
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 $\sim 4s \sim e_g$). 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 $\alpha \sim \gamma$ -transitions for the impurity concentration x .

1. Band and Covalent Electrons in Metals with the Magnetic Order

The different applications require intent attention to the smallest details of physical and chemical properties of Fe alloys. The strong influence of the spin order on their phase diagrams, see [1, 2], is accompanied by 'giant' changes of properties not only in the order-disorder transitions, but also in the order-order transitions. These are invar effects [3, 4], 'giant' magnetoresistance [1], magnetostriction [3], etc. Even the lowering of the symmetry of the atomic (fcc or bcc) lattice is caused in many cases by the vector spin order.

The translational symmetry sets the band structure of external electrons. The localization of internal shells and nonhomogeneity of the electron density distribution in interatomic space [5] require a choosing of local orbits (bonding and antibonding) of electrons. The usual term (covalent) for these electrons [6] at

their statistical treatment requires the consideration of CBF [7].

The phase diagram of Fe is investigated by all known experimental methods. The large role is played by magnetic measurements [8, 9]. The exchange energy and its strong dependence on temperature T , pressure P , impurity, etc. influences Fe mono-, poly- and nanocrystals (sometimes this influence is determining). Therefore, atomic and magnetic phase diagrams should be considered as a unit, see [10, 11]. On the contrary, the division of phase spaces of quantum statistics into coordinate and spin ones allows one to construct a noncontradictory multielectronic theory of Fe. Here we consider γ -Fe. It is possible to consider this phase as weak antiferromagnetic (spin 1/2) with the low Neel temperature $T_N \leq 10^2$ K [9, 12]. It is possible to keep the Fe γ -phase up to low temperatures only in special cases (nano-inclusions in an fcc lattice, for example, Cu, oligatomic layers, etc.) [12].

In the fcc lattice of γ -Fe, we have band 4s-electrons, playing a main role in metal chemical bond, and the splitting of 3d-states of electrons into e_g and t_{2g} [5, 13]. We suppose, following [14], that a 3d-hole of the low t_{2g} -level is partially collectivized in the 3d-band (with amplitude ξ_h), and partially (with amplitude ξ_d) participates in creation of a covalent bond, accordingly to [6]. The wave function of a t_{2g} -electron (the Fermi-operator $a_{\mathbf{r}}^+$) in a site \mathbf{r}

$$a_{\mathbf{r}\sigma}^+ = \xi_{h\sigma} h_{\mathbf{r}\sigma}^+ + \hat{D}_{\mathbf{r}\sigma} \xi_d, \quad \hat{D}_{\mathbf{r}\sigma} = c_{\mathbf{r}\sigma} d_{\mathbf{r}\sigma} \quad (d)^+ = \bar{d}, \quad (1.1)$$

is expressed through the Fermi-operator $h_{\mathbf{r}\sigma}^+$, where σ is spin, and through the multielectronic operator spinor (MEOS) $\hat{D}_{\mathbf{r}}$ [7]. The electron localization on a covalent bond

$$d_{\mathbf{r}\sigma} \bar{d}_{\mathbf{r}\sigma} = 1, \quad d_{\mathbf{r}} = d_0 + \sum_{\mathbf{k}} d_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}},$$
$$d_{\mathbf{k}} = \sum_{\mathbf{r}} d_{\mathbf{r}} e^{-i\mathbf{k}\mathbf{r}} / N, \quad (1.2)$$

allows one to define the MEOS in the antisymmetric Fock space with the exact commutation ratio (N is the number of lattice sites)

$$[d_{\mathbf{k}}, \bar{d}_{\mathbf{q}}]_{+} = \delta_{\mathbf{kq}} / N, \quad [d_{\mathbf{r}}, d_{\mathbf{r}'}]_{+} = \delta_{\mathbf{r}\mathbf{r}'}. \quad (1.3)$$

The MEOS spin factor

$$c_{\mathbf{r}\sigma}^2 = (1 + \sigma \mathbf{s}_{\mathbf{r}}) / 2 \quad (1.4)$$

is expressed through the Pauli matrix σ and spin polarization of covalent electrons $\mathbf{s}_{\mathbf{r}}$. The MEOS orbital factor is here neglected (we suppose it is equal to 1), including the Lande factor $g=2$.

