Sn – Zr (Tin – Zirconium)

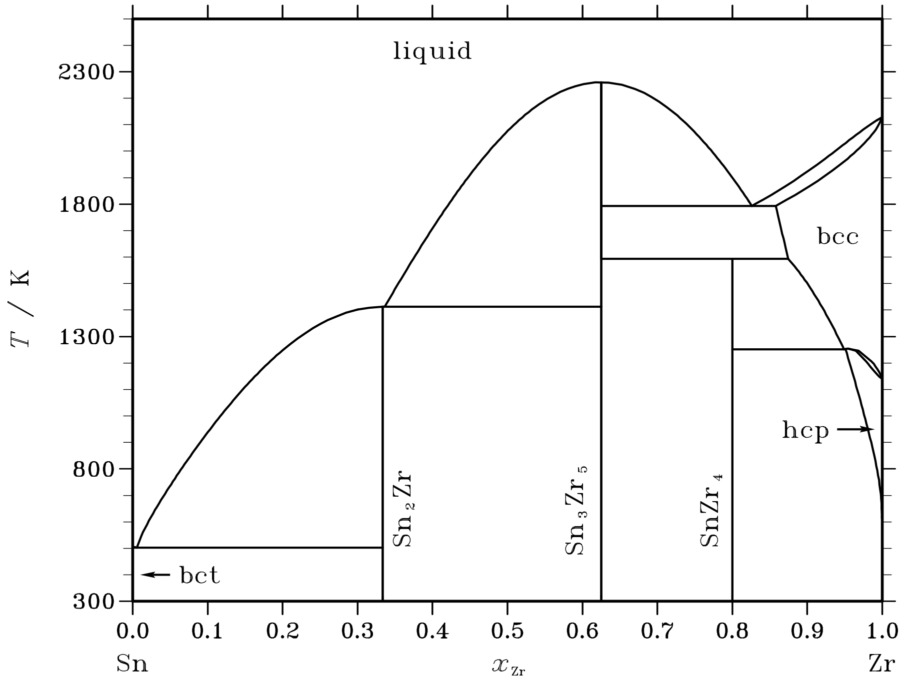

Fig. 1. Calculated phase diagram for the system Sn-Zr.

The Sn-Zr system is of great importance in nuclear industry as Sn is the major alloying element in Zr alloys used for cladding. Sn increases the strength of Zr alloys and stabilises the hexagonal phase and does not cause problems in the high-neutron densities in the nuclear reactor. The Sn_3Zr_5 phase is modelled as a stoichiometric compound although it certainly has considerable solubility but the experimental data on the defect structure makes it difficult to do anything better. An assessment of the Sn-Zr system has been reported in [98Sub].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Sn,Zr)_1$
bct	$A5$	βSn	$tI4$	$I4_1/amd$	BCT_A5	Sn_1
Sn_2Zr	$C54$	$TiSi_2$	$oF24$	$Fddd$	C54_SN2ZR	Sn_2Zr_1
Sn_3Zr_5	$D8_8$	Mn_5Si_3	$hP16$	$P6_3/mcm$	D88_SN3ZR5	Sn_3Zr_5
$SnZr_4$	$A15$	Cr_3Si	$cP8$	$Pm\overline{3}n$	A15_SNZR4	Sn_1Zr_4
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Sn,Zr)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Sn,Zr)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_r H$ / (J/mol)
liquid ⇌ Sn_3Zr_5	congruent	2260.2	0.625	0.625		−58746
liquid ⇌ Sn_3Zr_5 + bcc	eutectic	1792.7	0.826	0.625	0.858	−26574
Sn_3Zr_5 + bcc ⇌ $SnZr_4$	peritectoid	1593.1	0.625	0.875	0.800	−17597
liquid ⇌ Sn_2Zr	congruent	1412.0	0.333	0.333		−39926
liquid ⇌ Sn_2Zr + Sn_3Zr_5	eutectic	1411.9	0.336	0.333	0.625	−39969
bcc ⇌ hcp	congruent	1254.9	0.956	0.956		−2692
bcc ⇌ $SnZr_4$ + hcp	eutectoid	1252.1	0.949	0.800	0.951	−2940
liquid ⇌ bct + Sn_2Zr	eutectic	503.0	0.006	0.000	0.333	−7265

