Fe – Zn (Iron – Zinc)

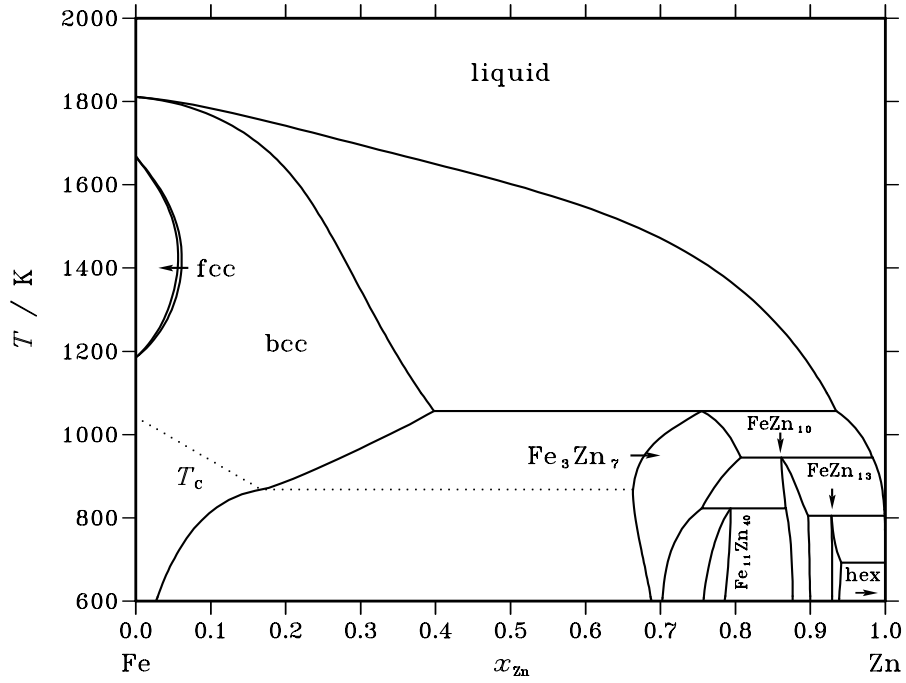

Fig. 1. Calculated phase diagram for the system Fe-Zn.

The Fe-Zn system was critically assessed by G. Reumont *et al.* [00Reu]. The solubility of Zn in bcc-Fe reaches up to about 42 at.% Zn at the peritectic temperature [64Spe, 79Ko, 79Nis, 81Tom, 82Kub], while the solubility of Fe in hcp-Zn is very limited (∼0.001 at.% Fe). The maximum solubility of Zn in fcc-Fe is reported as 5.68 at.% Zn at ∼1423 K and a characteristic "gamma-loop" is formed [73Kir]. The Fe-Zn system contains four intermetallic phases Fe_3Zn_7, $Fe_{11}Zn_{40}$, $FeZn_{10}$ and $FeZn_{13}$, which are complex variants of the bcc-Fe phase with very similar chemical stabilities. These compounds are nonstoichiometric phases which are modelled with two sublattices containing Fe as well as Zn. Fe_3Zn_7 is stable below its peritectic temperature. It has a maximum range of 69 to 83 at.% Zn at 945 K [74Bas, 80Gel, 81Tom]. The $FeZn_{10}$ and $FeZn_{13}$ phases decompose peritectically at 945 and 803 K respectively and the phase $Fe_{11}Zn_{40}$ is formed peritectoidly at 823 K. The experimentally determined zinc activities by [81Tom] in the bcc-phase are reproduced well by the assessed data [00Reu]. The calculated phase diagram and thermodynamic properties are in good agreement with available experimental data.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Zn)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Zn)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Zn)_1$
Fe_3Zn_7	$D8_2$	Cu_5Zn_8	$cI52$	$I\overline{4}3m$	D82_FEZN	$(Fe,Zn)_3(Fe,Zn)_7$
$Fe_{11}Zn_{40}$	···	$Fe_{11}Zn_{40}$	$cF408$	$F\overline{4}3m$	FE11ZN40	$(Fe,Zn)_1(Fe,Zn)_3$
$FeZn_{10}$	···	$FeZn_{10}$	$hP555$	$P6_3mc$	FEZN_DELTA	$(Fe,Zn)_1(Fe,Zn)_7$
$FeZn_{13}$	···	$CoZn_{13}$	$mC28$	$C2/m$	FEZN_ZETA	$(Fe,Zn)_1(Fe,Zn)_{13}$
hex	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_ZN	Zn_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zn}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc + liquid $\rightleftharpoons$ Fe_3Zn_7	peritectic	1056.7	0.398	0.934	0.755	−11618
Fe_3Zn_7 + liquid $\rightleftharpoons$ $FeZn_{10}$	peritectic	944.5	0.807	0.983	0.861	−4227
Fe_3Zn_7 + $FeZn_{10}$ $\rightleftharpoons$ $Fe_{11}Zn_{40}$	peritectoid	822.5	0.755	0.867	0.794	−1637
$FeZn_{10}$ + liquid $\rightleftharpoons$ $FeZn_{13}$	peritectic	805.2	0.897	0.999	0.928	−2101
liquid $\rightleftharpoons$ $FeZn_{13}$ + hex	eutectic	692.7	1.000	0.941	1.000	−7323

Table IIIa. Integral quantities for the stable phases at 1066 K.

