Fe – Zr (Iron – Zirconium)

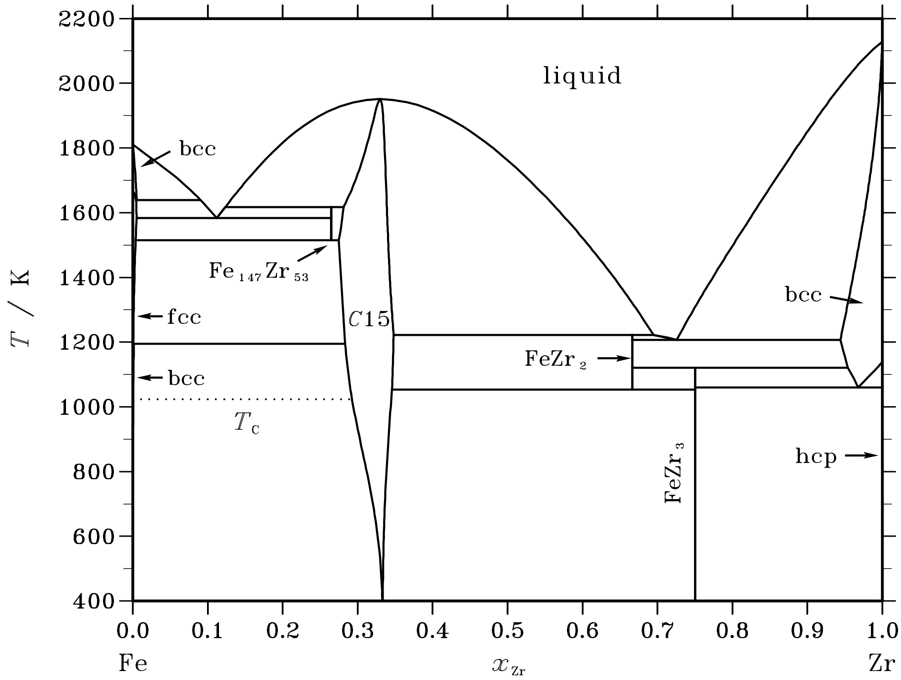

Fig. 1. Calculated phase diagram for the system Fe-Zr.

The Fe-Zr system has been assessed by Chevalier and Fischer [03Che]. The phase diagram of the Fe-Zr system presents a complete solubility of the elements in the liquid state, but a limited solid solubility of zirconium in the iron rich solid solutions (bcc, fcc), and of iron in zirconium rich solid solutions (bcc, hcp). According to Stein *et al.* [02Ste], the true equilibrium intermetallic phases are the hexagonal $C36$ ($x_{\rm Zr}$ = 0.265 - 0.27) and the cubic $C15$ ($x_{\rm Zr}$ = 0.275 - 0.344) polymorphs of the Laves phase Fe_2Zr, tetragonal $FeZr_2$ ($x_{\rm Zr}$ = 0.667 - 0.672) and orthorhombic $FeZr_3$ ($x_{\rm Zr}$ = 0.748 - 0.754). The previously identified compounds Fe_4Zr, Fe_3Zr or $Fe_{23}Zr_6$ were either non-equilibrium or ternary stabilised phases.

The solubility of iron in hcp zirconium has been determined by Stupel *et al.* [85Stu], Borrelly *et al.* [90Bor] and Zou *et al.* [94Zou]. The iron-rich part of the diagram has been precised by Granovsky and Arias [96Gra]. The temperatures of invariant reactions and liquidus of two alloys were determined. The invariant reactions both in the iron and zirconium rich domains were clarified by Stein *et al.* [02Ste].

The overall agreement with the most recent experimental work [02Ste] is about 5 K for the invariant reactions. The temperature independent calculated enthalpy of mixing of the liquid phase is in satisfactory agreement with the experimental results of [87Sud], [90Wan] and [95Ros]. The calculated activities of elements agree with the experimental results of [71Pei] at 2500 K.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Zr)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Zr)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Zr)_1$
$Fe_{147}Zr_{53}$	$C36$	$MgNi_2$	$hP24$	$P6_3/mmc$	FE147ZR53	$Fe_{147}Zr_{53}$
$C15$	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	LAVES_C15	$(Fe,Zr)_2(Fe,Zr)_1$
$FeZr_2$	$C16$	Al_2Cu	$tI12$	$I4/mcm$	FEZR2_C16	$(Fe,Zr)_1(Fe,Zr)_2$
$FeZr_3$	$E1_a$	BRe_3	$oC16$	$Cmcm$	FEZR3_E1A	$(Fe,Zr)_1(Fe,Zr)_3$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Fe,Zr)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_r H$ / (J/mol)
liquid ⇌ $C15$	congruent	1950.9	0.330	0.330		−24190
bcc ⇌ fcc + liquid	metatectic	1639.3	0.005	0.004	0.090	−530
liquid + $C15$ ⇌ $Fe_{147}Zr_{53}$	peritectic	1617.4	0.124	0.281	0.265	−1107
liquid ⇌ fcc + $Fe_{147}Zr_{53}$	eutectic	1583.1	0.112	0.005	0.265	−14273
$Fe_{147}Zr_{53}$ ⇌ fcc + $C15$	eutectoid	1514.4	0.265	0.004	0.275	−363
$C15$ + liquid ⇌ $FeZr_2$	peritectic	1222.2	0.348	0.695	0.667	−11700
liquid ⇌ $FeZr_2$ + bcc	eutectic	1206.5	0.725	0.667	0.944	−11609
fcc + $C15$ ⇌ bcc	peritectoid	1194.5	0.001	0.283	0.001	−894
$FeZr_2$ + bcc ⇌ $FeZr_3$	peritectoid	1121.4	0.667	0.954	0.750	−7719
bcc ⇌ $FeZr_3$ + hcp	eutectoid	1059.9	0.968	0.750	1.000	−5756
$FeZr_2$ ⇌ $C15$ + $FeZr_3$	eutectoid	1052.8	0.667	0.346	0.750	−4872

