Fe – Ni (Iron – Nickel)

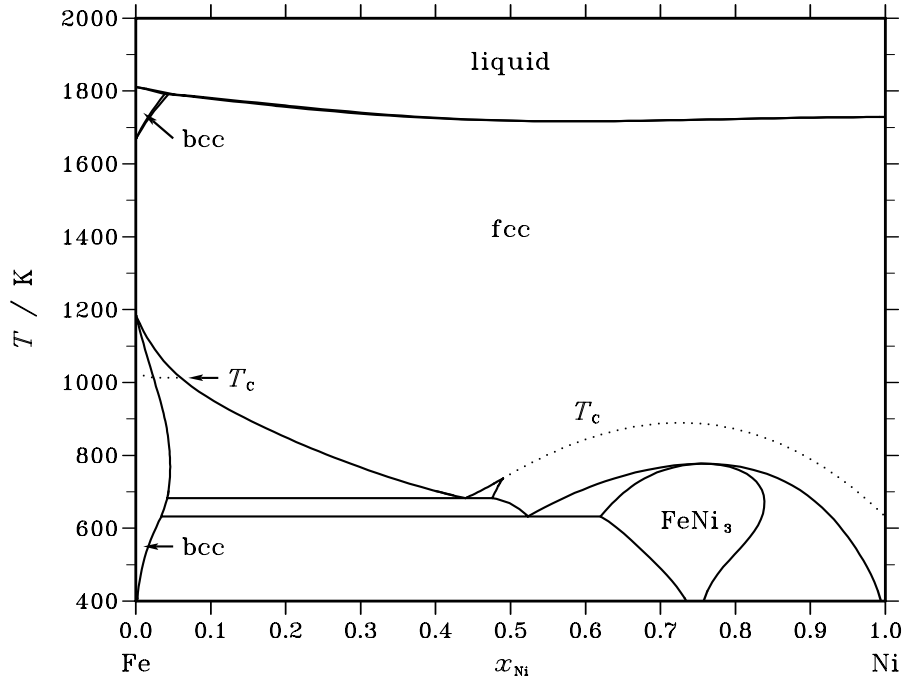

Fig. 1. Calculated phase diagram for the system Fe-Ni.

The fcc and liquid phases form complete solutions across the Fe-Ni system and the solubility of Ni in bcc is quite low. At low temperature there is an ordered $FeNi_3$ phase with $L1_2$ structure. There are many important features in this system, in particular the magnetic properties which causes the Invar effect close to equiatomic compositions. When Fe is added to Ni the temperature for the ferro-magnetic transformation, the Curie temperature, first increases towards a maximum around x_{Ni}=0.75 and then decreases again. In the calculated phase diagram, the interaction of the magnetic transition with the bcc/fcc two-phase field results in the formation of a so-called Nishizawa-horn.
The assessment of the liquid, bcc and fcc phases for this system [86Din] is quite old and has never been published. The ordered phase has been added later [95Ans] also as unpublished work. The present assessment is the most widely used in steel and superalloy databases.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Ni)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Ni)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Ni)_1$
$FeNi_3$	$L1_2$	$AuCu_3$	$cP4$	$Pm\overline{3}m$	FCC_L12	4(Fe,Ni)

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ni}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc + liquid $\rightleftharpoons$ fcc	peritectic	1791.5	0.039	0.049	0.044	−8157
liquid $\rightleftharpoons$ fcc	congruent	1716.7	0.581	0.581		−14762
fcc $\rightleftharpoons$ $FeNi_3$	congruent	777.3	0.756	0.756		−3206
fcc $\rightleftharpoons$ fcc′ + fcc″	critical	737.3	0.490	0.490	0.490	0
fcc′ $\rightleftharpoons$ bcc + fcc″	monotectoid	682.9	0.440	0.042	0.476	−1370
fcc″ $\rightleftharpoons$ bcc + $FeNi_3$	eutectoid	632.8	0.523	0.034	0.620	−4008

Table IIIa. Integral quantities for the liquid phase at 1873 K.

x_{Ni}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−5512	−990	2.415	−450	−0.288	0.000
0.200	−8675	−2055	3.535	−883	−0.626	0.000
0.300	−10780	−3084	4.109	−1267	−0.970	0.000
0.400	−12053	−3968	4.317	−1572	−1.279	0.000
0.500	−12561	−4595	4.253	−1767	−1.510	0.000
0.600	−12301	−4854	3.976	−1820	−1.620	0.000
0.700	−11214	−4635	3.513	−1701	−1.566	0.000
0.800	−9172	−3827	2.854	−1379	−1.307	0.000
0.900	−5885	−2319	1.904	−822	−0.799	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(liquid), Ni(liquid)

Table IIIb. Partial quantities for Fe in the liquid phase at 1873 K.