The high level e_g hybridizes with $4s$ -electrons. For an e_g -hole, we suppose

$$\Psi_{\mathbf{r}}^e = \hat{D}_{\mathbf{r}}^e \Psi_0, \quad \hat{D}_{\mathbf{r}}^e = [c_{\mathbf{r}\sigma} d_{\mathbf{r}\sigma}], \quad (1.5)$$

where the operator factor $d_{\mathbf{r}\sigma}$ is determined similarly to (1.3), and the spin factor

$$c_{\mathbf{r}\sigma}^2 = (1 + \sigma \mathbf{S}_{\mathbf{r}}) / 2 \quad (1.6)$$

is expressed through the local spin $\mathbf{S}_{\mathbf{r}}$. It will be based below, why we consider that e_g -electrons are magnetic (responsible for antiferromagnetic (AFM) order).

The condition for MEOS localization (1.2) reduces the coordinate part of the Hubbard operator to a constant, and the spin part to the Casimir operator. The intraionic Hamiltonian of e_g -holes is equal to the sum of the Hubbard and the Hund operators

$$H_i^e = (U_e / 2) \sum_{\sigma} |c_{\mathbf{r}\sigma}|^4 - A_e (\mathbf{S}_{\mathbf{r}})^2 - \lambda (\mathbf{S}_{\mathbf{r}} \mathbf{L}_{\mathbf{r}}), \quad (1.7)$$

where $\mathbf{L}_{\mathbf{r}}$ - orbital moment, induced in $3d$ -metals by the spin-orbit interaction (λ). The intraionic Hamiltonian of t_{2g} -holes is similar to (1.7):

$$H_i^t = (U_t / 2) \mathbf{s}_{\mathbf{r}}^2 - A_t (\mathbf{S}_{\mathbf{r}} \mathbf{s}_{\mathbf{r}}), \quad U_{t,e} > 0, \quad (1.8)$$

where the contribution of the Hund exchange between t_{2g} -electrons is included in the expression for U_t . At $U_t \gg |A_t|$, spin polarization of t_{2g} -holes $|\mathbf{s}_{\mathbf{r}}| \ll \ll S = 1/2$. The inverse inequality $(U_e / 8) < A_e$ favours the formation of the local spin of an e_g -hole ($S = 1/2$).

2. The Electronic Spectrum of $4s - e_g$ -electrons

The hybridization of $4s - 3d$ -electrons is essential for the high (e_g) level, so the hybridization of $4s - t_{2g}$ is neglected in the first approximation. The MEOS for one covalent electron on a site allows us

to write down the binary transfer Hamiltonian of $4s$ - (the Fermi-amplitude $f_{\mathbf{k}\sigma}^+$) and e_g -fermions ($d_{\mathbf{k}\sigma}$)

$$H^{4s-e} = \sum \tilde{\xi}_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma}^+ f_{\mathbf{k}\sigma} + N \sum \Gamma_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} \bar{d}_{\mathbf{k}\sigma} + \sum (g_{\sigma} f_{\mathbf{r}\sigma}^+ \bar{d}_{\mathbf{r}\sigma} + \text{h.c.}), \quad (2.1)$$

where

$$\Gamma_{\mathbf{k}\sigma} = [\Gamma(0) - \Gamma(\mathbf{k})] \{c_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma}\}, \quad \Gamma(\mathbf{k}) = \sum \Gamma(|\mathbf{r} - \mathbf{r}'|) e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}')} \quad (2.2)$$

and $\Gamma(|\mathbf{r} - \mathbf{r}'|)$ - the transfer integral of e_g -holes (the energy of local covalent bond). The kinetic energy of $4s$ -electrons

$$\tilde{\xi}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}}(\sigma) - \varepsilon_{\mathbf{F}\sigma} \quad (2.3)$$

is counted from the Fermi level $\varepsilon_{\mathbf{F}}$, which is replaced in the Stoner approximation by the effective renormalized chemical potential of spin subbands $\sigma = \pm 1/2$. Braces in (2.2) mean the Fourier-image of the spin MEOS product. The part of covalent energy, omitted in (2.1), which does not depend on the wave vector \mathbf{k} ,

$$H_0^{\text{ch}} = - \sum \Gamma(|\vec{\rho}|) c_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma}, \quad \vec{\rho} \hat{=} \mathbf{r} - \mathbf{r}' \quad (2.4)$$

contains the exchange Hamiltonian, which will be received below in the case of two AFM sublattices.

