H-Ti (Hydrogen-Titanium)

H. Okamoto

A partial Ti-H phase diagram at 1 atm pressure in [Massalski2] was adopted from [87San]. Partly based on [87San], [91Fuk] proposed a Ti-H phase diagram for wider composition and temperature ranges under a high H pressure (≤30 MPa). The invariant reaction existing at 447 °C in a *P-T-X* diagram was speculated to be due to the L ↔ δ + L(H_2) reaction. Figure 1 is redrawn essentially from [91Fuk], but the (αTi)/(αTi) + (βTi) boundary is according to [87San] because the opening angle of (βTi) + (αTi) two-phase field at 0 at.% H in the phase diagram of [87San] is thermodynamically more plausible. Figure 1 is expected not to differ much from a diagram at 1 atm because the pressure is not very high.

Ti-H crystal structure data (Table 1) are accepted from [87San].

Cited References

87San: A. San-Martin and F.D. Manchester, *Bull. Alloy Phase Diagrams*, *8*(1), 30-42 (1987).

91Fuk: Y. Fukai, *Nippon Kinzoku Gakkai-shi*, *55*(1), 17-21 (1991) in Japanese.

Table 1 Ti-H Crystal Structure Data

Phase	Composition, at.% H	Pearson symbol	Space group	Strukturbericht designation	Prototype
(βTi)	0 to 50	*cI*2	$Im\bar{3}m$	*A*2	W
(αTi)	0 to 8.5	*hP*2	$P6_3/mmc$	*A*3	Mg
δ	50 to 66.7	*cF*12	$Fm\bar{3}m$	*C*1	CaF_2
ε	60 to 66.7	*tI*6	*I*4/*mmm*	$L'2_b$	ThH_2

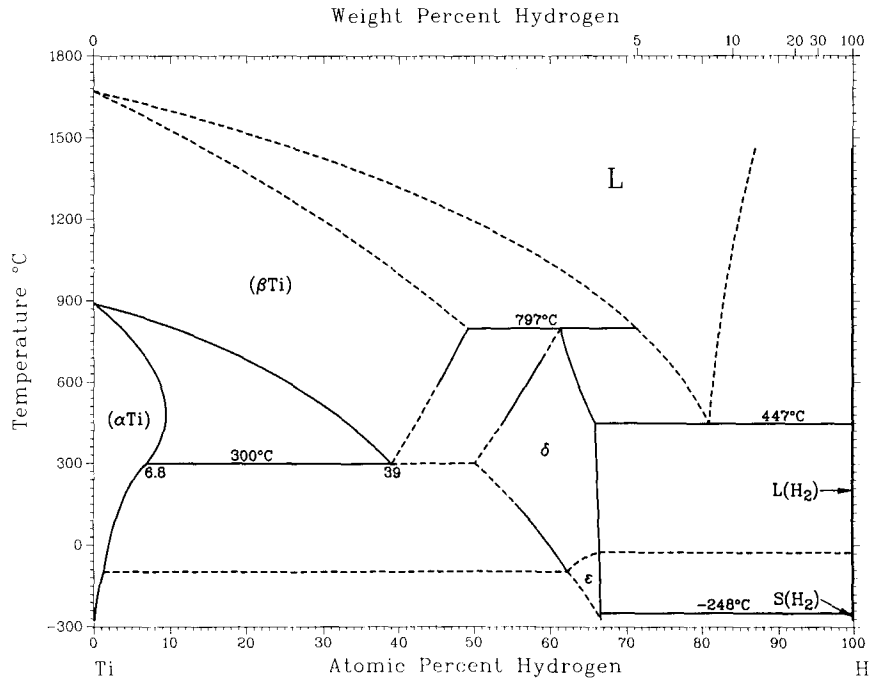

Fig. 1 Ti-H phase diagram.