Ir – Zr (Iridium – Zirconium)

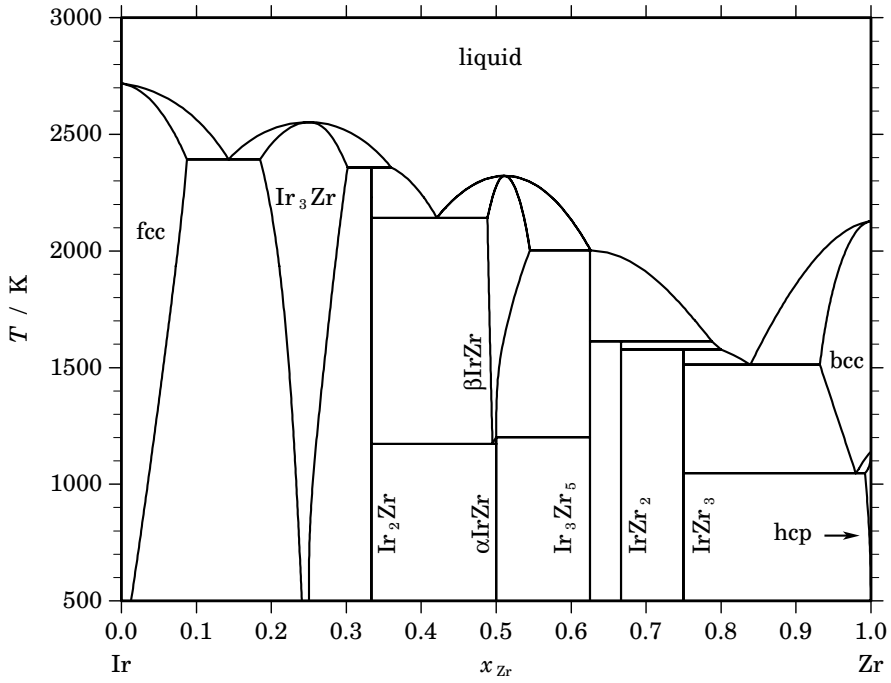

Fig. 1. Calculated phase diagram for the system Ir-Zr.

This system was assessed by Ran and Du [2006Ran], from the available experimental information on the phase diagram and thermodynamics. Iridium alloys are new materials with higher melting temperatures and superior oxidation resistance than Ni-based superalloys. The phase diagram was experimentally determined by Kuprina and Kuryachava [1974Kup], Eremenko *et al.* [1974Ere, 1978Ere1, 1978Ere2, 1980Ere]. The experimental phase diagram was assessed by Okamoto [1992Oka]. It presents four solution phases, the liquid with a complete miscibility range, the iridium based fcc phase and the zirconium rich terminal solution phases, bcc and hcp. There are three non-stoichiometric intermetallic compounds, Ir_3Zr, αIrZr and βIrZr, and four stoichiometric compounds, Ir_2Zr, Ir_3Zr_5, $IrZr_2$ and $IrZr_3$. The Ir_3Zr homogeneity range is equal to 19-30 at.% Zr at 2393 K [1980Ere]. βIrZr extends from 47 to 52 at.% Zr at 2143 K and from 49 to 50 at.% Zr below 1500 K. The crystal structures of the compounds were reported by Dwight and Beck [1959Dwi, 1961Dwi], Raman and Schubert [1964Ram], Schubert *et al.* [1964Sch], Biswas and Schubert [1967Bis], McCarthy [1971McC], Eremenko *et al.* [1978Ere2, 1980Ere], Matthias *et al.* [1961Mat], Cenzul and Parthe [1985Cen]. The enthalpy of formation of IrZr has been measured by Topor and Kleppa [1989Top].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ir,Zr)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Ir,Zr)_1$
Ir_3Zr	$L1_2$	$AuCu_3$	$cP4$	$Pm\overline{3}m$	IR3ZR	$(Ir,Zr)_3(Ir,Zr)_1$
Ir_2Zr	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	IR2ZR	Ir_2Zr_1
αIrZr	$\cdots$	$\cdots$	$\cdots$	$\cdots$	IRZR	$(Ir,Zr)_1Zr_1$
βIrZr	$B2$	CsCl	$cP2$	$Pm\overline{3}m$	IRZR_B2	$(Ir,Zr)_1(Ir,Zr)_1$
Ir_3Zr_5	$D8_8$	Mn_5Si_3	$hP16$	$P6_3/mcm$	IR3ZR5	Ir_3Zr_5
$IrZr_2$	$C16$	Al_2Cu	$tI12$	$I4/mcm$	IRZR2	Ir_1Zr_2
$IrZr_3$	$\cdots$	αV_3S	$tI32$	$I\overline{4}2m$	IRZR3	Ir_1Zr_3
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Ir,Zr)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Ir,Zr)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ Ir_3Zr	congruent	2553.0	0.250	0.250		−36496
liquid $\rightleftharpoons$ fcc + Ir_3Zr	eutectic	2393.0	0.143	0.088	0.185	−22262
Ir_3Zr + liquid $\rightleftharpoons$ Ir_2Zr	peritectic	2358.4	0.302	0.360	0.333	−19625
liquid $\rightleftharpoons$ βIrZr	congruent	2323.0	0.511	0.511		−33162
liquid $\rightleftharpoons$ Ir_2Zr + βIrZr	eutectic	2142.6	0.421	0.333	0.488	−29582
βIrZr + liquid $\rightleftharpoons$ Ir_3Zr_5	peritectic	2003.1	0.545	0.626	0.625	−51090
Ir_3Zr_5 + liquid $\rightleftharpoons$ $IrZr_2$	peritectic	1613.0	0.625	0.788	0.667	−14992
$IrZr_2$ + liquid $\rightleftharpoons$ $IrZr_3$	peritectic	1578.2	0.667	0.800	0.750	−26785
liquid $\rightleftharpoons$ $IrZr_3$ + bcc	eutectic	1512.6	0.839	0.750	0.932	−30410
βIrZr $\rightleftharpoons$ αIrZr	congruent	1201.4	0.500	0.500		−2723
βIrZr $\rightleftharpoons$ αIrZr + Ir_3Zr_5	eutectoid	1201.4	0.500	0.500	0.625	−2723
βIrZr $\rightleftharpoons$ Ir_2Zr + αIrZr	eutectoid	1173.0	0.495	0.333	0.500	−2758
bcc $\rightleftharpoons$ $IrZr_3$ + hcp	eutectoid	1047.7	0.980	0.750	0.992	−7136