Diagonalization of the binary form (2.1) according to Bogolyubov gives 2×2 branches of a spectrum. Pairs of spin subband (collective and CBF)

$$E_{\mathbf{k}\sigma}^{\pm} = \{\Gamma_{\mathbf{k}\sigma} + \tilde{\xi}_{\mathbf{k}\sigma} \pm [(\Gamma_{\mathbf{k}\sigma} - \tilde{\xi}_{\mathbf{k}\sigma})^2 + 4 |g_{c\sigma}|^2]^{1/2}\} / 2 \quad (2.5)$$

are analyzed in the Stoner approximation, replacing the spin operator $\mathbf{S}_{\mathbf{r}}$ in (1.6) and (2.4) by the mean spin $S_{jT} = \pm S_T$ of a sublattice $j = 1, 2$. The Lionce model (see [5]) of antiparallel spins of neighbouring sites in the approximation of nearest neighbours gives

$$|g_{c\sigma}|^2 = |g|^2 \sqrt{1 - S^2} / 2, \quad \Gamma_{\mathbf{k}\sigma} \approx \Gamma_{\mathbf{k}} (1 - S^2)^{1/2} / 2. \quad (2.6)$$

Therefore, in AFM and paramagnetic phases, the energies of bands have the same form without spin splitting on subbands (in contrast to the ferromagnetic α -Fe).

In the limit of small $k \ll k_{\mathbf{F}}$ ($\tilde{\xi} \approx -\varepsilon_{\mathbf{F}}$), the spectra of CBF and band holes are received

$$E_{\mathbf{k}}^{\pm}(S_T) \approx \begin{cases} \Gamma_{\mathbf{k}\sigma} + |g_{c\sigma}|^2 / \varepsilon_{\mathbf{F}}, & k \ll k_{\mathbf{F}}, \\ \tilde{\xi}_{\mathbf{k}\sigma} - |g_{c\sigma}|^2 / \varepsilon_{\mathbf{F}}, & \end{cases} \quad (2.7)$$