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G_{\mathrm{Fe}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Fe}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1644	56	0.908	−3	0.032	0.900	1.000
0.800	−3530	77	1.926	−55	0.071	0.797	0.996
0.700	−5772	−159	2.997	−217	0.031	0.690	0.986
0.600	−8507	−874	4.075	−552	−0.172	0.579	0.965
0.500	−11915	−2288	5.140	−1120	−0.623	0.465	0.931
0.400	−16255	−4623	6.210	−1986	−1.408	0.352	0.880
0.300	−21959	−8101	7.399	−3210	−2.612	0.244	0.814
0.200	−29918	−12944	9.063	−4854	−4.319	0.146	0.732
0.100	−42840	−19372	12.530	−6981	−6.615	0.064	0.639
0.000	$-\infty$	−27607	∞	−9653	−9.586	0.000	0.538

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Ni in the liquid phase at 1873 K.

x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ni}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ni}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
0.000	$-\infty$	−9151	∞	−4482	−2.493	0.000	0.750
0.100	−40327	−10402	15.977	−4468	−3.168	0.075	0.751
0.200	−29256	−10581	9.971	−4192	−3.411	0.153	0.764
0.300	−22466	−9910	6.704	−3717	−3.307	0.236	0.788
0.400	−17372	−8610	4.678	−3103	−2.940	0.328	0.819
0.500	−13208	−6902	3.367	−2413	−2.396	0.428	0.856
0.600	−9665	−5008	2.487	−1710	−1.761	0.538	0.896
0.700	−6609	−3149	1.848	−1055	−1.118	0.654	0.935
0.800	−3985	−1547	1.302	−510	−0.554	0.774	0.968
0.900	−1779	−424	0.723	−138	−0.153	0.892	0.991
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ni(liquid)

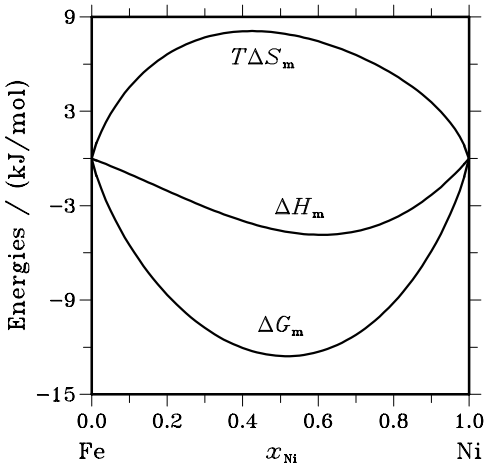

Fig. 2. Integral quantities of the liquid phase at T=1873 K.

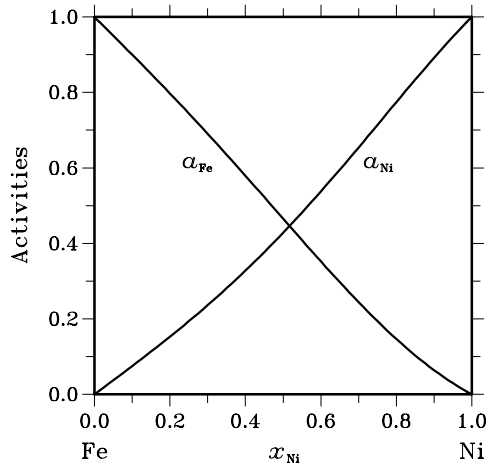

Fig. 3. Activities in the liquid phase at T=1873 K.

Table IVa. Integral quantities for the stable phases at 1473 K.

