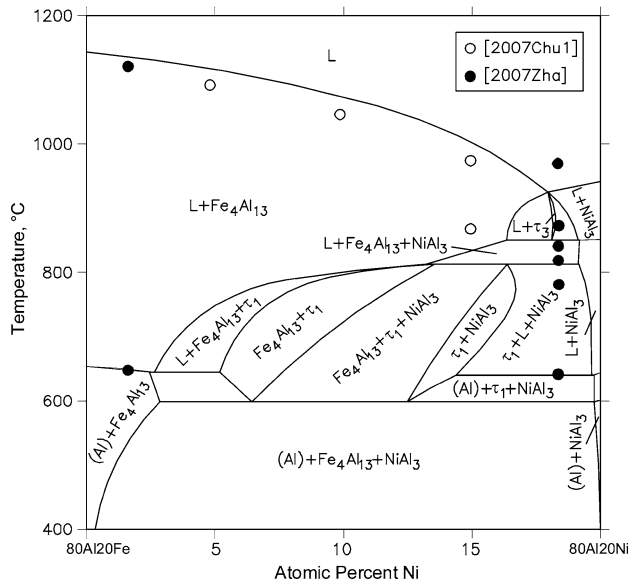

Fig. 7 Al-Fe-Ni computed vertical section at 80 at.% Al [2009Zha]

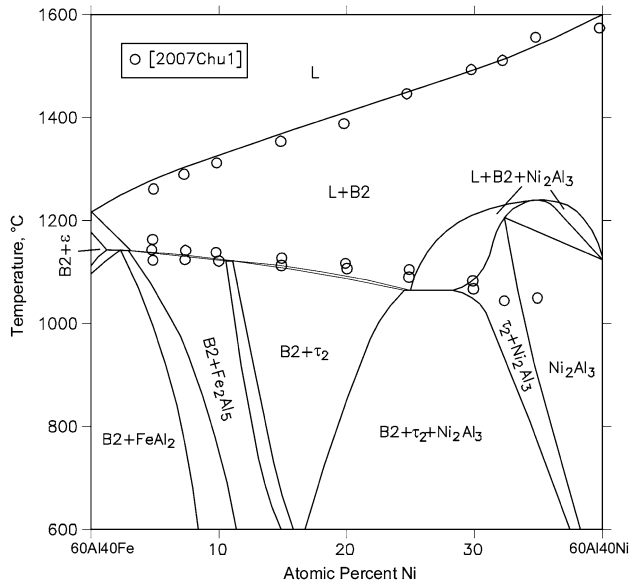

Fig. 8 Al-Fe-Ni computed vertical section at 60 at.% Al [2009Zha]

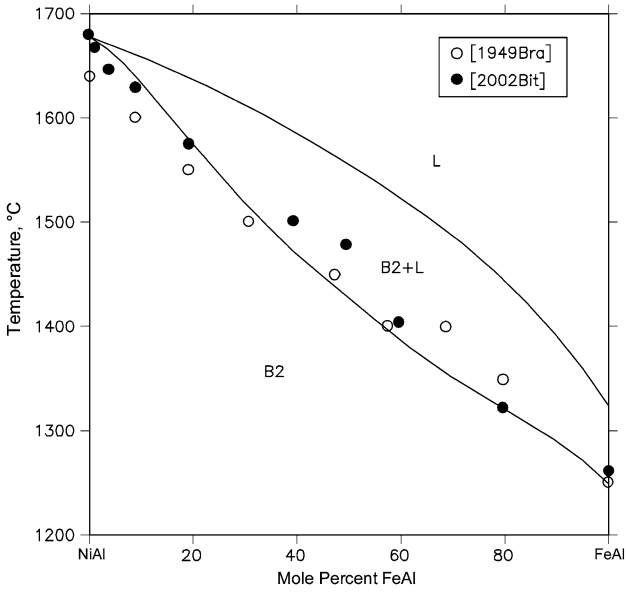

Fig. 9 Al-Fe-Ni computed vertical section along the NiAl-FeAl join [2009Zha]

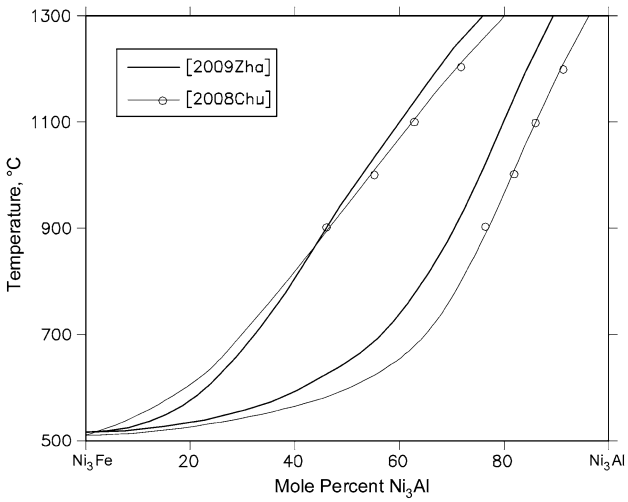

Fig. 10 Al-Fe-Ni computed vertical section along the Ni_3Fe-Ni_3Al join [2009Zha]