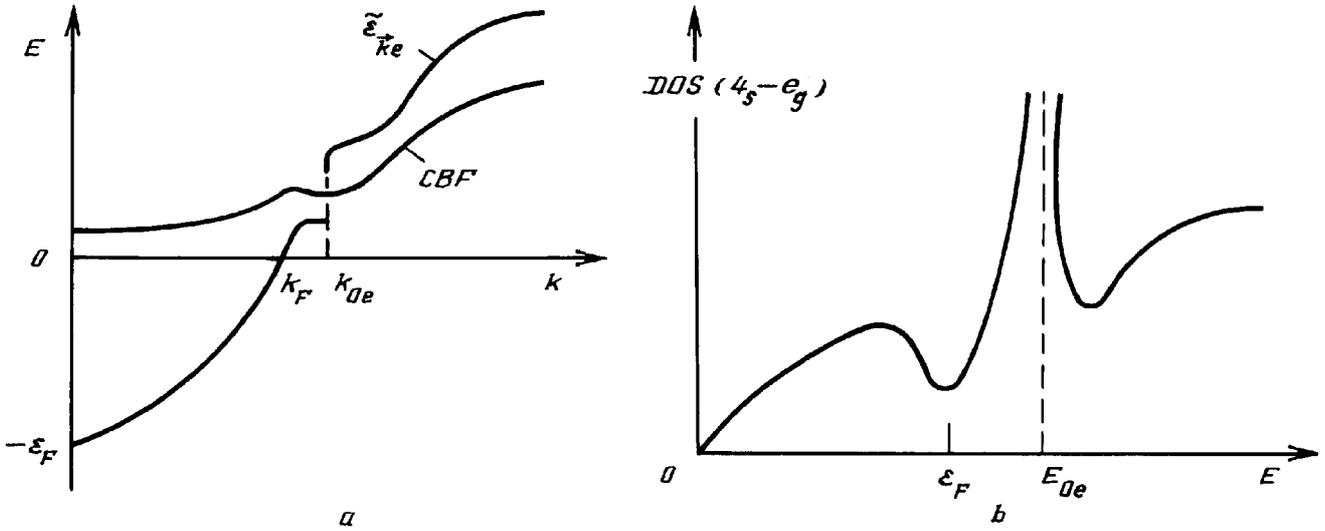


Fig. 1. Dispersion curves of hybridized 4s- and 3d (e_g)-electrons: a - dependence of the energies $E(k)$ of the CBF branch of e_g -electrons and hybridized 4s - 3d (e_g)-band branch ($\tilde{\xi}_{ke}$) on the wave vector \mathbf{k} , b - DOS in 4s - 3d (e_g)-band; k_F - the Fermi momentum of 4s - 3d (e_g)-electrons, $E_{0e}(k_{0e})$ - the singularity of the spectra

and hybridization strengthens here both metal bonds (lowers the band fermions' energy), and covalent ones, entering the activation energy in the CBF spectrum.

However, the part of the spectrum near the Fermi surface is major. For the further analysis, we suppose

$$|\Gamma(0)| \ll \epsilon_F, \quad \tilde{\xi}_{k\sigma} \rightarrow 0 \text{ at } k \rightarrow k_F. \quad (2.8)$$

Near the Fermi surface ($\mathbf{k} = \mathbf{k}_F$), the spectrum

$$E_{\mathbf{k}}^{\pm} \approx \pm |g_{c\sigma}| + (\Gamma_{k\sigma} + \tilde{\xi}_{k\sigma})/2, \quad |k| \rightarrow k_F \quad (2.9)$$

becomes anomalous (Fig. 1,a). Neglecting the weak dependence on spin ($S_T < S = 1/2$) and taking into account covalent bonds of different sites (ensuring $\Gamma_{\mathbf{k}} > 0$), the crossing of band (e_g) and CBF branches above abscissa is received, Fig. 1,a. Band extrema give sharp anomalies of DOS ($4s - e_g$): the antipeak near ϵ_F (its role is analyzed by Irkhin, see [13]) and the peak above the Fermi level, observed experimentally in various Fe alloys, see [15].

3. Collective Bands and CBF of t_{2g} -electrons

The transfer Hamiltonian of t_{2g} -electrons, binary in the Fermi-amplitudes (1.1)

$$H' = - \sum V(|\mathbf{r} - \mathbf{r}'|) a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}'} \quad (3.1)$$

in representation (1.1) - (1.3), without account of the spin σ , looks like

$$H' = H'_0 + \xi_d^2 \sum_{\mathbf{k}} V_{\mathbf{k}} d_{\mathbf{k}} \bar{d}_{\mathbf{k}} + \xi_h^2 \sum_{\mathbf{k}} (V_{\mathbf{k}} - \epsilon_F) h_{\mathbf{k}}^{\dagger} h_{\mathbf{k}} +$$

$$+ \xi_d \xi_h \sum_{\mathbf{k}} (V_{\mathbf{k}} d_{\mathbf{k}} h_{\mathbf{k}} + \text{h.c.}). \quad (3.2)$$

The orthogonality

$$d_{\mathbf{r}} h_{\mathbf{r}} = 0 \quad (3.2')$$

of band and covalent t_{2g} -electrons is supposed. In opposite case, a spectrum as (2.5) is received. Assuming that the t_{2g} -level is lower (in relation to e_g) [5, 13, 14], we consider the hybridization 4s - t_{2g} as the effect of a higher order and here neglect it.