Phase	x_{Ni}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
fcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−4348	−327	2.730	−366	0.027	−0.004
	0.200	−6892	−904	4.066	−764	−0.095	−0.008
	0.300	−8644	−1626	4.765	−1163	−0.314	0.003
	0.400	−9773	−2393	5.010	−1530	−0.586	0.068
	0.500	−10312	−3091	4.903	−1823	−0.860	0.209
	0.600	−10230	−3568	4.522	−1987	−1.073	0.370
	0.700	−9436	−3644	3.932	−1955	−1.147	0.428
	0.800	−7785	−3150	3.147	−1656	−1.014	0.314
	0.900	−5009	−1969	2.064	−1027	−0.639	0.120
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(fcc), Ni(fcc)

Table IVb. Partial quantities for Fe in the stable phases at 1473 K.

Phase	x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Fe}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Fe}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
fcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1271	142	0.959	20	0.083	0.901	1.002
	0.800	−2690	429	2.117	43	0.262	0.803	1.004
	0.700	−4363	660	3.410	5	0.444	0.700	1.000
	0.600	−6434	622	4.790	−178	0.543	0.591	0.986
	0.500	−9119	−12	6.183	−630	0.420	0.475	0.950
	0.400	−12744	−1720	7.484	−1522	−0.134	0.353	0.883
	0.300	−17777	−4936	8.718	−3032	−1.293	0.234	0.781
	0.200	−24994	−9732	10.361	−5283	−3.020	0.130	0.650
	0.100	−36570	−15959	13.992	−8370	−5.152	0.050	0.505
	0.000	$-\infty$	−24116	∞	−12534	−7.862	0.000	0.359

Reference state: Fe(fcc)

Table IVc. Partial quantities for Ni in the stable phases at 1473 K.

Phase	x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ni}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ni}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
fcc	0.000	$-\infty$	−1682	∞	−3428	1.185	0.000	0.756
	0.100	−32043	−4550	18.665	−3843	−0.480	0.073	0.731
	0.200	−23703	−6234	11.860	−3992	−1.522	0.144	0.722
	0.300	−18635	−6959	7.926	−3889	−2.084	0.218	0.728
	0.400	−14781	−6917	5.339	−3559	−2.279	0.299	0.748
	0.500	−11506	−6169	3.623	−3016	−2.140	0.391	0.782
	0.600	−8553	−4800	2.548	−2297	−1.699	0.497	0.829
	0.700	−5861	−3091	1.881	−1493	−1.085	0.620	0.885
	0.800	−3483	−1505	1.343	−750	−0.512	0.752	0.941
	0.900	−1502	−414	0.738	−212	−0.138	0.885	0.983
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ni(fcc)

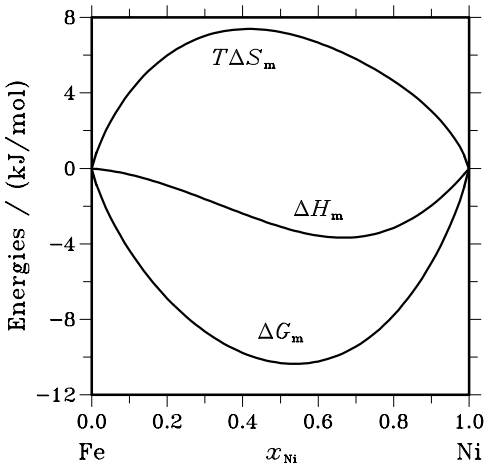

Fig. 4. Integral quantities of the stable phases at T=1473 K.

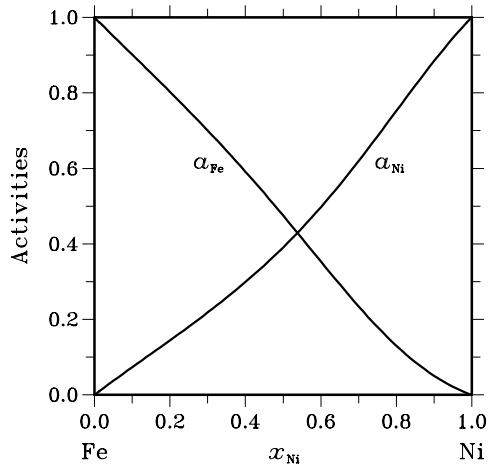

Fig. 5. Activities in the stable phases at T=1473 K.

Table V. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_{Ni}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C_P^{\circ}$ / (J/(mol·K))
$FeNi_3$	0.750	−10599	−13547	−9.888	0.006

References

[86Din] A.T. Dinsdale, T. Chart: unpublished assessment, 1986.
[95Ans] I. Ansara: unpublished assessment, 1995.