Four computed vertical sections at 80, 60, and 50 at.% Al and at 75 at.% Ni, respectively, are shown in Fig. 7-10. The sections in Fig. 7 and 8 are compared with the results of [2007Chu1] and [2007Zha] and the agreement is satisfactory. The same is seen in Fig. 9, where the computed section is compared with the data of [1949Bra] and [2002Bit]. In Fig. 10, the vertical section along the Ni_3Fe-Ni_3Al join computed by [2009Zha] is compared with the most recent experimental results of [2008Chu] from EPMA measurements. The experimental data points from various other sources indicated by [2009Zha] show a wide scatter and are not shown in Fig. 10. [2009Zha] also computed a liquidus projection and a reaction sequence for solidification reactions. The computed invariant reactions and their temperatures generally agree with those reported by [2007Chu1] and reviewed in the update by [2008Rag], but with some differences.

References

1949Bra: A.J. Bradley, Microscopic Studies on the Iron-Nickel-Aluminum System. Part 1: α + β Alloys and Isothermal Section of the Phase Equilibrium Diagram, *J. Iron Steel Inst. (Lond.)*, 1949, **163**(1), p 19-30

1988Ray: G.V. Raynor and V.G. Rivlin, Al-Fe-Ni, *Phase Equilibria in Iron Ternary Alloys*, Institute of Metals, London, 1988, p 107-121

1993Kat: U.R. Kattner and B.P. Burton, Al-Fe (Aluminum-Iron), *Phase Diagrams of Binary Iron Alloys*, H. Okamoto, Ed., ASM International, Materials Park, OH, 1993, p 12-28

1993Oka: H. Okamoto, Al-Ni (Aluminum-Nickel), *J. Phase Equilib.*, 1993, **14**(2), p 257-259

1994Rag: V. Raghavan, Al-Fe-Ni (Aluminum-Iron-Nickel), *J. Phase Equilib.*, 1994, **15**(4), p 411-413

2002Bit: H. Bitterlich, W. Loeser, and L. Schultz, Reassessment of Al-Ni and Ni-Fe-Al Solidus Temperatures, *J. Phase Equilib.*, 2002, **23**(4), p 301-304

2005Cac: G. Cacciamani, R. Ferro, B. Grushko, P. Perrot, and R. Schmid-Fetzer, Aluminum-Iron-Nickel, *Landolt-Bornstein New Series IV*, Vol 11A2, G. Effenberg and S. Ilyenko, Ed., Springer-Verlag, Berlin, 2005, p 329-358

2005Rag: V. Raghavan, Al-Fe-Ni (Aluminum-Iron-Nickel), *J. Phase Equilb. Diffus.*, 2005, **26**(1), p 70-71

2006Ele: L. Eleno, K. Frisk, and A. Schneider, Assessment of the Fe-Ni-Al System, *Intermetallics*, 2006, **14**, p 1276-1290

2006Rag: V. Raghavan, Al-Fe-Ni (Aluminum-Iron-Nickel), *J. Phase Equilib. Diffus.*, 2006, **27**(5), p 489-490

2007Chu1: I. Chumak, K.W. Richter, and H. Ipser, The Fe-Ni-Al Phase Diagram in the Al-Rich (>50 At.% Al) Corner, *Intermetallics*, 2007, **15**, p 1416-1424

2007Chu2: I. Chumak, K.W. Richter, S.G. Fries, and H. Ipser, Experimental Phase Diagram Investigations in the Ni-Rich Part of Al-Fe-Ni and Comparison with Calculated Phase Equilibria, *J. Phase Equilib. Diffus.*, 2007, **28**(5), p 417-421

2007Zha: L. Zhang and Y. Du, Thermodynamic Description of the Al-Fe-Ni System Over the Whole Composition and Temperature Ranges: Modeling Coupled with Key Experiment, *CALPHAD*, 2007, **31**, p 529-540

2008Chu: I. Chumak, K.W. Richter, and H. Ipser, Isothermal Sections in the (Fe,Ni)-Rich Part of the Fe-Ni-Al Phase Diagram, *J. Phase Equilib. Diffus.*, 2008, **29**(4), p 300-304

2008Rag: V. Raghavan, Al-Fe-Ni (Aluminum-Iron-Nickel), *J. Phase Equilib. Diffus.*, 2008, **29**(2), p 180-184

2008Zha: L. Zhang, Y. Du, H. Xu, C. Tang, H. Chen, and W. Zhang, Phase Equilibria of the Al-Fe-Ni System at 850°C and 627°C, *J. Alloys Compd.*, 2008, **454**, p 129-135

2009Rag1: V. Raghavan, Al-Fe-Ni (Aluminum-Iron-Nickel), *J. Phase Equilib. Diffus.*, 2009, **30**(1), p 85-88

2009Rag2: V. Raghavan, Al-Fe-Ni (Aluminum-Iron-Nickel), *J. Phase Equilb. Diffus.*, 2009, **30**(4), p 375-377

2009Zha: L. Zhang, J. Wang, Y. Du, R. Hu, P. Nash, X.G. Lu, and C. Jiang, Thermodynamic Properties of the Al-Fe-Ni System Acquired via a Hybrid Approach Combining Calorimetry, First-Principles and CALPHAD, *Acta Mater.*, 2009, **57**, p 5324-5341