Mo – Zr (Molybdenum – Zirconium)

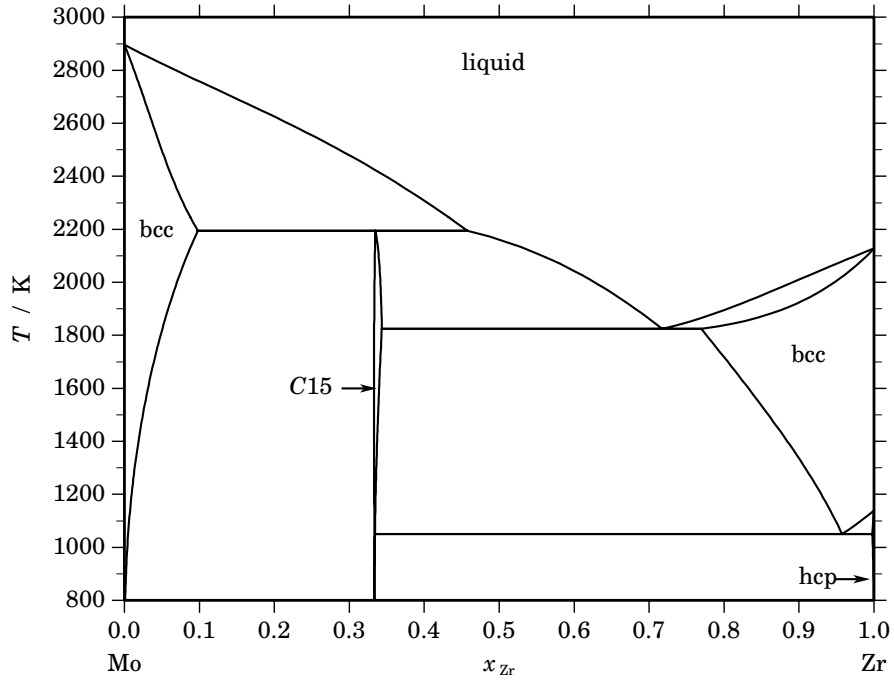

Fig. 1. Calculated phase diagram for the system Mo-Zr.

Mo is added in certain amounts to zirconium based alloys for the nuclear power industry in order to enhance their mechanical properties. Similarly, zirconium belongs to the group of alloying elements for Mo-based metals in order to further increase their strength and creep resistance at high temperatures. The literature on the Mo-Zr system has been reviewed in [1976Kub, 2002Zin, 2003Jer] and thermodynamic assessments have been reported in [2002Zin, 2003Jer]. The phase equilibria in the Mo-Zr system have been studied in several investigations but no measurements of thermodynamic data have been reported. The assessment of [2003Jer] is preferred here because in the dataset of [2002Zin] the liquid and the bcc phases are modelled with quite high excess entropies which seem to be unrealistic. This causes the slopes of the boundaries for the single-phase bcc regions to be too steep and in the liquid an artificial inverse miscibility gap opens above 4660 K. Although this is in some distance above the liquidus it indicates a certain weakness in the optimisation.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mo,Zr)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Mo,Zr)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mo,Zr)_1$
$C15$	$C15$	$MgCu_2$	$cF24$	$Fd\overline{3}m$	LAVES_C15	$(Mo,Zr)_2(Mo,Zr)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc + liquid $\rightleftharpoons C15$	peritectic	2194.2	0.098	0.457	0.335	−22868
liquid $\rightleftharpoons C15$ + bcc	eutectic	1824.9	0.717	0.343	0.769	−18826
bcc $\rightleftharpoons C15$ + hcp	eutectoid	1050.2	0.957	0.334	0.998	−5583

Table IIIa. Integral quantities for the liquid phase at 2900 K.

x_{Zr}	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)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−7244	−2534	1.624	595	−1.079	0.000
0.200	−11290	−4342	2.396	776	−1.765	0.000
0.300	−14081	−5483	2.965	649	−2.114	0.000
0.400	−15909	−6020	3.410	319	−2.186	0.000
0.500	−16821	−6014	3.727	−108	−2.037	0.000
0.600	−16754	−5527	3.871	−526	−1.724	0.000
0.700	−15559	−4620	3.772	−830	−1.307	0.000
0.800	−12980	−3356	3.318	−914	−0.842	0.000
0.900	−8511	−1795	2.316	−672	−0.387	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Mo in the liquid phase at 2900 K.

