La – Ni (Lanthanum – Nickel)

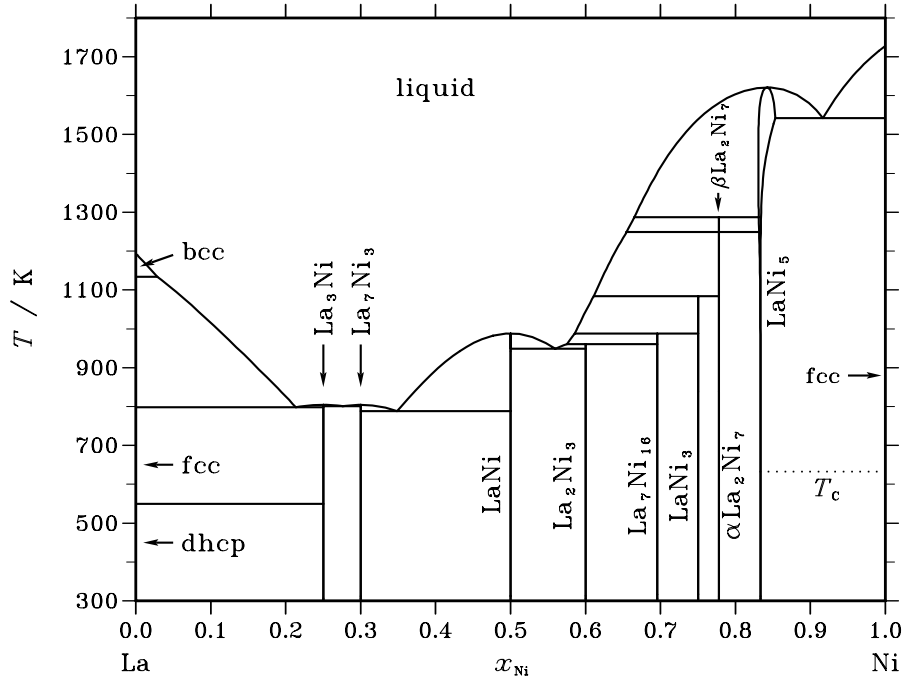

Fig. 1. Calculated phase diagram for the system La-Ni.

