Ce – Ni (Cerium – Nickel)

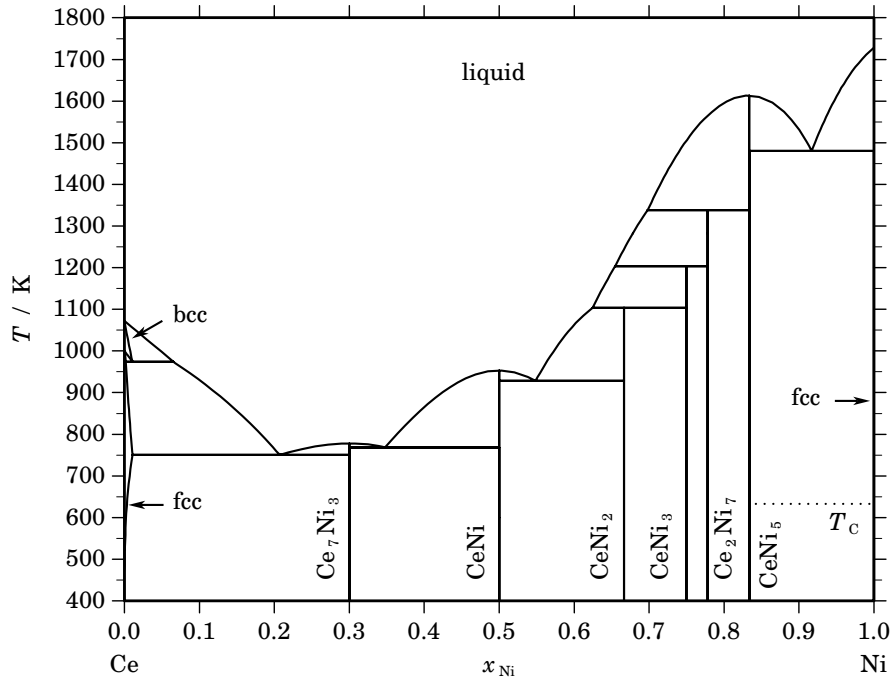

Fig. 1. Calculated phase diagram for the system Ce-Ni.

The interest in the Ce-Ni system is related to its potential use in hydrogen storage materials or in permanent magnets. A review on the thermodynamic literature of the Ce-Ni system has been given by Nash and Tung [1991Nas] and a thermodynamic optimisation has been prepared by Du *et al.* [2004Du]. The optimisation is based mainly on experimental information on the phase diagram [1947Vog, 1964Dus, 1965Per, 1967Geb]. No thermodynamic data are available for the melt. Calorimetric data for the standard enthalpy of formation for intermetallic compounds have been reported only for $CeNi_5$ [1983Col, 1998Guo] and for CeNi [1998Guo].

Table I. Phases, structures and models.

Phase	Strukturbericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ce,Ni)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Ce,Ni)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Ce,Ni)_1$
Ce_7Ni_3	$D10_2$	Fe_3Th_7	$hP20$	$P6_3mc$	CE7NI3	Ce_7Ni_3
CeNi	$B33$	CrB	$oC8$	$Cmcm$	CENI	Ce_1Ni_1
$CeNi_2$	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	CENI2	Ce_1Ni_2
$CeNi_3$	···	$CeNi_3$	hP*	$P6_3/mmc$	CENI3	Ce_1Ni_3
Ce_2Ni_7	···	$CeNi_3$	hP*	$P6_3/mmc$	CE2NI7	Ce_2Ni_7
$CeNi_5$	$D2_d$	$CaCu_5$	$hP6$	$P6/mmm$	CENI5	Ce_1Ni_5

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ni}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ $CeNi_5$	congruent	1613.2	0.833	0.833		−21520
liquid $\rightleftharpoons$ $CeNi_5$ + fcc	eutectic	1480.4	0.917	0.833	1.000	−17066
liquid + $CeNi_5$ $\rightleftharpoons$ Ce_2Ni_7	peritectic	1337.9	0.698	0.833	0.778	−5737
liquid + Ce_2Ni_7 $\rightleftharpoons$ $CeNi_3$	peritectic	1203.3	0.655	0.778	0.750	−2925
liquid + $CeNi_3$ $\rightleftharpoons$ $CeNi_2$	peritectic	1103.3	0.625	0.750	0.667	−7964
bcc $\rightleftharpoons$ fcc + liquid	metatectic	974.1	0.011	0.002	0.065	−1778
liquid $\rightleftharpoons$ CeNi	congruent	953.3	0.500	0.500		−13001
liquid $\rightleftharpoons$ CeNi + $CeNi_2$	eutectic	928.2	0.548	0.500	0.667	−11999
liquid $\rightleftharpoons$ Ce_7Ni_3	congruent	778.2	0.300	0.300		−16211
liquid $\rightleftharpoons$ Ce_7Ni_3 + CeNi	eutectic	768.2	0.348	0.300	0.500	−14826
liquid $\rightleftharpoons$ fcc + Ce_7Ni_3	eutectic	750.2	0.207	0.011	0.300	−13593

