# **Mn – Zr** (Manganese – Zirconium)

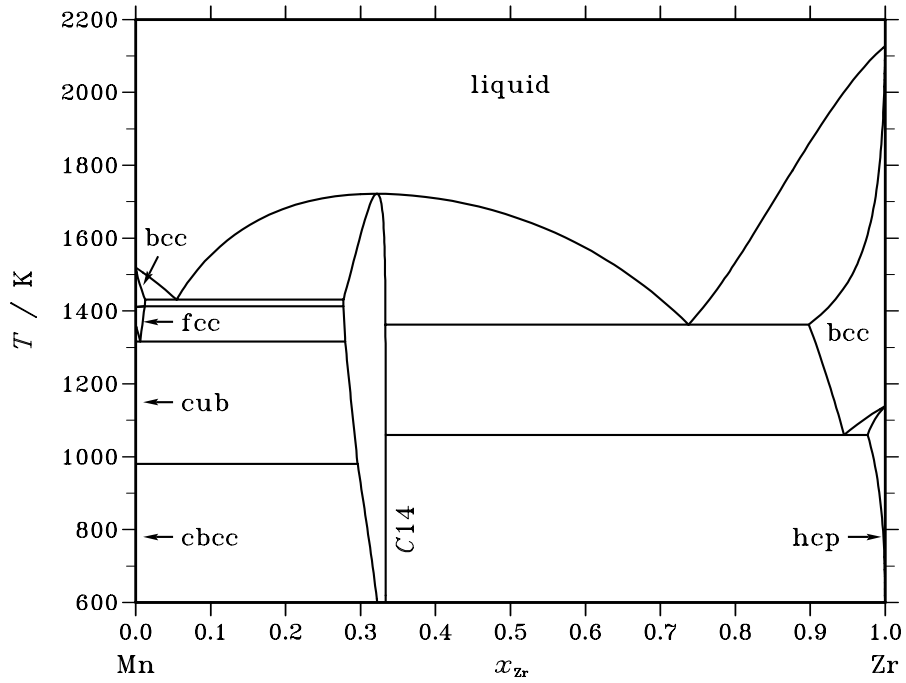


**Fig. 1.** Calculated phase diagram for the system Mn-Zr.

The Mn-Zr binary system has been investigated in the framework of the COST 507 project on light metal alloys. The system is characterised by a congruent melting $C14$ Laves phase, $Mn_2Zr$ and two eutectics on either side. Two thermodynamic assessments are available in the literature: Hack [98Hac], which has been accepted in the COST 507 compilation and Flandorfer *et al.* [97Fla]. For the first assessment, no precise information is given on the selected underlying experimental data. In the case of Flandorfer's work, the authors based their assessment on the available literature data and own experimental work which was mainly focused on the solubility limit of the $C14$ Laves phase. The work of [97Fla] agrees better with the available phase diagram data and has therefore been selected.

**Table I.** Phases, structures and models.

| Phase | Struktur-bericht | Prototype | Pearson symbol | Space group | SGTE name | Model |
|---|---|---|---|---|---|---|
| liquid | | | | | LIQUID | $(Mn,Zr)_1$ |
| fcc | $A1$ | Cu | $cF4$ | $Fm\overline{3}m$ | FCC_A1 | $(Mn,Zr)_1$ |
| bcc | $A2$ | W | $cI2$ | $Im\overline{3}m$ | BCC_A2 | $(Mn,Zr)_1$ |
| cbcc | $A12$ | $\alpha$Mn | $cI58$ | $I\overline{4}3m$ | CBCC_A12 | $(Mn,Zr)_1$ |
| cub | $A13$ | $\beta$Mn | $cP20$ | $P4_132$ | CUB_A13 | $(Mn,Zr)_1$ |
| $C14$ | $C14$ | $MgZn_2$ | $hP12$ | $P6_3/mmc$ | C14_MN2ZR | $(Mn,Zr)_2(Mn,Zr)_1$ |
| hcp | $A3$ | Mg | $hP2$ | $P6_3/mmc$ | HCP_A3 | $(Mn,Zr)_1$ |