x_{Mo}	ΔG_{Mo} [J/mol]	ΔH_{Mo} [J/mol]	ΔS_{Mo} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Mo}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Mo}}$ [J/(mol·K)]	a_{Mo}	γ_{Mo}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2316	−374	0.670	224	−0.206	0.908	1.009
0.800	−4623	−1414	1.107	757	−0.749	0.826	1.032
0.700	−7213	−2996	1.454	1387	−1.511	0.741	1.059
0.600	−10415	−4998	1.868	1902	−2.380	0.649	1.082
0.500	−14621	−7297	2.526	2092	−3.238	0.545	1.091
0.400	−20348	−9768	3.648	1746	−3.970	0.430	1.075
0.300	−28379	−12290	5.548	651	−4.462	0.308	1.027
0.200	−40209	−14738	8.783	−1402	−4.599	0.189	0.943
0.100	−60146	−16990	14.881	−4626	−4.264	0.083	0.825
0.000	$-\infty$	−18923	∞	−9231	−3.342	0.000	0.682

Reference state: Mo(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 2900 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	$-\infty$	−29187	∞	8369	−12.950	0.000	1.415
0.100	−51593	−21979	10.212	3927	−8.933	0.118	1.177
0.200	−37957	−16052	7.553	850	−5.828	0.207	1.036
0.300	−30104	−11284	6.490	−1074	−3.521	0.287	0.956
0.400	−24150	−7551	5.724	−2056	−1.895	0.367	0.918
0.500	−19021	−4731	4.928	−2308	−0.836	0.454	0.909
0.600	−14357	−2699	4.020	−2040	−0.227	0.551	0.919
0.700	−10065	−1334	3.011	−1464	0.045	0.659	0.941
0.800	−6172	−511	1.952	−792	0.097	0.774	0.968
0.900	−2774	−107	0.919	−233	0.043	0.891	0.990
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

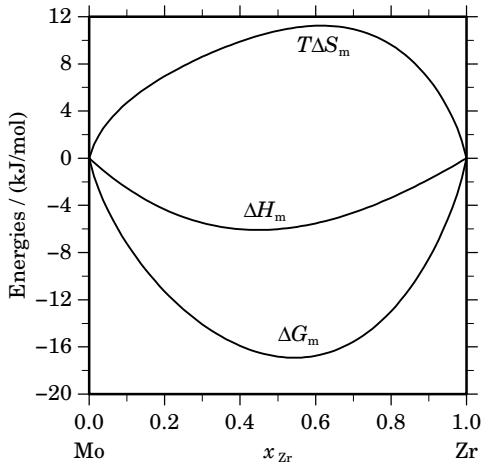

Fig. 2. Integral quantities of the liquid phase at T=2900 K.

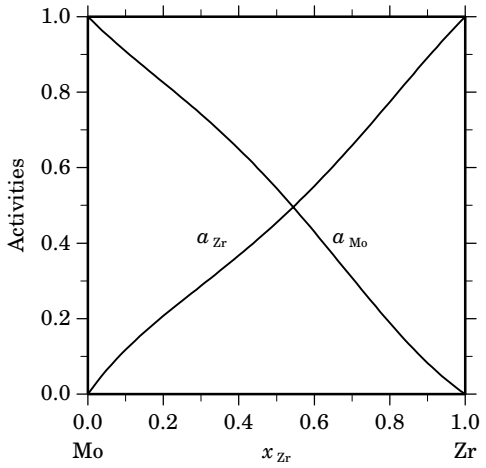

Fig. 3. Activities in the liquid phase at T=2900 K.

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))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
$C15$	0.333	−7231	−7245	−0.048	0.000

References

[1976Kub] O. Kubaschewski, O. von Goldbeck in: "Zirconium: Physico-Chemical Properties of its Compounds and Alloys", O. Kubaschewski (ed.), Atomic Energy Rev. Spec. Issue 6, IAEA, Vienna, 1976, pp. 96–97.

[2002Zin] M. Zinkevich, N. Mattern: J. Phase Equilibria **23** (2002) 156–161.

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