Intermetallic compounds of rare-earth metals with transition metals are of interest due to their magnetic properties and because of the reversible absorption of hydrogen gas which is required for hydrogen storage materials. Thermodynamic assessments for the La-Ni system are given by [98Du] and [00Liu]. The work of [00Liu] has been selected because it includes an improved description of the $LaNi_5$ phase. The assessment is based on experimental data on the phase equilibria from several investigations, mixing enthalpy data for the liquid at 1376 K and the enthalpy of formation for the intermetallic compounds. Except for $LaNi_5$, all intermetallic phases are described as stoichiometric compounds.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(La,Ni)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(La,Ni)_1$
fcc	$A1$	Cu	$cF4$	$Fm3\overline{3}m$	FCC_A1	$(La,Ni)_1$
dhcp	$A3'$	αLa	$hP4$	$P6_3/mmc$	DHCP	$(La,Ni)_1$
La_3Ni	$D0_{11}$	Fe_3C	$oP16$	$Pnma$	LA3NI	La_3Ni_1
La_7Ni_3	$D10_2$	Fe_3Th_7	$hP20$	$P6_3mc$	LA7NI3	La_7Ni_3
LaNi	$B33$	CrB	$oC8$	$Cmcm$	LANI	La_1Ni_1
La_2Ni_3	···	···	$oC20$	$Cmca$	LA2NI3	La_2Ni_3
La_7Ni_{16}	···	···	$tI46$	$I\overline{4}2m$	LA7NI16	La_7Ni_{16}
$LaNi_3$	···	Ni_3Pu	$hR24$	$R\overline{3}m$	LANI3	La_1Ni_3
αLa_2Ni_7	···	Ce_2Ni_7	$hP36$	$P6_3/mmc$	LA2NI7_ALFA	La_2Ni_7
βLa_2Ni_7	···	Gd_2Co_7	$hR18$	$R\overline{3}m$	LA2NI7_BETA	La_2Ni_7
$LaNi_5$	$D2_d$	$CaCu_5$	$hP6$	$P6/mmm$	LANI5	$(La,Ni)_1(La,Ni)_2Ni_3$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ni}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ $LaNi_5$	congruent	1620.9	0.842	0.842		−18548
liquid $\rightleftharpoons$ $LaNi_5$ + fcc	eutectic	1542.2	0.917	0.853	1.000	−14666
liquid + $LaNi_5$ $\rightleftharpoons$ βLa_2Ni_7	peritectic	1287.4	0.665	0.831	0.778	−2144
βLa_2Ni_7 $\rightleftharpoons$ αLa_2Ni_7	polymorphic	1248.8	0.778	0.778		−2630
bcc + liquid $\rightleftharpoons$ fcc	degenerate	1134.0	0.000	0.029	0.000	−3121
liquid + αLa_2Ni_7 $\rightleftharpoons$ $LaNi_3$	peritectic	1084.3	0.611	0.778	0.750	−2510
liquid $\rightleftharpoons$ LaNi	congruent	988.1	0.500	0.500		−11700
liquid + $LaNi_3$ $\rightleftharpoons$ La_7Ni_{16}	peritectic	987.4	0.586	0.750	0.696	−5254
liquid + La_7Ni_{16} $\rightleftharpoons$ La_2Ni_3	peritectic	960.2	0.575	0.696	0.600	−8932
liquid $\rightleftharpoons$ LaNi + La_2Ni_3	eutectic	948.5	0.560	0.500	0.600	−11216
liquid $\rightleftharpoons$ La_3Ni	congruent	805.0	0.250	0.250		−10158
liquid $\rightleftharpoons$ La_7Ni_3	congruent	804.6	0.300	0.300		−10036
liquid $\rightleftharpoons$ La_3Ni + La_7Ni_3	eutectic	800.9	0.276	0.250	0.300	−10075
liquid $\rightleftharpoons$ fcc + La_3Ni	eutectic	797.8	0.214	0.000	0.250	−10299
liquid $\rightleftharpoons$ La_7Ni_3 + LaNi	eutectic	788.0	0.349	0.300	0.500	−9842
fcc + La_3Ni $\rightleftharpoons$ dhcp	degenerate	550.0	0.000	0.250	0.000	−364

Table IIIa. Integral quantities for the liquid phase at 1800 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	−14690	−5265	5.236	−9824	2.533	0.000
0.200	−24592	−11758	7.130	−17103	2.969	0.000
0.300	−31114	−18581	6.963	−21972	1.884	0.000
0.400	−34639	−24833	5.448	−24567	−0.148	0.000
0.500	−35397	−29615	3.212	−25024	−2.551	0.000
0.600	−33551	−32029	0.846	−23479	−4.750	0.000
0.700	−29210	−31173	−1.091	−20068	−6.170	0.000
0.800	−22417	−26150	−2.074	−14927	−6.235	0.000
0.900	−13058	−16058	−1.667	−8193	−4.370	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for La in the liquid phase at 1800 K.

x_{La}	ΔG_{La} [J/mol]	ΔH_{La} [J/mol]	ΔS_{La} [J/(mol·K)]	G^E_{La} [J/mol]	S^E_{La} [J/(mol·K)]	a_{La}	γ_{La}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2872	764	2.020	−1296	1.144	0.825	0.917
0.800	−8340	1858	5.666	−5001	3.810	0.573	0.716
0.700	−16182	1481	9.813	−10844	6.847	0.339	0.485
0.600	−26198	−2164	13.352	−18553	9.105	0.174	0.289
0.500	−38230	−10876	15.196	−27856	9.433	0.078	0.155
0.400	−52195	−26456	14.300	−38481	6.681	0.031	0.076
0.300	−68176	−50701	9.708	−50157	−0.302	0.011	0.035
0.200	−86697	−85410	0.715	−62610	−12.667	0.003	0.015
0.100	−110031	−132383	−12.418	−75570	−31.563	0.001	0.006
0.000	−∞	−193418	∞	−88765	−58.141	0.000	0.003

