# The Zr (Zirconium) System

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**By J. P. Abriata and J. C. Bolcich**
**Centro Atómico Bariloche, Comisión Nacional de Energía Atómica**

Three allotropic solid phases were shown to exist in pure Zr under pressure: $\alpha$, $\beta$, and (hexagonal) $\omega$. The main features of the temperature-pressure phase diagram of pure Zr (Fig. 1) include: the temperature 863 ± 5 °C for the $\alpha/\beta$ equilibrium at zero pressure [76Alc], the pressure 22 ± 3 kbar for the $\alpha/\omega$ equilibrium at room temperature [73Zil, 75Zil, 81Min], the coordinates ~700 °C and ~60 kbar for the $\alpha/\beta/\omega$ triple point [63Jay, 75Kut], and the (estimated) slope $(dT/dp)^{\beta/\omega} \approx 2.1$ °C/kbar [75Kut].

Within experimental error, the $\alpha/\beta$ and $\beta/\omega$ equilibrium curves are straight lines [63Jay, 75Zil]. The $\alpha \rightleftarrows \omega$ transformation was associated with considerable hysteresis [73Zil], and the $\alpha/\omega$ equilibrium curve also was assumed to be a straight line [73Zil, 75Zil].

[70Kau] gave a first approximation calculation of the temperature-pressure phase diagram for pure Zr, where the relative stabilities of the $\alpha$, $\beta$, and $\omega$ phases were quantitatively described by:

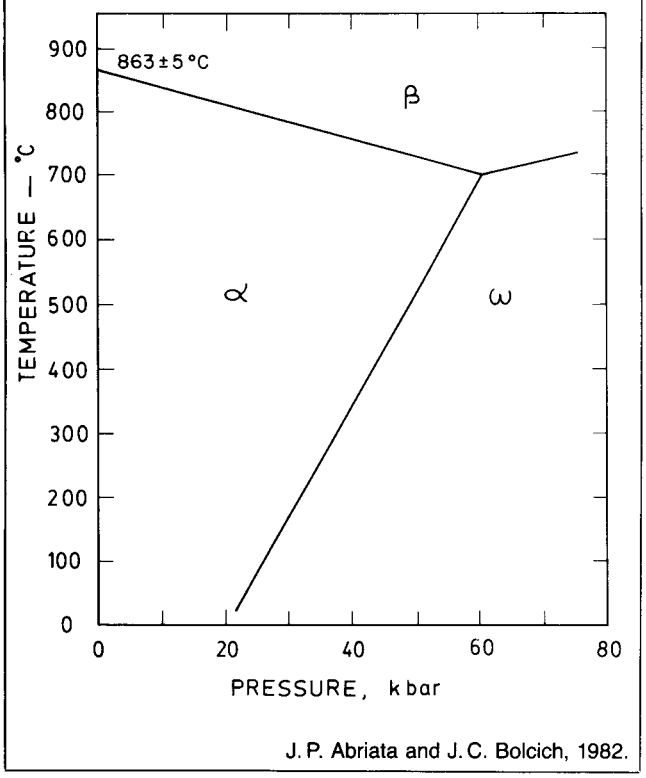
$$\Delta F_{Zr}^{\alpha \rightarrow \beta} \approx 3.8\,(1143 - T) - 9.6\,P$$

and

$$\Delta F_{Zr}^{\omega \rightarrow \alpha} \approx -0.335\,(4500 + T) + 32\,P$$

where $\Delta F$ are the free energy differences in J/mol, $T$ is the temperature in K, and $P$ is the pressure in kbar. The general adjustment of the results by [70Kau] to the previously described $T$-$P$ diagram is acceptable, except for the calculated $\alpha/\omega$ equilibrium at room temperature, which is too displaced toward high pressures.

**Fig. 1 Zr Temperature–Pressure Phase Diagram**

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Zr evaluation contributed by **J. P. Abriata** and **J. C. Bolcich,** Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, 8400 – S. C. de Bariloche, Rio Negro, Argentina. Literature searched through October 1981. Dr. Abriata is the ASM/NBS Data Program Category Editor for binary zirconium alloys.