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The BCC-FCC Structural Phase Transition in Semimetal Systems

Nguyen The Lam*

Faculty of Physics, Hanoi Pedagogical University No.2, Vinh Phuc, Vietnam

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Abstract: It will show that, the second structural phase transition (BCC-FCC) may be took place in the semimetals cause of extra condition as temperature or doping… The first structural phase transition occurs is due to nesting vector Q = π. The free energy of system in some crystal structures are depended on temperature and doping. In this case, the temperatiure or doping is increased, the free energy of system in this crystal structure is lower than itself in other crystal structure. So the second structural phase transition may be occurred.

Keyword: BBC-FCC transition, structure phase transaction.

1. Introduction

In some semimetals, these are structural transition more once, for example, Iron in temperature increase higher than 911^0C, these is the first phase transition from BCC to FCC, then when temperature is higher 1392^0C, the second phase transition takes place again form FCC to BCC [1]. The alloys of Iron, these are many phase transition take place when doing density increases. Investigation of electronic structure of Iron, we see that, these is overlap between conduction band (level *s*) and valence band (level *d*). The Fermi face is also indicates that level 3*d* is not occupied completely (holes), while in the level 4s these are electrons [2]. From investigation of electronic band of Iron, we may consider Iron as a semimetal.

In semimetal systems, when nesting vector Q = π [3], these is the dielectric gap Δ in energy band , this may accompany the charge density wave (CDW) and the first structural phase transition take place. The gap Δ maximum corresponds to energy of system is minimum. When temperature or doping increases, the system is not stable. It makes the gap Δ decrease and energy of system increases. The decreasing of Δ in the different crystals are not the same. This may lead to the second structural phase transition occur. Our study started with after the first structural phase transition, the crystal of system is BCC or FCC. When the temperature or doping increasing, both gaps Δ for the BCC and FCC are decreasing. At first the gap of this crystal higher (lower) than the other but then it is lower (higher) than the other. So the FCC – BCC structure phase may be occurred.

* Tel.: 84- 989387131
Email: nguyenthelam@yahoo.com

In the semimetal the energy spectrum may be written in form:

$$\varepsilon_1(\vec{k}) = \delta\mu + \varepsilon(\vec{k}) \quad (1)$$

$$\varepsilon_2(\vec{k}) = \delta\mu + \varepsilon(\vec{k} + \vec{Q}) \quad (2)$$

where $\delta\mu$ is the shift of Fermi level, $\vec{Q}$ is nesting vector

In the tight-building approximation, we received the energy spectrum for BCC

$$\varepsilon(\vec{k}) = -\alpha - 8\gamma \cos\frac{1}{2}k_x a \cos\frac{1}{2}k_y a \cos\frac{1}{2}k_z a \quad (3)$$

and for FCC

$$\varepsilon(\vec{k}) = -\alpha - 4\gamma\left[\cos\frac{1}{2}k_y a \cos\frac{1}{2}k_z a + \cos\frac{1}{2}k_z a \cos\frac{1}{2}k_x a + \cos\frac{1}{2}k_x a \cos\frac{1}{2}k_y a\right] \quad (4)$$

where α is ground energy, γ is the width of energy band and a is lattice spacing.

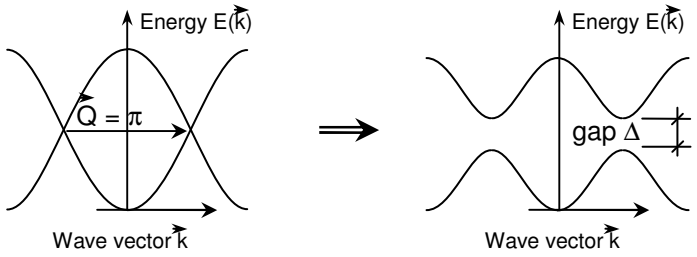

Fig 1. The first structural phase transition in semimetal system.

2. Basic equations

Following [3] the Hamiltonian for semimetal system have form

$$H = \sum_{\vec{k}\sigma i} \varepsilon(\vec{k}) a_\delta^+(\vec{k}) a_\sigma(\vec{k}) + \sum_{\vec{q}} \omega_{\vec{q}} (b_{\vec{q}}^+ b_{-\vec{q}} + \frac{1}{2})$$
$$+ \frac{1}{2} \sum_{\sigma 1 \sigma 2 \vec{k} p 1 \vec{k} 2 \vec{q}} \lambda a_{\sigma 1}^+(\vec{k}_1 + \vec{q}) a_{\sigma 2}^+(\vec{k}_2 - \vec{q}) a_{\sigma 2}(\vec{k}_2) a_{\sigma 1}(\vec{k}_1) + \sum_{\vec{k},\vec{q},\sigma} g(b_{\vec{q}}^+ + b_{-\vec{q}}) a_\sigma^+(\vec{k}) a_\sigma(\vec{k} + \vec{q}) \quad (5)$$