The spectrum branches

$$E_{\mathbf{k}}^{(d,h)} = \{V_{\mathbf{k}} - \epsilon_F \pm [(V_{\mathbf{k}} - \epsilon_F)^2 + 4\xi_d^2 V_{\mathbf{k}} \epsilon_F]^{1/2}\} / 2 \quad (3.3)$$

are crossed (Fig. 2,a). In the limit of small momenta $k \ll k_F$

$$E_{\mathbf{k}}^{(d,h)} \approx \begin{cases} \xi_d^2 V_{\mathbf{k}}, \\ V_{\mathbf{k}} \xi_h^2 - \epsilon_F, \quad k \ll k_F \end{cases} \quad (3.4)$$

there are an upper (positive) CBF branch and a lower branch of band t_{2g} -electrons. Assuming

$$V(\mathbf{k}) = \sum_{\mathbf{r}} V(|\mathbf{r}|) e^{i\mathbf{k}\mathbf{r}} > 0, \quad V_{\mathbf{k}} = V(0) - V(\mathbf{k}) > 0, \quad (3.4')$$

the positive effective mass of band fermions (3.4) is received.

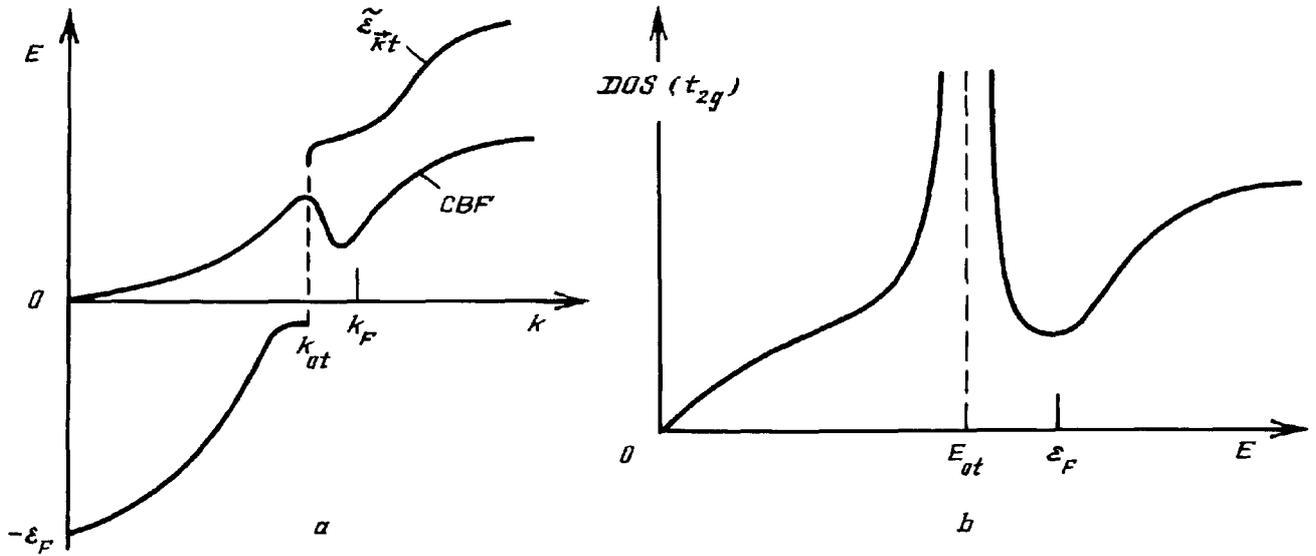


Fig. 2. Dispersion curves of band (ϵ_{kr}) and covalent (CBF) $3d(t_{2g})$ -electrons: a - dependences of the energies $E(k)$ of band $3d(t_{2g})$ -electrons and CBF branch, b - DOS of band $3d(t_{2g})$ -electrons; k_F - the Fermi momentum, $E_{0t}(k_{0t})$ - the singularity of the spectra

Near the Fermi surface, the crossing of d - and h -branches (3.3) are expected. At $V_{\mathbf{k}} \rightarrow \epsilon_F$, dispersion (3.3) becomes anomalous

$$E_{\mathbf{k}}^{(d,h)} \approx \pm |\xi_d| \sqrt{V_{\mathbf{k}} \epsilon_F} + (V_{\mathbf{k}} - \epsilon_F)/2. \quad (3.5)$$