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)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−14339	−6471	4.371	−9474	1.668	0.000
0.200	−25006	−13551	6.364	−17517	2.203	0.000
0.300	−33018	−20473	6.969	−23876	1.890	0.000
0.400	−38371	−26469	6.612	−28298	1.016	0.000
0.500	−40905	−30772	5.630	−30532	−0.133	0.000
0.600	−40394	−32612	4.324	−30322	−1.272	0.000
0.700	−36559	−31223	2.965	−27417	−2.114	0.000
0.800	−29053	−25837	1.787	−21564	−2.374	0.000
0.900	−17374	−15685	0.939	−12509	−1.764	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Ce}	ΔG_{Ce} [J/mol]	ΔH_{Ce} [J/mol]	ΔS_{Ce} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ce}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ce}}$ [J/(mol·K)]	a_{Ce}	γ_{Ce}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2250	433	1.490	−673	0.614	0.860	0.956
0.800	−6370	707	3.932	−3030	2.076	0.653	0.817
0.700	−12915	−712	6.779	−7577	3.814	0.422	0.603
0.600	−22464	−5361	9.501	−14819	5.254	0.223	0.372
0.500	−35636	−14775	11.589	−25262	5.826	0.092	0.185
0.400	−53126	−30490	12.575	−39412	4.957	0.029	0.072
0.300	−75795	−54042	12.085	−57776	2.075	0.006	0.021
0.200	−104946	−86966	9.989	−80859	−3.393	0.001	0.005
0.100	−143627	−130797	7.128	−109166	−12.017	0.000	0.001
0.000	$-\infty$	−187072	∞	−143205	−24.371	0.000	0.000

Reference state: Ce(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)]	$G^{\mathrm{E}}_{\mathrm{Ni}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ni}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
0.000	$-\infty$	−59100	∞	−101047	23.304	0.000	0.001
0.100	−123138	−68603	30.298	−88678	11.153	0.000	0.003
0.200	−99550	−70585	16.091	−75463	2.710	0.001	0.006
0.300	−79926	−66583	7.413	−61907	−2.598	0.005	0.016
0.400	−62232	−58132	2.278	−48518	−5.341	0.016	0.039
0.500	−46175	−46768	−0.330	−35801	−6.093	0.046	0.091
0.600	−31907	−34027	−1.178	−24262	−5.425	0.119	0.198
0.700	−19744	−21444	−0.944	−14406	−3.910	0.267	0.382
0.800	−10080	−10554	−0.264	−6740	−2.119	0.510	0.637
0.900	−3346	−2895	0.251	−1769	−0.625	0.800	0.888
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ni(liquid)

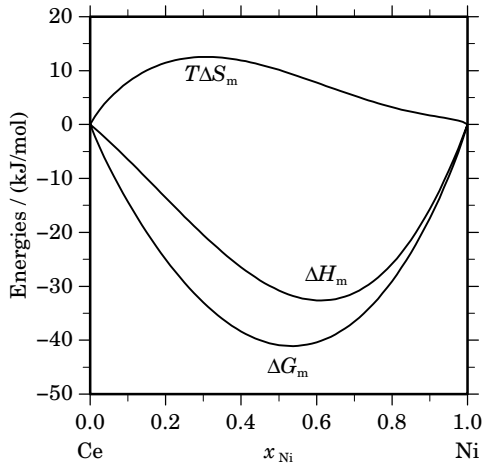

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

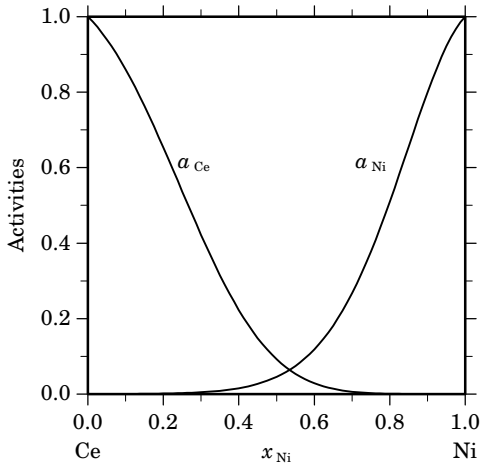

Fig. 3. Activities in the liquid phase at T=1800 K.

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))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
Ce_7Ni_3	0.300	−24116	−25508	−4.667	−0.229
Ce_1Ni_1	0.500	−31122	−30422	2.345	−0.382
Ce_1Ni_2	0.667	−30676	−29654	3.427	−0.510
Ce_1Ni_3	0.750	−29610	−28955	2.198	−0.573
Ce_2Ni_7	0.778	−29044	−28532	1.717	−0.595
Ce_1Ni_5	0.833	−27602	−27521	0.274	−0.637

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