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Fe-P-Ti (Iron-Phosphorus-Titanium)

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The previous review of the experimental data on this ternary system by [1988Rag], based on mainly on the work of [1959Vog] and [1965Kan], presented a liquidus projection, an isothermal section at 25 °C and a reaction scheme for the Fe-FeP-Ti region. Recently, [2006Oht] made a CALPHAD-type thermodynamic analysis of the entire system, incorporating first-principles energy calculations.

Binary Systems

The Fe-P phase diagram [2006Oht, Massalski2] has the following compounds at ambient pressure: Fe_3P ($D0_e$, Ni_3P-type tetragonal), Fe_2P ($C22$, Fe_2P-type hexagonal), FeP ($B31$, MnP-type orthorhombic), FeP_2 ($C18$, FeS_2-marcasite type orthorhombic), and FeP_4 (monoclinic). There are two intermediate phases in Fe-Ti system: Fe_2Ti ($C14$, $MgZn_2$-type hexagonal) and FeTi ($B2$, CsCl-type cubic). The computed P-Ti phase diagram [2006Oht] shows the following intermediate phases: Ti_3P (tetragonal, space group $P4_2/n$), Ti_2P (hexagonal, space group $P6/mmm$), $Ti_{1.7}P$ (orthorhombic, space group $P2_12_12_1$), Ti_5P_3 ($D8_8$, Mn_5Si_3-type hexagonal), Ti_4P_3 ($D7_3$, Th_3P_4-type cubic?), TiP (B_i, AsTi-type hexagonal), and TiP_2 (orthorhombic, space group $Pnma$).

The Computed Ternary Phase Equilibria

In their thermodynamic modeling, [2006Oht] used a regular solution model for the liquid, face-centered cubic (fcc), body-centered cubic (bcc), and close-packed hexagonal (cph) phases. The $C14$ phase (Fe_2Ti) was described by a three sub-lattice model to account for its wide homogeneity range. The slight solubility of Ti in Fe_3P and Fe_2P and the homogeneity ranges of Ti_5P_3 and TiP were taken into account, by using a two sublattice model. The other binary compounds were modeled as stoichiometric phases. The small homogeneity range of the ternary compound FeTiP (anti $PbCl_2$-type orthorhombic) was accounted for, by adopting a three sublattice model. The enthalpies of formation of the binary phosphides and the ternary phosphide FeTiP were evaluated from the electron band energy calculations, using the Full Potential Linearized Augmented Plane Wave (FLAPW) method. See [2006Oht] for details.

The experimental phase diagram data of [1959Vog] and [1965Kan] were used in the optimization and the derived interaction parameters were listed. Four vertical sections along the Fe_3P-FeTiP and Fe-FeTiP joins and at constant 7.5 mass % P and 7.5 mass % Ti respectively, computed by [2006Oht] are compared with the experimental data of [1959Vog] in Fig. 1-4. The agreement is fair. A liquidus

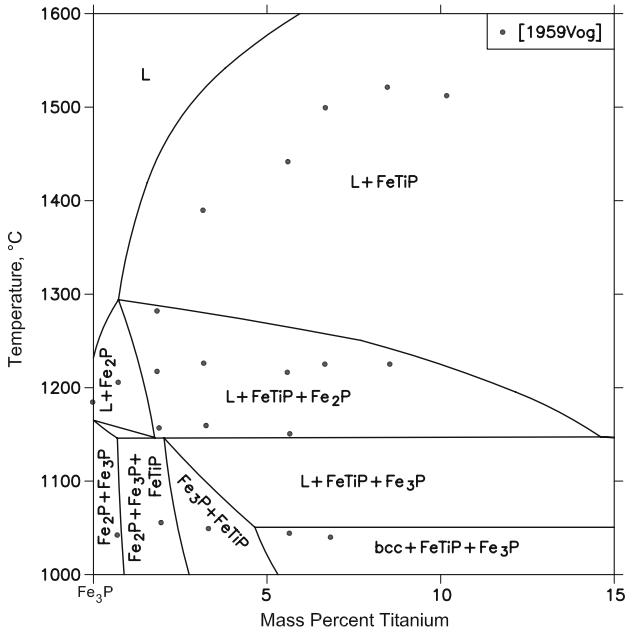

Fig. 1 Fe-P-Ti computed vertical section along the Fe_3P-FeTiP join [2006Oht]

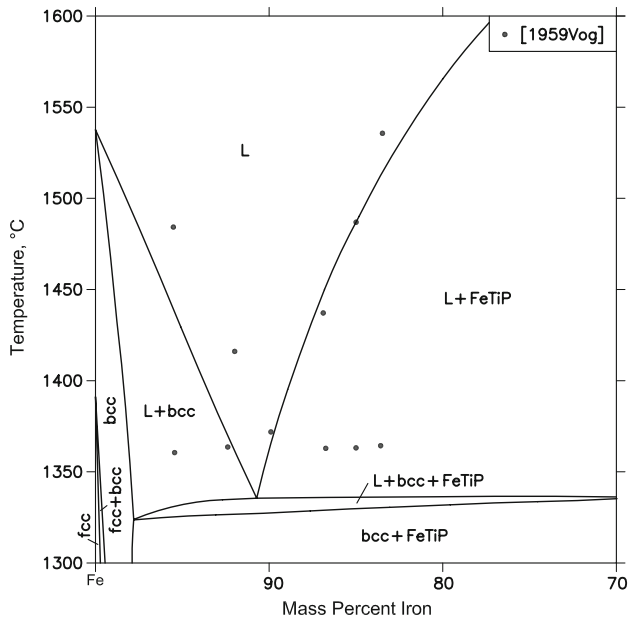

Fig. 2 Fe-P-Ti computed vertical section along the Fe-FeTiP join [2006Oht]

projection for the entire composition range was computed. The computed part in the Fe-FeP-Ti region agrees with the assessed projection of [1988Rag]. Full isothermal sections were also computed at 800 and 25 °C and compared with the partial sections at 800 °C by [1965Kan] and 25 °C by [1959Vog]. In Fig. 5, the full computed section at 800 °C [2007Oht] is compared with the few experimental points of [1965Kan].