The effective mass changes a sign. DOS of the t_{2g} -band is

$$\text{DOS}(t_{2g}) \sim k_F^2 / (\partial E_{\mathbf{k}}^{(h)} / \partial \mathbf{k}) \approx k_F^2 / (V_0 k \pm D_0) \quad (3.6)$$

on both sides of the Fermi surface, where the square dispersion law $V_{\mathbf{k}}(\mathbf{k})$ is accepted and

$$D_0 \approx |\xi_d| \sqrt{V_0 \epsilon_F}. \quad (3.7)$$

Expression (3.6), fig. 2, b , is similar to DOS of spectrum (2.9), though the singularities (antipeak and peak) (3.6) may be smoothed.

4. The Covalent Bond of Sublattices and AFM Exchange of the Nearest Neighbours

The various symmetry of $3d$ -functions in the fcc lattice of the t_{2g} - and e_g -type allows us to assume a stronger (attractive) bond along edges of the fcc cell (in the second coordination sphere). It corresponds to the bonding covalent interaction $\Gamma(|\vec{\rho}_{jj}^{\rightarrow}|) > 0$ inside the AFM j -sublattice. The interaction between the nearest neighbours $\tilde{\Gamma}(|\vec{\rho}_{12}^{\rightarrow}|) < 0$, belonging to different spin j -sublattices, is considered to be antibonding and weaker

$$0 < -\tilde{\Gamma}(|\vec{\rho}_{12}^{\rightarrow}|) = \Gamma(|\vec{\rho}_{12}^{\rightarrow}|) \ll \Gamma(|\vec{\rho}_{jj}^{\rightarrow}|), \quad j = 1, 2. \quad (4.1)$$

The latter creates direct AFM exchange between sublattices.

The Hamiltonian of the covalent e_g - e_g -bond under condition (1.1) is equal to

$$H_e^{\text{ch}} = - \sum \Gamma(|\vec{\rho}_{jj}^{\rightarrow}|) \hat{D}_{j\mathbf{r}} \hat{D}_{j\mathbf{r}'} + \sum \Gamma(|\vec{\rho}_{12}^{\rightarrow}|) d_{1\mathbf{r}} \bar{d}_{2\mathbf{r}'} [1 + (\mathbf{S}_{1\mathbf{r}} \mathbf{S}_{2\mathbf{r}'})/4],$$

$$\mathbf{r}' = \mathbf{r} + \vec{\rho}, \quad \hat{D}_{j\mathbf{r}} \hat{D}_{j\mathbf{r}'} = d_{j\mathbf{r}} \bar{d}_{j\mathbf{r}'} [1 + (\mathbf{S}_{j\mathbf{r}} \mathbf{S}_{j\mathbf{r}'})/4]/2, \quad (4.2)$$

according to (1.6). The spin part (4.2), even in the AFM phase, gives a small renormalization of covalent constants ($\sim \mathbf{S}_{j\mathbf{r}}^2/4 \leq 0,06$) of γ -Fe and is not taken into account in the calculation of electronic spectra ($S = 1/2$) in Sections 2, 3. The last term (4.2) also influences weakly the CBF dispersion. However, its influence on a spin configuration is decisive.

Direct d - d -exchange inside and between sublattices is selected from (4.2) as

$$H^{\text{ex}} = - \sum A_{jj} (|\vec{\rho}_{jj}^{\rightarrow}|) \mathbf{S}_{j\mathbf{r}} \mathbf{S}_{j\mathbf{r}'} + \sum A_{12} (|\vec{\rho}_{12}^{\rightarrow}|) \mathbf{S}_{1\mathbf{r}} \mathbf{S}_{2\mathbf{r}'}. \quad (4.3)$$

