# **Ce-Fe-P** (Cerium-Iron-Phosphorus)

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Recently, Chikhrii et al. [1997Chi] determined isothermal sections for this system at  $\sim$ 800 °C for 0-30 at.% Ce and at  $\sim$ 590 °C for 30-70 at.% Ce.

#### **Binary Systems**

The Ce-Fe phase diagram [1993Zha] depicts two stoichiometric compounds,  $Ce_2Fe_{17}$  and  $CeFe_2$ , both forming peritectically.  $Ce_2Fe_{17}$  has two crystal modifications (hexagonal and rhombohedral).  $CeFe_2$  has the cubic MgCu<sub>2</sub> type structure. The Ce-P phase diagram is not known. Three intermediate compounds are known: CeP (cubic, NaCl type),  $CeP_2$  (monoclinic), and  $CeP_5$  (monoclinic). A partial phase diagram is known for the Fe-P system [1982Kub]. The intermediate compound  $Fe_3P$  forms through a peritectic reaction at 1166 °C between liquid and  $Fe_2P$ .  $Fe_2P$  forms congruently at 1370 °C.  $Fe_3P$  is body-centered tetragonal with the Ni<sub>3</sub>P type of structure.  $Fe_2P$  has the hexagonal C22 structure. The other intermediate phases at higher P contents are FeP (orthorhombic MnP type), FeP<sub>2</sub> [orthorhombic FeS<sub>2</sub> (marcasite) type], and FeP<sub>4</sub> (monoclinic).

### **Ternary Compounds**

Three ternary compounds are known in this system. CeFe<sub>2</sub>P<sub>2</sub> ( $\tau_1$ ) has the Al<sub>4</sub>Ba-type tetragonal structure [1985Jei]. Ce<sub>2</sub>Fe<sub>12</sub>P<sub>7</sub> ( $\tau_2$ ) has the Zr<sub>2</sub>Fe<sub>12</sub>P<sub>7</sub>-type hexagonal structure [1984Jei].  $CeFe_4P_{12}$  ( $\tau_3$ ) has the LaFe\_4P\_{12}-type cubic structure [1977Jei]. Table 1 lists the structural details of these compounds.

## **Ternary Isothermal Section**

With starting materials of purity of 99.9% Ce, 99.99% Fe, and 99.89% P, [1997Chi] prepared 36 alloy compositions. For compositions up to 33.3 at.% P, the alloys were melted in an arc furnace. For higher P contents, the powder mixtures were sintered by slow heating up to 800 °C. The samples were finally annealed for 500 h at 1070 K for compositions with  $\leq$ 30 at.% Ce and at 870 K for compositions with 30-70 at.% Ce and quenched in water. The phase equilibria were studied by x-ray powder diffraction. The isothermal sections determined by [1997Chi] at 797 °C (1070 K) for 0-30 at.% Ce and at ~590 °C for 30-70 at.% Ce are presented as a composite section in Fig. 1. The temperature of anneal for the higher Ce content alloys is assumed here to be just below the eutectic temperature (592 °C) of the Fe-Ce system, as no liquid phase is indicated by [1997Chi]. The ternary compounds  $\tau_1$  and  $\tau_2$  are present at 797 °C. The composition of the ternary compound  $\tau_3$  falls outside the range investigated by [1997Chi]. No homogeneity ranges were found for the ternary compounds. The third component solubility in the binary compounds is negligible.



Fig. 1 Ce-Fe-P isothermal section at 797 °C (0-30 at.% Ce) and at ~590 °C (30-70 at.% Ce) [1997Chi]. Narrow two-phase regions around tie-triangles are omitted.

	Composition,				Lattice	
Phase	at.%	Pearson Symbol	Space Group	Prototype	Parameter, nm	Reference
CeFe <sub>2</sub> P <sub>2</sub>	20 Ce	<i>tI</i> 10	I4/mmm	Al <sub>4</sub> Ba	a = 0.3852	1985Jei
$(\tau_1)$	40 P				c = 1.0314	
$Ce_2Fe_{12}P_7$	9.5 Ce	hP21	$P\overline{6}$	$Zr_2Fe_{12}P_7$	a = 0.9135	1984Jei
$(\tau_2)$	33.3 P				c = 0.3677	
CeFe <sub>4</sub> P <sub>12</sub>	5.9 Ce	<i>cI</i> 34	Im3	LaFe <sub>4</sub> P <sub>12</sub>	a = 0.7792	1977Jei
$(\tau_3)$	70.6 P					

 Table 1
 Ce-Fe-P
 Crystal Structure and Lattice Parameter Data

#### References

- 1977, Jei: W. Jeitschko and D. Braun: "LaFe<sub>4</sub>P<sub>12</sub> with Filled CoAs<sub>3</sub> Type Structure and Isotypic Lanthanoid-Transition Metal Polyphosphides," Acta Crsytallogr., B, 1977, 33B(11), pp. 3401-06. 1982Kub: O. Kubaschewski: "Iron-Phosphorus" in Iron-Binary
- Phase Diagrams, Springer-Verlag, Berlin, 1982, pp. 84-86.
- 1984Jei: W. Jeitschko, U. Meisen, and U.D. Scholtz: "Ternary Lanthanoid Iron Phosphides With YCo5P3 and Zr2Fe12P7 Type Structures," J. Solid State Chem., 1984, 55, pp. 331-36.

1985Jei: W. Jeitschko, U. Meisen, M.H. Moeller, and M. Reehius:

"On LaCo<sub>2</sub>P<sub>2</sub> and Other New Compounds with ThCr<sub>2</sub>Si<sub>2</sub> and CaBe2Ge2 Type Structure," Z. Anorg. Allg. Chem., 1985, 527, pp. 73-84 (in German).

- 1993Zha: W. Zhang, G. Liu, and K. Han: "Ce-Fe (Cerium-Iron)" in Phase Diagrams of Binary Iron Alloys, H. Okamoto, ed., ASM International Materials Park, OH, 1993, pp. 89-92.
- 1997Chi: S.I. Chikhrii and O.V. Shevchuk: "Phase Equilibria in the (La,Ce)-Fe-P Systems," Zhur. Neorg. Khim., 1997, 42(8), pp. 1384-86 (in Russian); TR: Russ. J. Inorg. Chem., 1997, 42(8), pp. 1258-60.