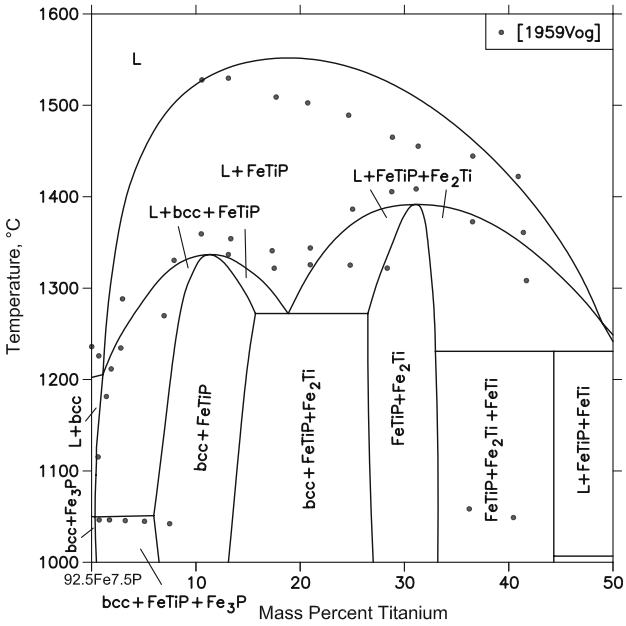

Fig. 3 Fe-P-Ti computed vertical section at 7.5 mass % P [2006Oht]

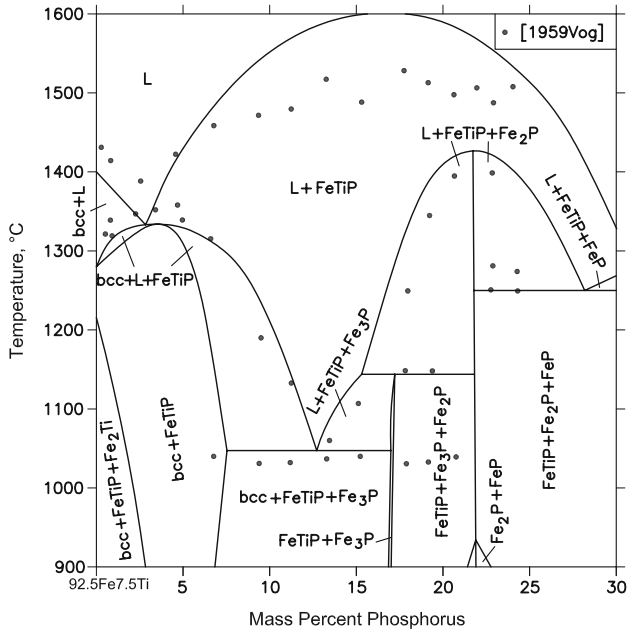

Fig. 4 Fe-P-Ti computed vertical section at 7.5 mass % Ti [2006Oht]

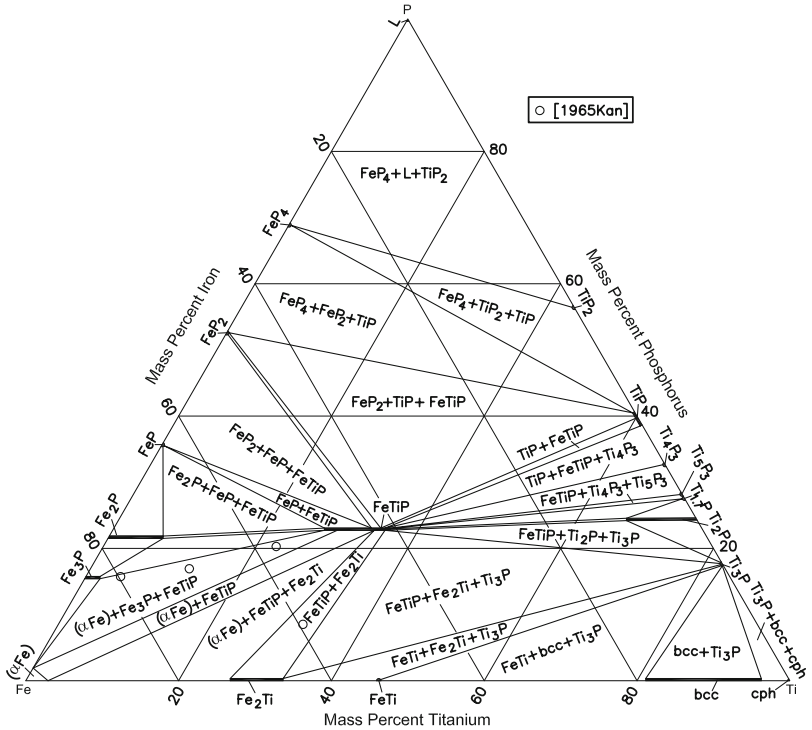

Fig. 5 Fe-P-Ti computed isothermal section at 800 °C [2007Oht]

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