The exchange parameters

$$A_{jj} \approx \Gamma(|\vec{\rho}_{jj}^{\rightarrow}|) \langle d_{j\mathbf{r}} \bar{d}_{j\mathbf{r}'} \rangle / 4 \gg A_{12} = \Gamma(|\vec{\rho}_{12}^{\rightarrow}|) \langle d_{1\mathbf{r}} \bar{d}_{2\mathbf{r}'} \rangle / 4 \quad (4.4)$$

are expressed through covalent ones ($\hat{\Gamma}$) and depend on temperature T , as they contain CBF correlators. Not stopping on a specific AFM spin configuration, which the form of a γ -Fe particle or a film can influence, we shall note the influence of this form on the value $\Gamma(|\vec{\rho}_{ij}^z|)$. In contrast to the direct short-range interaction $\Gamma(|\vec{\rho}_{12}^z|)$, the exchange parameter $\Gamma(|\vec{\rho}_{ij}^z|)$ should strongly depend on nonideality of atomic configurations of next neighbours. Except strong deformations of a film or a nanoparticle of γ -Fe in a Cu-matrix (for example), it is necessary to take into account a probable rough defectivity of their surface. Thus, our theory can explain the observable experimental difference of T_N [12]. The dominant value of intrasublattice exchange is responsible for it (in agreement with (4.4) and (4.1)), which strongly depends on nonideality of a lattice.

5. γ -Fe Stability. Discussion of Results and Conclusions

The CBF excitation and occurrence of CBF soft modes destabilize covalent bonds and lower the stability of a lattice. The occurrence of a CBF soft mode is possible as a result of the crossing of CBF branches with band branches of electrons (holes). This crossing is the most probable near the Fermi surfaces, see Fig. 1, 2. Anomalies of the electron DOS near the Fermi surface are indicators of the effect (Fig. 1,*b* and 2,*b*). The closer the DOS peak to the Fermi level, the more probable is the occurrence of the CBF soft mode. In the case of γ -Fe, the analysis of solution (2.7) and (2.9) for the low (e_g) CBF branch does not find out an appreciable softening. In addition, the activation energy of the CBF branch in (2.7) appreciably stabilizes the Fe fcc phase concerning to a growth in T .

On the contrary, at T lowering, the antibonding part of the covalent (e_g) energy in (4.2) begins to play a role. It is responsible for the AFM order of the nearest neighbours, but also for instability of the fcc phase at T lowering relative to the γ - α -transition. The

bonding covalent energy of nearest neighbours of the bcc α -Fe lattice (responsible for ferromagnetism [16]) favours this transition).

Specific conclusions of the theory:

1. Covalent electrons of the high e_g -level in an fcc lattice hybridize with band $4s$ -electrons. Repulsion of fermion branches (CBF and band $4s$ -branch) in the vicinity of the center of the Brillouin zone ($k < k_F$) creates the CBF activation energy. It stabilizes an fcc lattice at heating.

2. The crossing of branches of CBF and $4s$ -band causes DOS anomalies near the Fermi surfaces.

3. Electrons of the low t_{2g} -level are partially delocalized, forming the $3d$ -band. The rest participate in covalent bonds, forming the second CBF branch. The crossing of this CBF branch with the $3d$ -band branch is responsible for appreciable DOS anomalies of band fermions both below (antipeak) and above (peak) the Fermi level because of the strong interaction. In such a way, our theory explains the observable DOS singularities near Fermi surfaces.

4. External pressure can strengthen these anomalies, favouring the occurrence of the CBF soft mode and destabilization of the fcc phase.

5. The strong Coulomb (Hubbard) repulsion of t_{2g} -electrons prevents their spontaneous local polarization. The domination of the Hund exchange of e_g -electrons favours the formation of local spin $S = 1/2$. The covalent nature of the weak antibonding interaction of e_g -electrons of the nearest neighbours results to the AFM bond of their spins $S_{j\mathbf{r}}$, belonging to different sublattices j .

6. The antibonding covalent (AFM) interaction of the nearest neighbours of the fcc lattice favours the occurrence of its instability relative to the γ - α -transition at T lowering ($T < T_0$). The strong bonding covalent (FM) interaction of the nearest neighbours of the Fe bcc lattice makes it stable at low temperatures $T < T_0$.