Where a and a^+ are annihilation and creation electron operators respectively with spin σ, b and b^+ are annihilation and creation phonon operators respectively, ω is phonon frequency, λ is screen Coulomb interaction, g is electron – phonon interaction and i, j are band index

The Green functions are defined

$$G_1(\vec{k}, t) = < T(a^+(\vec{k}, t) a(\vec{k}, 0)) >$$
$$G_2(\vec{k}, \vec{Q}, t) = < T(a^+(\vec{k} - \frac{\vec{Q}}{2}, t) a(\vec{k} + \frac{\vec{Q}}{2}, 0)) > \quad (6)$$

Where $G_1(\vec{k},\omega)$ is Green function for exciton pairs with the same orientation of spin for both electrons and holes. It may lead to the appearance of CDW and structural phase transition. Where $G_2(\vec{k},\omega)$ is Green function for exciton pairs with different orientation of spin for electron and holes.

By Green function method, combine Hamiltonian (5) with the definitions (6), in the self-consistent field approximation. We have

$$\begin{aligned}&[-i\omega_n+\varepsilon_1(\vec{k})G_1(\vec{k},\omega_n)+\Delta G_2(\vec{k},\omega_n)]=1\\&\Delta^* G_1(\vec{k},\omega_n)+[-i\omega_n+\varepsilon_2(\vec{k})]G_2(\vec{k},\omega_n)=0\end{aligned} \quad (7)$$

where, $G_1(\vec{k},\omega)$, $G_2(\vec{k},\omega)$ are Fourier transform coefficients of $G_1(\vec{k},t)$, $G_2(\vec{k},t)$ respectively. The gap Δ is defined

$$\Delta = T\sum_{\vec{k},\omega}\lambda_1 G_2(\vec{k},\omega) \quad (8)$$

and $\omega_n=(2n_0+1)\pi T$ with n_0 are integers and T is temperature.

The difference of electron and hole density is defined as doping. This is due to the displacement of Fermi level.

$$n=-\frac{1}{2}\sum_{k,\omega}[G_2(\vec{k},\omega)-G_1(\vec{k},\omega)] \quad (9)$$

Solving the system of equations (7) for $G_1(\vec{k},\omega)$, $G_2(\vec{k},\omega)$. Substituting $G_1(\vec{k},\omega)$, $G_2(\vec{k},\omega)$ into (8) and (9), we get the equations for dielectric gap and doping

$$1=\lambda_0\sum_{\vec{k}}\frac{1}{4E}\left[th\frac{E+\delta\mu}{2T}+th\frac{E-\delta\mu}{2T}\right] \quad (10)$$

$$n=-\frac{1}{2}\sum_{\vec{k}}\left[th\frac{E+\delta\mu}{2T}-th\frac{E-\delta\mu}{2T}\right] \quad (11)$$

Where n is carrier density, and is the difference between electron and hole. The excitation spectrum of one particle is given

$$\omega_{\pm\sigma}(\vec{k})=\delta\mu\pm E(\vec{k}) \quad (12)$$

With $E(\vec{k})=[\varepsilon^2(\vec{k})+\Delta^2]^{\frac{1}{2}}$ with $\varepsilon(\vec{k})$ is given in equations (3) and (4), $\lambda_0=\lambda+\frac{4|g|^2}{\omega_o}$ where ω_0 is the cut-off phonon frequency and g is electron-phonon constant.

3. Numerrical results and disussion

Solving equation (10) numerically with the energy spectrums (3) and (4) respectively, we obtain the dependence of energy gaps for FCC and BCC on temperature (fig.1). In figure 2, Both of curves are decreasing when the temperature increasing. At arbitrary temperature T_0, two curves crossed each other.

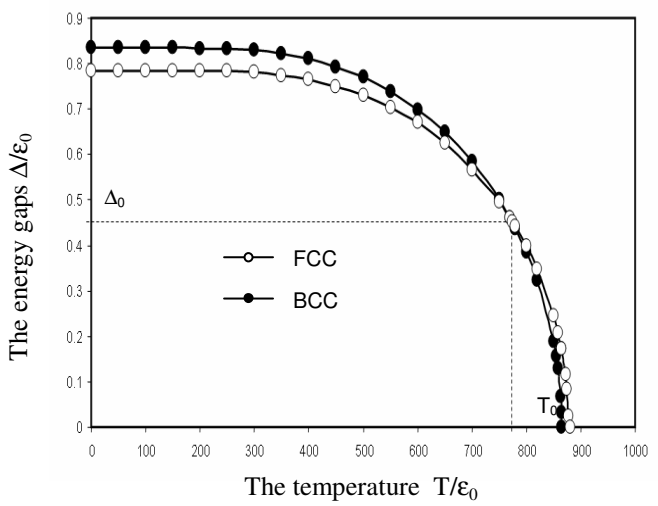

Fig. 2. The dependence of energy gaps FCC and BCC on Temperature. For both FCC and BCC With $\lambda = 0.0045$. Where the open circles for FCC and the solid circles for BCC. The parameters in unit of ε_0, it is the width of conduction band.

