Ni – Zr (Nickel – Zirconium)

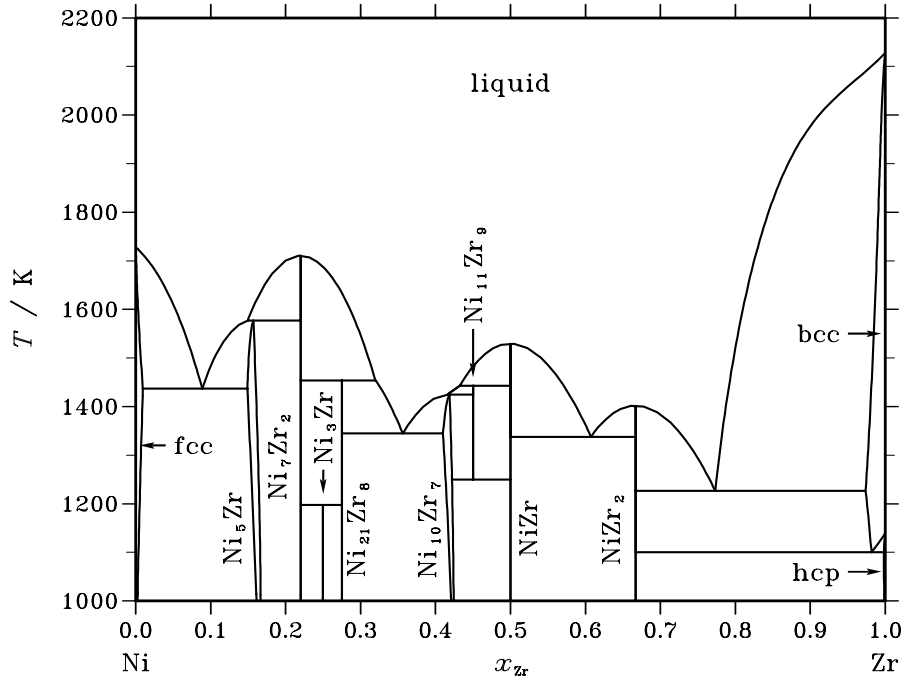

Fig. 1. Calculated phase diagram for the system Ni-Zr.

The diagram has many intermetallic phases most of which are formed peritectically. Some of the compounds have the solubility range modelled. Ni is added in small amounts to Zr-alloys as a hardening element. The assessment has been reported in [94Gho].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ni,Zr)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Ni,Zr)_1$
Ni_5Zr	$C15_b$	$AuBe_5$	$cF24$	$F\overline{4}3m$	C15B_NI5ZR	$(Ni,Zr)_5(Zr,\Box)_1$
Ni_7Zr_2	···	···	$mC36$	$C2/m$	NI7ZR2	$Ni_{39}Zr_{11}$
Ni_3Zr	$D0_{19}$	Ni_3Sn	$hP8$	$P6_3/mmc$	D019_NI3ZR	$(Ni,Zr)_3(Zr,\Box)_1$
$Ni_{21}Zr_8$	···	Hf_8Ni_{21}	$a*$*	···	NI21ZR8	$Ni_{29}Zr_{11}$
$Ni_{10}Zr_7$	···	···	$oC68$	$Pbca$	NI10ZR7	$(Ni,Zr)_{23}(Zr,\Box)_{17}$
$Ni_{11}Zr_9$	···	···	$tI40$	$I4/m$	NI11ZR9	$Ni_{11}Zr_9$
NiZr	$B33$	CrB	$oC8$	$Cmcm$	B33_NIZR	Ni_1Zr_1
$NiZr_2$	$C16$	Al_2Cu	$tI12$	$I4/mcm$	C16_NIZR2	Ni_1Zr_2
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Ni,Zr)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Ni,Zr)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ Ni_7Zr_2	congruent	1710.7	0.220	0.220		−17977
liquid + Ni_7Zr_2 $\rightleftharpoons$ Ni_5Zr	peritectic	1577.3	0.149	0.220	0.157	−13117
liquid $\rightleftharpoons$ NiZr	congruent	1529.6	0.500	0.500		−18972
Ni_7Zr_2 + liquid $\rightleftharpoons$ $Ni_{21}Zr_8$	peritectic	1453.8	0.220	0.320	0.275	−9020
liquid + NiZr $\rightleftharpoons$ $Ni_{11}Zr_9$	peritectic	1443.0	0.432	0.500	0.450	−10888
liquid $\rightleftharpoons$ fcc + Ni_5Zr	eutectic	1437.1	0.089	0.010	0.149	−12233
liquid + $Ni_{11}Zr_9$ $\rightleftharpoons$ $Ni_{10}Zr_7$	peritectic	1424.9	0.416	0.450	0.419	−14373
liquid $\rightleftharpoons$ $NiZr_2$	congruent	1402.4	0.667	0.667		−14573
liquid $\rightleftharpoons$ $Ni_{21}Zr_8$ + $Ni_{10}Zr_7$	eutectic	1344.5	0.356	0.275	0.410	−13752
liquid $\rightleftharpoons$ NiZr + $NiZr_2$	eutectic	1337.9	0.607	0.500	0.667	−14670
$Ni_{11}Zr_9$ $\rightleftharpoons$ $Ni_{10}Zr_7$ + NiZr	eutectoid	1250.1	0.450	0.422	0.500	−1019
liquid $\rightleftharpoons$ $NiZr_2$ + bcc	eutectic	1226.7	0.773	0.667	0.974	−9663
Ni_7Zr_2 + $Ni_{21}Zr_8$ $\rightleftharpoons$ Ni_3Zr	peritectoid	1197.7	0.220	0.275	0.250	−638
bcc $\rightleftharpoons$ $NiZr_2$ + hcp	eutectoid	1100.3	0.982	0.667	0.998	−4535

