

THE COVALENT THEORY OF fcc Fe STABILITY

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Stability of the Fe fcc phase (γ -Fe) is defined by metal bonds of $4s$ - and a part $3d(t_{2g})$ -electrons and by covalent interactions of $3d(e_g)$ - and a part of $3d(t_{2g})$ -electrons. The hybridization of electrons of the high (e_g) $3d$ -level and $4s$ -band results in DOS peaks and antipeaks of band electrons (DOS $\sim 4s - e_g$). In exactly the same way, the total transfer integral for band and covalent $3d(t_{2g})$ -electrons results in anomalies of DOS $\sim t_{2g}$ near the Fermi surface. Bonding covalent energies of parts of e_g - and t_{2g} -electrons provide the stability of γ -Fe at heating, though the occurrence of a soft mode of chemical (covalent) bond fluctuations (CBF) under pressure P , which destabilizes the fcc lattice, is possible. The antibonding covalent energy of the nearest neighbours is responsible for γ -Fe antiferromagnetism. It gives the excess of the fcc lattice free energy above those for a bcc lattice, in which the bonding covalent energy of the nearest neighbours is responsible for α -Fe ferromagnetism. This excess explains the distinction of magnetic states of γ -Fe and α -Fe and the stability of bcc α -Fe at low temperatures $T < T_0$, where $T_0(P, x)$ is the line of polymorphous $\alpha - \gamma$ -transitions for the impurity concentration x .