Table IIIa. Integral quantities for the liquid phase at 2800 K.

x_{Zr}	ΔG_m [J/mol]	ΔH_m [J/mol]	ΔS_m [J/(mol·K)]	G_m^E [J/mol]	S_m^E [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−40194	−40246	−0.019	−32625	−2.722	0.000
0.200	−71963	−66275	2.031	−60313	−2.129	0.000
0.300	−96417	−80063	5.841	−82196	0.762	0.000
0.400	−113075	−83589	10.531	−97407	4.935	0.000
0.500	−121215	−78831	15.137	−105078	9.374	0.000
0.600	−120012	−67766	18.659	−104344	13.063	0.000
0.700	−108557	−52373	20.066	−94336	14.987	0.000
0.800	−85837	−34629	18.288	−74187	14.128	0.000
0.900	−50599	−16512	12.174	−43031	9.471	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ir in the liquid phase at 2800 K.

x_{Ir}	ΔG_{Ir} [J/mol]	ΔH_{Ir} [J/mol]	ΔS_{Ir} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ir}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ir}}$ [J/(mol·K)]	a_{Ir}	γ_{Ir}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−4777	−7439	−0.950	−2324	−1.827	0.814	0.905
0.800	−15648	−27117	−4.096	−10454	−5.951	0.511	0.638
0.700	−34425	−55080	−7.377	−26122	−10.342	0.228	0.326
0.600	−62956	−87372	−8.720	−51064	−12.967	0.067	0.112
0.500	−103150	−120036	−6.031	−87013	−11.794	0.012	0.024
0.400	−157036	−149118	2.828	−135704	−4.791	0.001	0.003
0.300	−226901	−170661	20.086	−198872	10.075	0.000	0.000
0.200	−315718	−180710	48.217	−278249	34.836	0.000	0.000
0.100	−429178	−175309	90.667	−375572	71.522	0.000	0.000
0.000	$-\infty$	−150503	∞	−492574	122.168	0.000	0.000

Reference state: Ir(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 2800 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	$-\infty$	−480143	∞	−348051	−47.176	0.000	0.000
0.100	−358940	−335514	8.366	−305334	−10.779	0.000	0.000
0.200	−297219	−222904	26.541	−259751	13.160	0.000	0.000
0.300	−241064	−138356	36.681	−213035	26.671	0.000	0.000
0.400	−188253	−77915	39.406	−166921	31.788	0.000	0.001
0.500	−139280	−37626	36.305	−123143	30.542	0.003	0.005
0.600	−95329	−13532	29.213	−83437	24.966	0.017	0.028
0.700	−57838	−1678	20.057	−49535	17.091	0.083	0.119
0.800	−28366	1891	10.806	−23172	8.951	0.296	0.370
0.900	−8535	1132	3.452	−6082	2.576	0.693	0.770
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