Table IIIa. Integral quantities for the liquid phase at 2200 K.

x_{Zr}	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	−22318	−23090	−0.351	−16371	−3.054	0.000
0.200	−38803	−38151	0.296	−29650	−3.864	0.000
0.300	−50180	−46843	1.517	−39007	−3.562	0.000
0.400	−56279	−50495	2.629	−43968	−2.967	0.000
0.500	−57099	−50113	3.176	−44420	−2.588	0.000
0.600	−52914	−46374	2.973	−40604	−2.623	0.000
0.700	−44292	−39631	2.119	−33118	−2.960	0.000
0.800	−32074	−29910	0.984	−22921	−3.177	0.000
0.900	−17271	−16908	0.165	−11324	−2.538	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ni in the liquid phase at 2200 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}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−3305	−4317	−0.460	−1378	−1.336	0.835	0.927
0.800	−10879	−14896	−1.826	−6798	−3.681	0.552	0.690
0.700	−23906	−28911	−2.275	−17382	−5.240	0.271	0.387
0.600	−42528	−44516	−0.904	−33184	−5.151	0.098	0.163
0.500	−65861	−60844	2.281	−53182	−3.483	0.027	0.055
0.400	−92047	−78007	6.382	−75287	−1.236	0.007	0.016
0.300	−118356	−97096	9.664	−96333	−0.347	0.002	0.005
0.200	−141527	−120182	9.702	−112087	−3.680	0.000	0.002
0.100	−159360	−150316	4.111	−117241	−15.034	0.000	0.002
0.000	−∞	−191525	∞	−105417	−39.140	0.000	0.003

Reference state: Ni(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 2200 K.

x_{Zr}	ΔG_{Zr} [J/mol]	ΔH_{Zr} [J/mol]	ΔS_{Zr} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Zr}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Zr}}$ [J/(mol·K)]	a_{Zr}	γ_{Zr}
0.000	−∞	−277375	∞	−175515	−46.300	0.000	0.000
0.100	−193427	−192039	0.631	−151309	−18.514	0.000	0.000
0.200	−150499	−131171	8.785	−121060	−4.596	0.000	0.001
0.300	−111487	−88683	10.365	−89464	0.355	0.002	0.008
0.400	−76906	−59463	7.929	−60145	0.310	0.015	0.037
0.500	−48337	−39381	4.071	−35658	−1.692	0.071	0.142
0.600	−26826	−25286	0.700	−17482	−3.547	0.231	0.385
0.700	−12551	−15003	−1.115	−6026	−4.081	0.504	0.719
0.800	−4711	−7341	−1.196	−629	−3.051	0.773	0.966
0.900	−1483	−2085	−0.274	444	−1.150	0.922	1.025
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

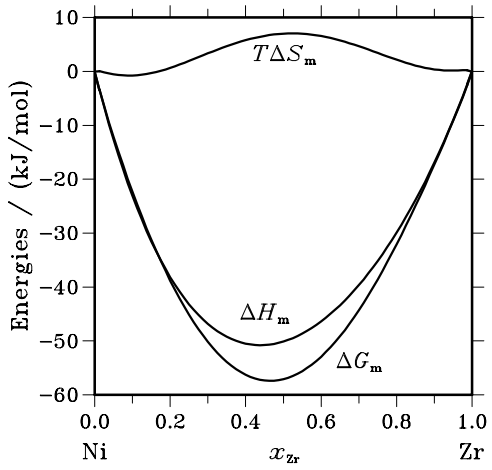

Fig. 2. Integral quantities of the liquid phase at T=2200 K.

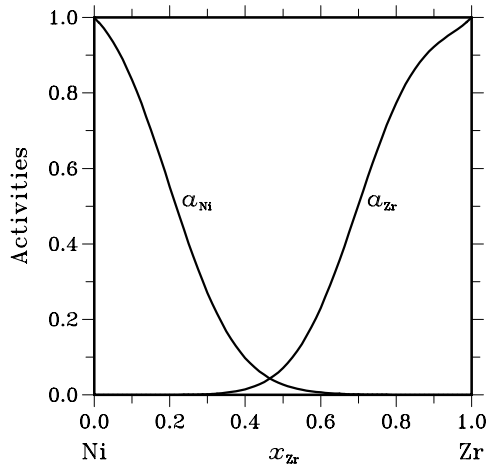

Fig. 3. Activities in the liquid phase at T=2200 K.

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

Compound	x_{Zr}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
Ni_5Zr	0.167	−31363	−30452	3.054	−0.756
Ni_7Zr_2	0.220	−38910	−37732	3.951	−0.753
Ni_3Zr	0.250	−41339	−40313	3.440	−0.752
$Ni_{21}Zr_8$	0.275	−42476	−41281	4.006	−0.751
$Ni_{10}Zr_7$	0.425	−47882	−46360	5.104	−0.743
$Ni_{11}Zr_9$	0.450	−47402	−45599	6.050	−0.742
NiZr	0.500	−49177	−47700	4.953	−0.739
$NiZr_2$	0.667	−37004	−35161	6.180	−0.731

References

[94Gho] G. Ghosh: J. Mater. Res. **9** (1994) 598–616.