Ni – Si (Nickel – Silicon)

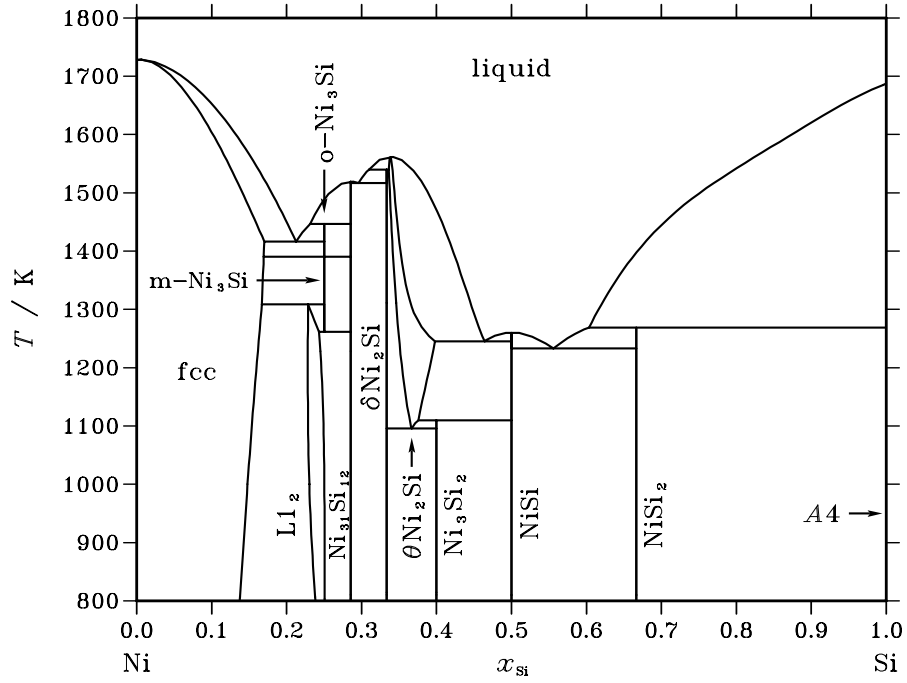

Fig. 1. Calculated phase diagram for the system Ni-Si.