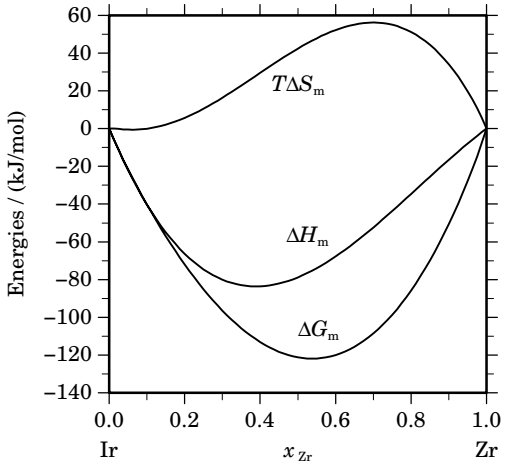

Fig. 2. Integral quantities of the liquid phase at T=2800 K.

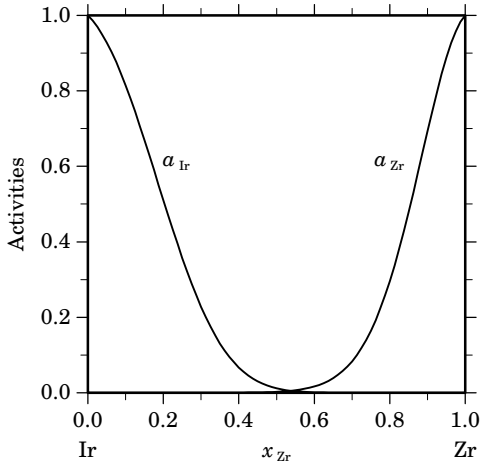

Fig. 3. Activities in the liquid phase at T=2800 K.

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))
Ir_3Zr	0.250	−81038	−80773	0.892	0.000
Ir_2Zr_1	0.333	−87313	−85827	4.982	0.000
αIrZr	0.500	−92448	−89893	8.568	0.000
βIrZr	0.500	−90393	−87162	10.837	−0.231
Ir_3Zr_5	0.625	−93849	−92893	3.207	0.000
Ir_1Zr_2	0.667	−88518	−88473	0.150	0.000
Ir_1Zr_3	0.750	−69264	−69236	0.095	0.000

References

[1959Dwi] A.E. Dwight, P.A. Beck: Trans. Metall. Soc. AIME **215** (1959) 976–979.

[1961Dwi] A.E. Dwight: Trans. ASM **53** (1961) 479–500.

[1961Mat] B.T. Matthias, V.B. Compton, E. Corenzwit: J. Phys. Chem. Solids **19** (1961) 130–133.

[1964Ram] A. Raman, K. Schubert: Z. Metallkd. **55** (1964) 704–710.

[1964Sch] K. Schubert, A. Raman, W. Rosseteutscher: Naturwiss. **51** (1964) 506–507.

[1967Bis] T.K. Biswas, K. Schubert: Z. Metallkd. **58** (1967) 558–559.

[1971McC] S.L. McCarthy: J. Low Temp. Phys. **4** (1971) 489–501.

[1974Kup] V.V. Kuprina, G.I. Kuryachaya: Vestn. MGU, Ser. 2, Khim. **15** (1974) 371–373 ;transl.: Moscow Univ. Chem. Bull. **29** (1974) 88.

[1974Ere] V.N. Eremenko, T.D. Shtepa, E.L. Semenova in: R. Rykhal, M. L'vov (Eds.), "Tezisy Dokl. Vses. Konf. Kristallokhim. Intermet. Soedin.", 2nd ed., Inst. Probl. Materialoved, Kiev, 1974, 28.

[1978Ere1] V.N. Eremenko, E.L. Semenova, T.D. Shtepa: Izv. Akad. Nauk SSSR, Met. 2 (1978) 200–203; transl.: Russ. Metall. 2 (1978) 158.

[1978Ere2] V.N. Eremenko, E.L. Semenova, T.D. Shtepa, Yu.V. Kudryavtsev: Dop. Akad. Nauk. Ukr. RSR, Ser. A, Fiz.-Mat. Tekn., No. 10 (1978) 943–945.

[1980Ere] V.N. Eremenko, E.L. Semenova, T.D. Shtepa: Izv. Akad. Nauk SSSR, Met. 5 (1980) 237–241; transl.: Russ. Metall. 5 (1978) 210.

[1985Cen] K. Cenzual, O.J. Parthe: Acta Cryst. C **41C** (1985) 820–823.

[1989Top] L. Topor, O.J. Kleppa: J. Less-Common Met. **155** (1988) 61–73.

[1992Oka] H. Okamoto: J. Phase Equilibria **13** (1992) 653–656.

[2006Ran] H. Ran, Z. Du: J. Alloys Comp. **413** (2006) 101–105.