When temperature $T < T_0$, the energy gap of BCC (Δ_{BCC}) is greater than the energy gap of FCC (Δ_{FCC}). This means free energy of system in BCC structure is smaller than the free energy of system in FCC structure, so system will in BCC structure. When temperature $T > T_0$, the energy gap of BCC (Δ_{BCC}) is smaller than the energy gap of FCC (Δ_{FCC}). This also means free energy of system in BCC structure is greater than the free energy of system in FCC structure, so system will in FCC structure. So, when the temperature increasing $T > T_0$, the second structure phase transition occurs from BCC to FCC.

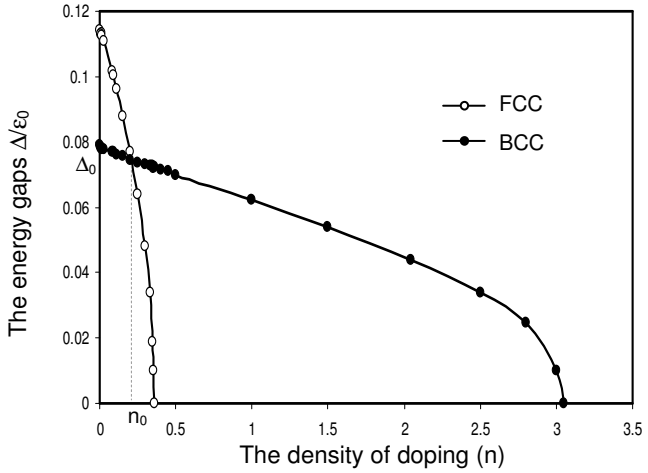

Fig. 3. The dependence of energy gaps FCC and BCC on doping. For FCC and BCC With $\lambda_{BCC} = 0.0072$ and $\lambda_{FCC} = 0.024$ respectively. Where the open circles for FCC and the solid circles for BCC. The energy gap in unit of ε_0, it is the width of conduction band.

Combination equation (10) and (11) we have system of equation, it describes the dependence of the dielectric gap on the temperature and doping. For investigation of doping, we solving numerically system equation (10) and (11) at T = 0K with energy spectrums (3) and (4) respectively. The dependence of energy gaps on the doping are shown in figure 3. From figure 3 we see that, When density of doping $n < n_0$, the energy gap of FCC (Δ_{BCC}) is greater than the energy gap of BCC (Δ_{FCC}). This means free energy of system in FCC structure is smaller than the free energy of system in BCC structure, so system will in FCC structure.

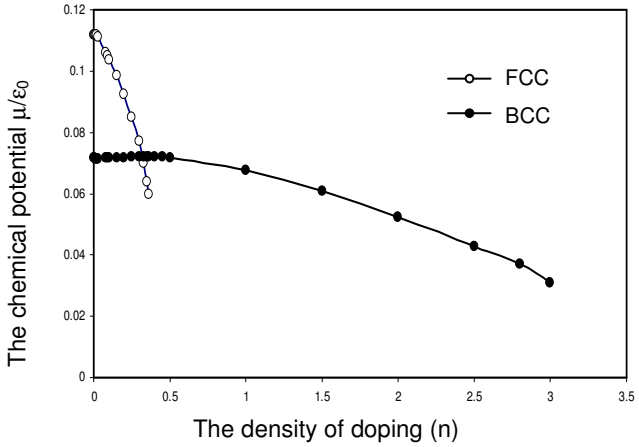

Fig. 4**.** The dependence of chemical potential of FCC and BCC on doping. For FCC and BCC With λ_{BCC} = 0.0072 and λ_{FCC} = 0.024 respectively. Where the open circles for FCC and the solid circles for BCC. The chemical potential in unit of ε_0, it is the width of conduction band.

When density of doping $n > n_0$, the energy gap of FCC (Δ_{BCC}) is smaller than the energy gap of BCC (Δ_{FCC}). This also means free energy of system in FCC structure is greater than the free energy of system in BCC structure, so system will in BCC structure. So, when the density of doping increasing $n > n_0$, the second structure phase transition occurs from FCC to BCC. The dependence of chemical potential on doping is also shown in figure 4.

4. Conclusion

In this paper, we have shown that, the second structural phase transition between BCC and FCC may be taken place in our model. The structural phase transition may be occurred is due to temperature or doping. The experiments also shows that, The are two structural phase transition from BBC to FCC at 911^0C and from FCC to BCC at 1392^0C [1]. In other way, from phase diagram of Fe-C alloy also has shown that, the critical temperature for transition is defended strongly on Carbon density. Some researches [4, 5] in other methods also have a good agreement with us.

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