

# Zn-Zr (Zinc-Zirconium)

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The Zn-Zr phase diagram in [Massalski2] was assessed by [1992Dut].

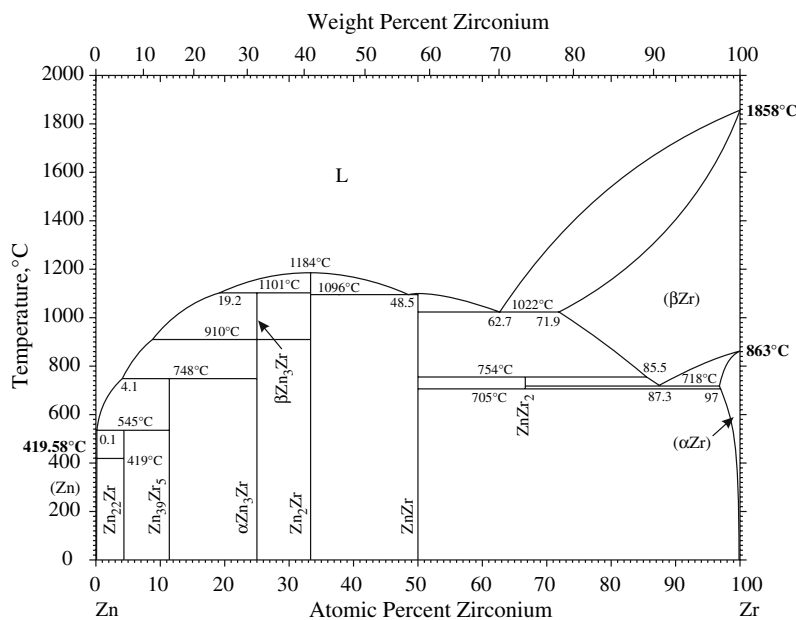
After this phase diagram was published, the existence of the  $ZnZr_2$  phase was discovered by [2004Wil]. This phase exists in a narrow temperature range from  $750 \pm 24$  and  $706 \pm 6$  °C according to optical metallography, SEM, and TEM investigations. This system was thermodynamically assessed by [2006Arr1]. Three possible thermodynamic models were considered. Because all calculated results are similar, the phase diagrams corresponding to their first model are shown in Fig. 1 and 2. Figure 1 shows the Zn-Zr phase diagram under constrained vapor conditions. The stability of various Zn-Zr phases was discussed by [2006Arr2].  $Zn_{14}Zr$  and  $Zn_6Zr$  shown in the diagram of [1992Dut] are  $Zn_{22}Zr$  and  $Zn_{39}Zr_5$ , respectively, according to [2006Arr2]. In addition to the phases in Fig. 1,  $Zn_2Zr_3$  may exist at high temperatures ( $>1000$  °C). [2006Arr1]

shows a phase diagram including  $Zn_2Zr_3$ . Figure 2 shows the Zn-Zr phase diagram at 1 bar.

Zn-Zr crystal structure data are given in Table 1.

## References

- 1992Dut:** J. Dutkiewicz, The Zn-Zr (Zinc-Zirconium) System, *J. Phase Equilib.*, 1992, **13**(4), p 430-433
- 2004Wil:** M.E. Williams, W.J. Boettinger, and U.R. Katner, Contribution to the Zr-Rich Part of the Zn-Zr Phase Diagram, *J. Phase Equilib. Diffusion*, 2004, **25**(4), p 355-363
- 2006Arr1:** R. Arroyave and Z.K. Liu, Thermodynamic Modeling of the Zn-Zr System, *Calphad*, 2006, **30**(1), p 1-13
- 2006Arr2:** R. Arroyave, A. van de Walle, and Z.K. Liu, First-Principles Calculations of the Zn-Zr System, *Acta Mater.*, 2006, **54**, p 473-482



**Fig. 1** Zn-Zr phase diagram under constrained vapor conditions

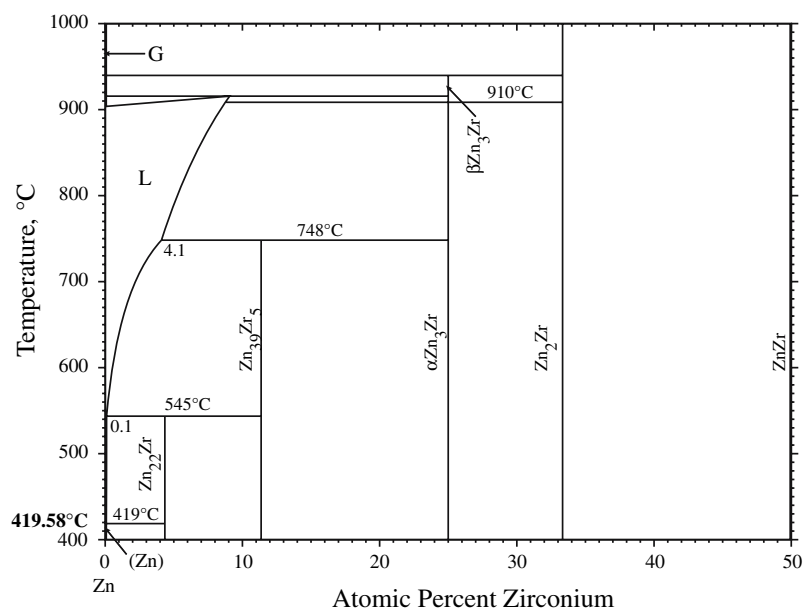


Fig. 2 Zn-Zr phase diagram at 1 bar

Table 1 Zn-Zr crystal structure data

Phase	Composition at.% Zr	Pearson symbol	Space group	Struktur-bericht designation	Prototype
(Zn)	0	<i>hP2</i>	<i>P6<sub>3</sub>/mmc</i>	<i>A3</i>	Mg
Zn <sub>22</sub> Zr	4.3	<i>cF184</i>	<i>Fd<math>\bar{3}m</math></i>	...	...
Zn <sub>39</sub> Zr <sub>5</sub>	11.4	<i>mC88</i>	<i>C2/m</i>	...	...
βZn <sub>3</sub> Zr	25	...	...	...	...
αZn <sub>3</sub> Zr	25	<i>t**</i>	...	...	...
Zn <sub>2</sub> Zr	33.3	<i>cF24</i>	<i>Fd<math>\bar{3}m</math></i>	<i>C15</i>	Cu <sub>2</sub> Mg
ZnZr	50	<i>cP2</i>	<i>Pm<math>\bar{3}m</math></i>	<i>B2</i>	CsCl
ZnZr <sub>2</sub>	66.7	<i>tI6</i>	<i>I4/mmm</i>	<i>D0<sub>22</sub></i>	MoSi <sub>2</sub>
(βZr)	71.9-100	<i>cI2</i>	<i>Im<math>\bar{3}m</math></i>	<i>A2</i>	W
(αZr)	96.8-100	<i>hP2</i>	<i>P6<sub>3</sub>/mmc</i>	<i>A3</i>	Mg