Reference state: La(liquid)

Table IIIc. Partial quantities for Ni in the liquid phase at 1800 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}
0.000	−∞	−43505	∞	−111424	37.733	0.000	0.001
0.100	−121044	−59525	34.177	−86583	15.032	0.000	0.003
0.200	−89598	−66221	12.987	−65511	−0.395	0.003	0.013
0.300	−65955	−65392	0.313	−47936	−9.698	0.012	0.041
0.400	−47300	−58837	−6.409	−33587	−14.028	0.042	0.106
0.500	−32565	−48355	−8.772	−22191	−14.535	0.114	0.227
0.600	−21122	−35744	−8.123	−13477	−12.370	0.244	0.406
0.700	−12511	−22805	−5.719	−7173	−8.684	0.433	0.619
0.800	−6346	−11335	−2.771	−3007	−4.627	0.654	0.818
0.900	−2283	−3133	−0.472	−706	−1.348	0.859	0.954
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ni(liquid)

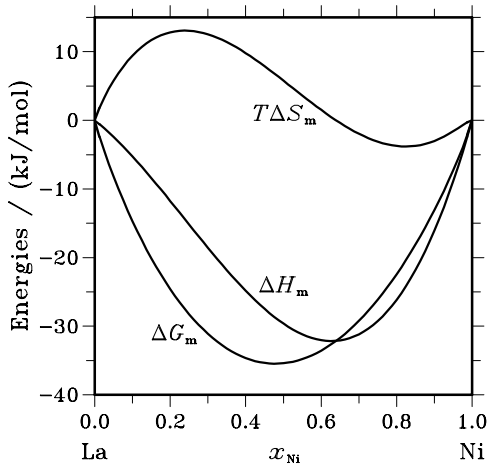

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

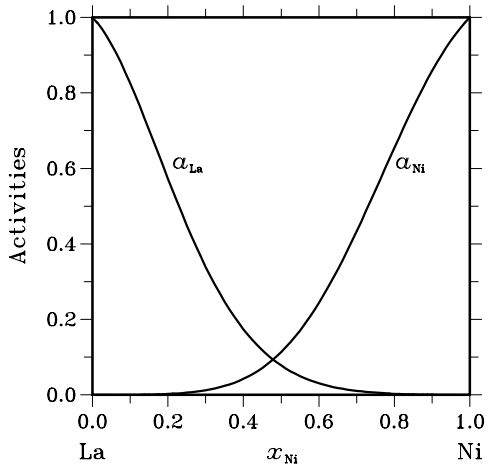

Fig. 3. Activities in the liquid phase at T=1800 K.

Table IV. 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))
La_3Ni_1	0.250	−14746	−13482	4.239	−0.191
La_7Ni_3	0.300	−17611	−16331	4.292	−0.229
La_1Ni_1	0.500	−27697	−26998	2.346	−0.382
La_2Ni_3	0.600	−28548	−28489	0.197	−0.459
La_7Ni_{16}	0.696	−29316	−30032	−2.401	−0.532
La_1Ni_3	0.750	−28156	−28686	−1.779	−0.573
αLa_2Ni_7	0.778	−27527	−28056	−1.772	−0.595
βLa_2Ni_7	0.778	−25525	−25426	0.334	−0.595
$LaNi_5$	0.833	−26202	−27008	−2.703	−0.637

References

[98Du] Z. Du, D. Wang, W. Zhang: J. Alloys. Compd. **264** (1998) 209–213.
[00Liu] L. Liu, Z. Jin: Z. Metallkd. **91** (2000) 739–743.