Ni and Si are both alloying elements in steels and other alloys. The solubility of Si in Ni is rather high and the ordered Ni_3Si phase ($L1_2$) is interesting for applications with heat resistant alloys. As in many metal-silicon systems there are several intermetallic phases but they have little or no practical interest. The assessment is taken from [96Lin].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ni,Si)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_L12	$(Ni,Si)_1$
$L1_2$	$L1_2$	Cu_3Au	$cP4$	$Pm\overline{3}m$	FCC_L12	$3(Ni,Si)_1 1(Ni,Si)_1$
o-Ni3Si	···	$GePt_3$	$mC16$	$C2/m$	NI3SI_ORTHO	Ni_3Si_1
m-Ni3Si	···	···	$oP16$	···	NI3SI_MONOCL	Ni_3Si_1
$Ni_{31}Si_{12}$	···	···	$hP14$	···	NI31SI12	$Ni_{31}Si_{12}$
δNi_2Si	$C37$	Co_2Si	$oP12$	$Pnma$	NI2SI	Ni_2Si_1
θNi_2Si	···	···	$hP6$	$C6_3m$	NI2SI_TETA	$Ni_1(Ni,\square)_1Si_1$
ϵNi_3Si_2	···	Ni_3Si_2	$oP80$	$Cmc2_1$	EPSILON_NI3SI2	Ni_3Si_2
$\epsilon' Ni_3Si_2$	···	···	···	···	NI3SI2	Ni_3Si_2
NiSi	$B31$	MnP	$oP8$	$Pnma$	B31_NISI	Ni_1Si_1
$NiSi_2$	$C1$	CaF_2	$cF12$	$Fm\overline{3}m$	C1_NISI2	Ni_1Si_2
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_FCC_A4	Si_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Si}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ $\theta$$Ni_2Si$	congruent	1561.8	0.338	0.338		−15747
liquid + $\theta$$Ni_2Si$ $\rightleftharpoons$ $\delta$$Ni_2Si$	peritectic	1539.8	0.310	0.336	0.333	−3876
liquid $\rightleftharpoons$ $Ni_{31}Si_{12}$	congruent	1519.3	0.286	0.286		−19951
liquid $\rightleftharpoons$ $Ni_{31}Si_{12}$ + $\delta$$Ni_2Si$	eutectic	1517.0	0.296	0.286	0.333	−19364
liquid + $Ni_{31}Si_{12}$ $\rightleftharpoons$ o-Ni_3Si	peritectic	1446.4	0.232	0.286	0.250	−10292
liquid $\rightleftharpoons$ fcc + o-Ni_3Si	eutectic	1416.3	0.213	0.170	0.250	−15561
o-Ni_3Si $\rightleftharpoons$ m-Ni_3Si	polymorphic	1390.4	0.250	0.169	0.250	−65
fcc + m-Ni_3Si $\rightleftharpoons$ $L1_2$	peritectoid	1308.7	0.167	0.250	0.229	−2343
liquid + $A4$ $\rightleftharpoons$ $NiSi_2$	peritectic	1269.0	0.604	1.000	0.667	−29062
m-Ni_3Si $\rightleftharpoons$ $L1_2$ + $Ni_{31}Si_{12}$	eutectoid	1261.7	0.250	0.243	0.286	−2568
liquid $\rightleftharpoons$ NiSi	congruent	1260.5	0.500	0.500		−21915
liquid $\rightleftharpoons$ $\theta$$Ni_2Si$ + NiSi	eutectic	1245.4	0.464	0.398	0.500	−18487
liquid $\rightleftharpoons$ NiSi + $NiSi_2$	eutectic	1232.8	0.556	0.500	0.667	−25881
$\theta$$Ni_2Si$ + NiSi $\rightleftharpoons$ Ni_3Si_2	peritectoid	1110.0	0.376	0.500	0.400	−4693
$\theta$$Ni_2Si$ $\rightleftharpoons$ $\delta$$Ni_2Si$ + Ni_3Si_2	eutectoid	1096.0	0.367	0.333	0.400	−3999

Table IIIa. Integral quantities for the liquid phase at 1853 K.

x_{Si}	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	−22638	−21314	0.715	−17630	−1.988	0.000
0.200	−37400	−39761	−1.274	−29690	−5.435	0.000
0.300	−45703	−51113	−2.920	−36292	−7.999	0.000
0.400	−48399	−54501	−3.293	−38030	−8.889	0.000
0.500	−46502	−51295	−2.587	−35822	−8.350	0.000
0.600	−41118	−43986	−1.547	−30749	−7.143	0.000
0.700	−33302	−35063	−0.950	−23890	−6.029	0.000
0.800	−23872	−25897	−1.093	−16163	−5.253	0.000
0.900	−13171	−15619	−1.321	−8162	−4.024	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ni in the liquid phase at 1853 K.

x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	G^E_{Ni} [J/mol]	S^E_{Ni} [J/(mol·K)]	a_{Ni}	γ_{Ni}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−4378	−393	2.151	−2755	1.275	0.753	0.836
0.800	−14595	−9187	2.918	−11157	1.063	0.388	0.485
0.700	−29672	−29240	0.233	−24177	−2.733	0.146	0.208
0.600	−47526	−55573	−4.343	−39656	−8.590	0.046	0.076
0.500	−65629	−79845	−7.672	−54950	−13.435	0.014	0.028
0.400	−81695	−94837	−7.092	−67578	−14.711	0.005	0.012
0.300	−94413	−98927	−2.436	−75864	−12.446	0.002	0.007
0.200	−104383	−100573	2.056	−79587	−11.325	0.001	0.006
0.100	−116100	−122788	−3.609	−80625	−22.754	0.001	0.005
0.000	−∞	−207620	∞	−83599	−66.930	0.000	0.004