Phase	x_{Zn}	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)]
bcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−1746	789	2.378	1136	−0.325	−7.193
	0.200	−2310	847	2.961	2126	−1.199	−9.214
	0.300	−2430	521	2.768	2985	−2.311	−9.432
	0.394	−2272	9	2.139	3672	−3.436	−8.814
liquid	0.932	−751	2064	2.641	1453	0.573	−1.049
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(bcc), Zn(liquid)

Table IIIb. Partial quantities for Fe in the stable phases at 1066 K.

Phase	x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Fe}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Fe}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−856	454	1.229	78	0.353	0.908	1.009
	0.800	−1700	1185	2.707	278	0.851	0.825	1.032
	0.700	−2558	1893	4.175	604	1.209	0.749	1.070
	0.606	−3386	2441	5.467	1055	1.300	0.682	1.126
liquid	0.068	−3386	29601	30.945	20426	8.607	0.682	10.020
	0.000	$-\infty$	31041	∞	22303	8.197	0.000	12.383

Reference state: Fe(bcc)

Table IIIc. Partial quantities for Zn in the stable phases at 1066 K.

Phase	x_{Zn}	ΔG_{Zn} [J/mol]	ΔH_{Zn} [J/mol]	ΔS_{Zn} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Zn}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Zn}}$ [J/(mol·K)]	a_{Zn}	γ_{Zn}
bcc	0.000	$-\infty$	14036	∞	12227	1.697	0.000	3.973
	0.100	−9751	3807	12.718	10657	−6.427	0.333	3.328
	0.200	−4748	−506	3.980	9517	−9.402	0.585	2.926
	0.300	−2131	−2680	−0.515	8540	−10.525	0.786	2.621
	0.394	−559	−3731	−2.976	7693	−10.716	0.939	2.382
liquid	0.932	−559	52	0.572	67	−0.014	0.939	1.008
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zn(liquid)

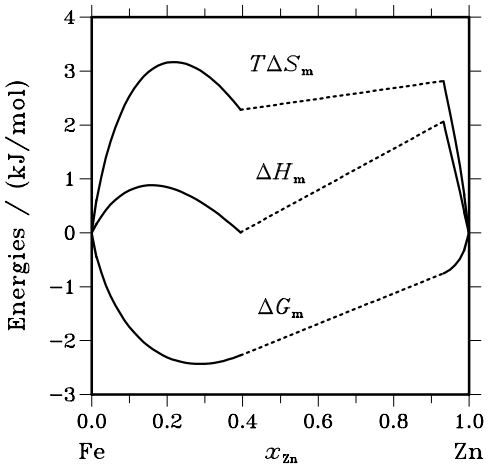

Fig. 2. Integral quantities of the stable phases at T=1066 K.

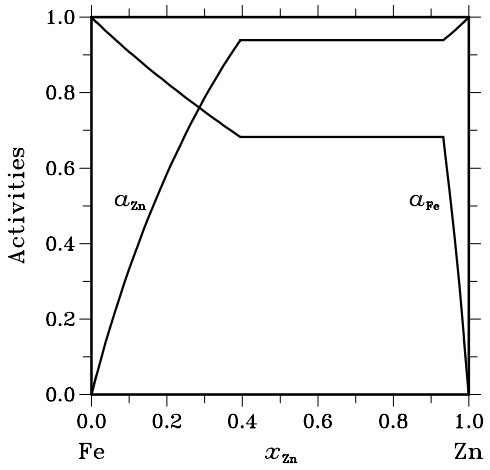

Fig. 3. Activities in the stable phases at T=1066 K.

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

Compound	x_{Zn}	$\Delta_{\mathrm{f}}G^\circ$ / (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_3Zn_7	0.700	−5717	−6602	−2.970	−0.124
$Fe_{11}Zn_{40}$	0.760	−5544	−6318	−2.595	−0.100
$FeZn_{10}$	0.900	−3110	−3041	0.233	−0.042
$FeZn_{13}$	0.929	−2268	−2052	0.724	−0.030

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