Table IIIa. Integral quantities for the liquid phase at 2173 K.

x_{Zr}	ΔG_m [J/mol]	ΔH_m [J/mol]	ΔS_m [J/(mol·K)]	G^E_m [J/mol]	S^E_m [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−9315	−8298	0.468	−3441	−2.235	0.000
0.200	−15673	−15006	0.307	−6632	−3.854	0.000
0.300	−19890	−19504	0.178	−8853	−4.901	0.000
0.400	−22069	−21692	0.173	−9909	−5.422	0.000
0.500	−22467	−21812	0.301	−9944	−5.462	0.000
0.600	−21412	−20257	0.532	−9252	−5.064	0.000
0.700	−19131	−17382	0.805	−8094	−4.274	0.000
0.800	−15551	−13327	1.023	−6510	−3.137	0.000
0.900	−10005	−7820	1.005	−4132	−1.698	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Fe in the liquid phase at 2173 K.

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	G^E_{Fe} [J/mol]	S^E_{Fe} [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1856	−638	0.561	47	−0.316	0.902	1.003
0.800	−5112	−3693	0.653	−1081	−1.202	0.754	0.942
0.700	−10387	−9529	0.395	−3943	−2.571	0.563	0.804
0.600	−17127	−17310	−0.084	−7898	−4.332	0.388	0.646
0.500	−24372	−25745	−0.632	−11849	−6.395	0.260	0.519
0.400	−31544	−33831	−1.053	−14989	−8.671	0.174	0.436
0.300	−39298	−41602	−1.060	−17545	−11.071	0.114	0.379
0.200	−50602	−50869	−0.123	−21524	−13.505	0.061	0.304
0.100	−73058	−65969	3.262	−31457	−15.882	0.018	0.175
0.000	$-\infty$	−94506	∞	−55142	−18.115	0.000	0.047

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 2173 K.

x_{Zr}	ΔG_{Zr} [J/mol]	ΔH_{Zr} [J/mol]	ΔS_{Zr} [J/(mol·K)]	G^E_{Zr} [J/mol]	S^E_{Zr} [J/(mol·K)]	a_{Zr}	γ_{Zr}
0.000	$-\infty$	−87171	∞	−31587	−25.579	0.000	0.174
0.100	−76442	−77236	−0.365	−34840	−19.510	0.015	0.145
0.200	−57916	−60259	−1.078	−28837	−14.460	0.041	0.203
0.300	−42062	−42777	−0.329	−20310	−10.339	0.097	0.325
0.400	−29481	−28265	0.560	−12926	−7.059	0.196	0.489
0.500	−20562	−17880	1.234	−8039	−4.529	0.320	0.641
0.600	−14657	−11207	1.588	−5428	−2.660	0.444	0.741
0.700	−10488	−7003	1.604	−4044	−1.362	0.560	0.799
0.800	−6788	−3941	1.310	−2756	−0.545	0.687	0.859
0.900	−2999	−1360	0.755	−1096	−0.121	0.847	0.941
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

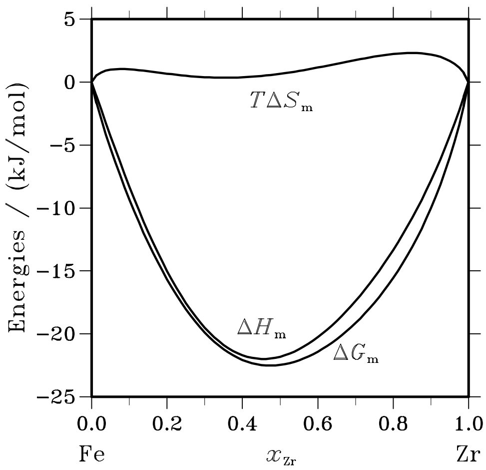

Fig. 2. Integral quantities of the liquid phase at T=2173 K.

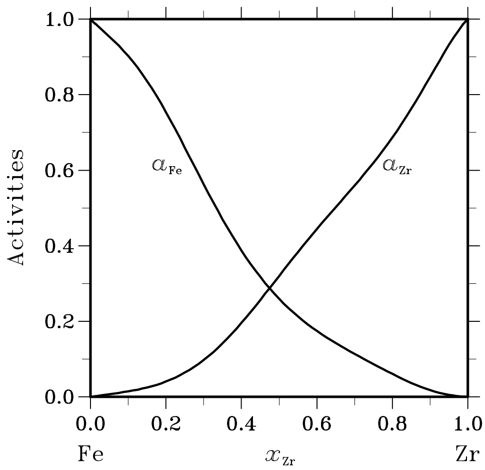

Fig. 3. Activities in the liquid phase at T=2173 K.

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))
$Fe_{147}Zr_{53}$	0.265	−17762	−16475	4.316	−0.307
$C15$	0.333	−24215	−23593	2.085	−0.368
Fe_1Zr_2	0.667	−12644	−12137	1.699	−0.147
Fe_1Zr_3	0.750	−14161	−15438	−4.285	−0.112

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