Reference state: Ni(liquid)

Table IIIc. Partial quantities for Si in the liquid phase at 1853 K.

x_{Si}	ΔG_{Si} [J/mol]	ΔH_{Si} [J/mol]	ΔS_{Si} [J/(mol·K)]	G^E_{Si} [J/mol]	S^E_{Si} [J/(mol·K)]	a_{Si}	γ_{Si}
0.000	−∞	−202740	∞	−202981	0.130	0.000	0.000
0.100	−186980	−209604	−12.209	−151505	−31.354	0.000	0.000
0.200	−128620	−162057	−18.045	−103824	−31.427	0.000	0.001
0.300	−83109	−102149	−10.275	−64560	−20.285	0.005	0.015
0.400	−49708	−52893	−1.719	−35591	−9.337	0.040	0.099
0.500	−27374	−22745	2.498	−16695	−3.265	0.169	0.338
0.600	−14067	−10085	2.149	−6197	−2.098	0.401	0.669
0.700	−7111	−7692	−0.314	−1616	−3.279	0.630	0.900
0.800	−3744	−7228	−1.880	−307	−3.735	0.784	0.980
0.900	−1734	−3711	−1.067	−111	−1.943	0.894	0.993
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Si(liquid)

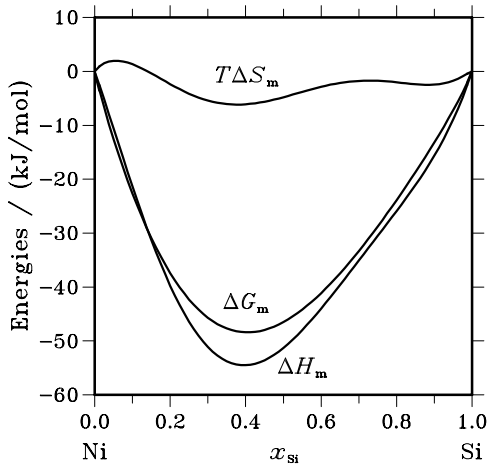

Fig. 2. Integral quantities of the liquid phase at T=1853 K.

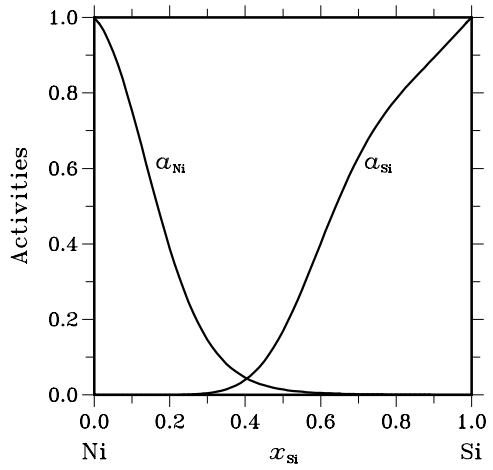

Fig. 3. Activities in the liquid phase at T=1853 K.

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

Compound	x_{Si}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
m-Ni_3Si	0.250	−38404	−38133	0.911	0.000
o-Ni_3Si	0.250	−38353	−38068	0.958	0.000
$Ni_{31}Si_{12}$	0.286	−43373	−43490	−0.391	0.000
δNi_2Si	0.333	−43448	−42923	1.760	0.000
Ni_3Si_2	0.400	−43559	−43852	−0.982	0.000
Ni_1Si_1	0.500	−39568	−39628	−0.200	0.000
Ni_1Si_2	0.667	−32866	−34583	−5.760	0.000

References

[96Lin] M. Lindholm, B. Sundman: Metall. Trans. A **26A** (1996) 2897–2903.