**Table II.** Invariant reactions.

| Reaction | Type | $T$ / K | Compositions / $x_{\mathrm{Zr}}$ | | | $\Delta_{\mathrm{r}}H$ / (J/mol) |
|---|---|---|---|---|---|---|
| liquid $\rightleftharpoons C14$ | congruent | 1721.8 | 0.322 | 0.322 | | −45655 |
| liquid $\rightleftharpoons$ bcc + $C14$ | eutectic | 1431.4 | 0.055 | 0.013 | 0.277 | −16051 |
| bcc + $C14 \rightleftharpoons$ fcc | peritectoid | 1413.0 | 0.012 | 0.277 | 0.012 | −1401 |
| liquid $\rightleftharpoons C14$ + bcc | eutectic | 1363.0 | 0.738 | 0.333 | 0.898 | −22267 |
| fcc $\rightleftharpoons$ cub + $C14$ | eutectoid | 1316.3 | 0.006 | 0.000 | 0.279 | −2772 |
| bcc $\rightleftharpoons C14$ + hcp | eutectoid | 1060.1 | 0.945 | 0.333 | 0.977 | −4155 |
| cub + $C14 \rightleftharpoons$ cbcc | degenerate | 980.0 | 0.000 | 0.296 | 0.000 | −2253 |

**Table IIIa.** Integral quantities for the liquid phase at 2200 K.

| $x_{\mathrm{Zr}}$ | $\Delta G_{\mathrm{m}}$ [J/mol] | $\Delta H_{\mathrm{m}}$ [J/mol] | $\Delta S_{\mathrm{m}}$ [J/(mol·K)] | $G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol] | $S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)] | $\Delta C_P$ [J/(mol·K)] |
|---|---|---|---|---|---|---|
| 0.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |
| 0.100 | −8987 | −5542 | 1.566 | −3041 | −1.137 | 0.000 |
| 0.200 | −14367 | −9008 | 2.436 | −5214 | −1.725 | 0.000 |
| 0.300 | −17953 | −10902 | 3.205 | −6779 | −1.874 | 0.000 |
| 0.400 | −20201 | −11624 | 3.899 | −7891 | −1.697 | 0.000 |
| 0.500 | −21273 | −11463 | 4.459 | −8594 | −1.304 | 0.000 |
| 0.600 | −21136 | −10601 | 4.789 | −8825 | −0.807 | 0.000 |
| 0.700 | −19588 | −9112 | 4.762 | −8414 | −0.317 | 0.000 |
| 0.800 | −16236 | −6961 | 4.216 | −7082 | 0.055 | 0.000 |
| 0.900 | −10389 | −4007 | 2.901 | −4443 | 0.198 | 0.000 |
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |

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

**Table IIIb.** Partial quantities for Mn in the liquid phase at 2200 K.

| $x_{\mathrm{Mn}}$ | $\Delta G_{\mathrm{Mn}}$ [J/mol] | $\Delta H_{\mathrm{Mn}}$ [J/mol] | $\Delta S_{\mathrm{Mn}}$ [J/(mol·K)] | $G^{\mathrm{E}}_{\mathrm{Mn}}$ [J/mol] | $S^{\mathrm{E}}_{\mathrm{Mn}}$ [J/(mol·K)] | $a_{\mathrm{Mn}}$ | $\gamma_{\mathrm{Mn}}$ |
|---|---|---|---|---|---|---|---|
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |
| 0.900 | −2414 | −1132 | 0.583 | −487 | −0.293 | 0.876 | 0.974 |
| 0.800 | −5627 | −3798 | 0.831 | −1545 | −1.024 | 0.735 | 0.919 |
| 0.700 | −9338 | −7150 | 0.995 | −2813 | −1.971 | 0.600 | 0.857 |
| 0.600 | −13600 | −10660 | 1.336 | −4256 | −2.911 | 0.475 | 0.792 |
| 0.500 | −18839 | −14128 | 2.142 | −6160 | −3.621 | 0.357 | 0.714 |
| 0.400 | −25899 | −17674 | 3.738 | −9138 | −3.880 | 0.243 | 0.607 |
| 0.300 | −36148 | −21747 | 6.546 | −14125 | −3.465 | 0.139 | 0.462 |
| 0.200 | −51821 | −27117 | 11.229 | −22381 | −2.153 | 0.059 | 0.294 |
| 0.100 | −77609 | −34877 | 19.424 | −35490 | 0.279 | 0.014 | 0.144 |
| 0.000 | $-\infty$ | −46447 | $\infty$ | −55361 | 4.051 | 0.000 | 0.048 |

Reference state: Mn(liquid)