Table IIIa. Integral quantities for the liquid phase at 2300 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	−31717	−15487	7.057	−25501	4.354	0.000
0.200	−54904	−27532	11.901	−45334	7.740	0.000
0.300	−71183	−36135	15.238	−59501	10.159	0.000
0.400	−80872	−41298	17.206	−68002	11.611	0.000
0.500	−84090	−43018	17.857	−70835	12.094	0.000
0.600	−80872	−41298	17.206	−68002	11.611	0.000
0.700	−71183	−36135	15.238	−59501	10.159	0.000
0.800	−54904	−27532	11.901	−45334	7.740	0.000
0.900	−31717	−15487	7.057	−25501	4.354	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Sn in the liquid phase at 2300 K.

x_{Sn}	ΔG_{Sn} [J/mol]	ΔH_{Sn} [J/mol]	ΔS_{Sn} [J/(mol·K)]	G^E_{Sn} [J/mol]	S^E_{Sn} [J/(mol·K)]	a_{Sn}	γ_{Sn}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−4848	−1721	1.360	−2833	0.484	0.776	0.862
0.800	−15601	−6883	3.790	−11334	1.935	0.442	0.553
0.700	−32321	−15487	7.320	−25501	4.354	0.184	0.264
0.600	−55103	−27532	11.988	−45334	7.740	0.056	0.093
0.500	−84090	−43018	17.857	−70835	12.094	0.012	0.025
0.400	−119525	−61946	25.034	−102002	17.416	0.002	0.005
0.300	−161861	−84316	33.715	−138837	23.705	0.000	0.001
0.200	−212116	−110127	44.343	−181338	30.961	0.000	0.000
0.100	−273539	−139379	58.330	−229505	39.185	0.000	0.000
0.000	$-\infty$	−172073	∞	−283340	48.377	0.000	0.000

Reference state: Sn(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 2300 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	$-\infty$	−172073	∞	−283340	48.377	0.000	0.000
0.100	−273539	−139379	58.330	−229505	39.185	0.000	0.000
0.200	−212116	−110127	44.343	−181338	30.961	0.000	0.000
0.300	−161861	−84316	33.715	−138837	23.705	0.000	0.001
0.400	−119525	−61946	25.034	−102002	17.416	0.002	0.005
0.500	−84090	−43018	17.857	−70835	12.094	0.012	0.025
0.600	−55103	−27532	11.988	−45334	7.740	0.056	0.093
0.700	−32321	−15487	7.320	−25501	4.354	0.184	0.264
0.800	−15601	−6883	3.790	−11334	1.935	0.442	0.553
0.900	−4848	−1721	1.360	−2833	0.484	0.776	0.862
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

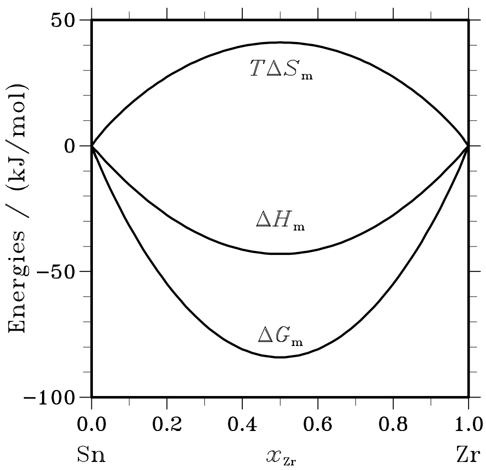

Fig. 2. Integral quantities of the liquid phase at T=2300 K.

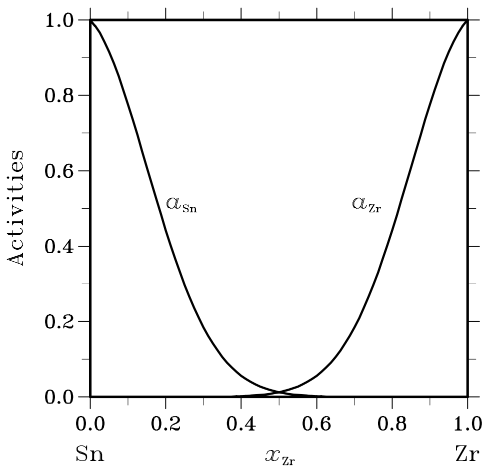

Fig. 3. Activities in the liquid phase at T=2300 K.

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))
Sn_2Zr_1	0.333	−67471	−67471	0.000	0.000
Sn_3Zr_5	0.625	−85762	−85279	1.619	0.000
Sn_1Zr_4	0.800	−57642	−59382	−5.835	0.000

References

[98Sub] N. Subasic: Calphad **22** (1998) 157–165.