**Table IIIc.** Partial quantities for Zr in the liquid phase at 2200 K.

| $x_{\mathrm{Zr}}$ | $\Delta G_{\mathrm{Zr}}$ [J/mol] | $\Delta H_{\mathrm{Zr}}$ [J/mol] | $\Delta S_{\mathrm{Zr}}$ [J/(mol·K)] | $G^{\mathrm{E}}_{\mathrm{Zr}}$ [J/mol] | $S^{\mathrm{E}}_{\mathrm{Zr}}$ [J/(mol·K)] | $a_{\mathrm{Zr}}$ | $\gamma_{\mathrm{Zr}}$ |
|---|---|---|---|---|---|---|---|
| 0.000 | $-\infty$ | −67763 | $\infty$ | −35895 | −14.486 | 0.000 | 0.141 |
| 0.100 | −68148 | −45237 | 10.414 | −26030 | −8.731 | 0.024 | 0.241 |
| 0.200 | −49329 | −29845 | 8.856 | −19889 | −4.525 | 0.067 | 0.337 |
| 0.300 | −38056 | −19658 | 8.362 | −16033 | −1.648 | 0.125 | 0.416 |
| 0.400 | −30103 | −13070 | 7.742 | −13343 | 0.124 | 0.193 | 0.482 |
| 0.500 | −23706 | −8798 | 6.776 | −11027 | 1.013 | 0.274 | 0.547 |
| 0.600 | −17960 | −5885 | 5.489 | −8616 | 1.241 | 0.375 | 0.624 |
| 0.700 | −12491 | −3696 | 3.998 | −5967 | 1.032 | 0.505 | 0.722 |
| 0.800 | −7340 | −1922 | 2.462 | −3258 | 0.607 | 0.669 | 0.837 |
| 0.900 | −2920 | −578 | 1.065 | −993 | 0.189 | 0.852 | 0.947 |
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |

Reference state: Zr(liquid)

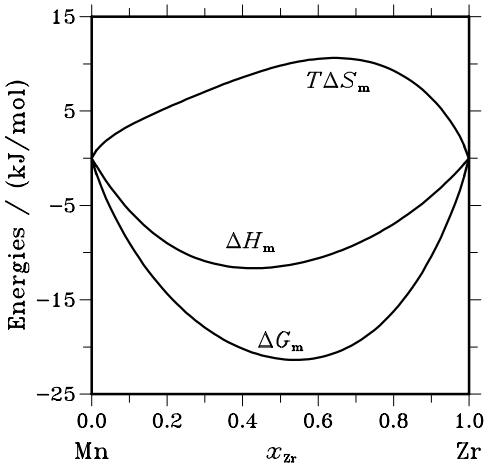


**Fig. 2.** Integral quantities of the liquid phase at $T$=2200 K.

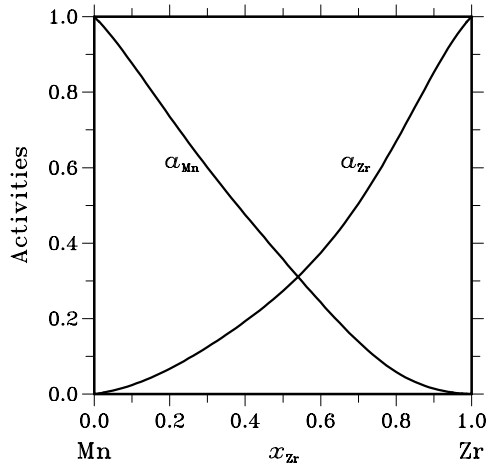


**Fig. 3.** Activities in the liquid phase at $T$=2200 K.

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

| Compound | $x_{\mathrm{Zr}}$ | $\Delta_{\mathrm{f}}G^{\circ}$ / (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)) |
|---|---|---|---|---|---|
| $C14$ | 0.333 | −36334 | −40004 | −12.309 | −0.003 |

## References

[97Fla] H. Flandorfer, J. Gröbner, A. Stamou, N. Hassiotis, A. Saccone, P. Rogl, R. Wouters, H. Seifert, D. Maccio, R. Ferro, G. Haidemenopoulos, L. Delaey, G. Effenberg: Z. Metallkd. **88** (1997) 529–538.

[98Hac] K. Hack, in: I. Ansara, A.T. Dinsdale, M.H. Rand (eds.): COST 507, "Thermochemical database for light metal alloys", Vol. 2, EUR 18499, 1998, 245–248.