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# The Structural Phase Transition of The Cubic to Tetragonal Superconductor Due to A Two-Fold Degenerate Electronic Band

W.Y.Chen( 陳惟堯 )
*Physics Department, Tamkang University, Taiwan*
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In this paper we report that there exists a structural phase transition between cubic and tetragonal superconductors. Calculation of the transition temperature $T_M$ is performed with a half-filled doubly degenerate $e_g$-band using BCS mean field theory. It is found that the transition temperature $T_M$ between the two superconductors reduces to that of the ordinary structural phase transition if the energy gap A is zero.

## 1. INTRODUCTION

It is well known that many intermetallic compounds exhibits a structural phase transition of the martansitic type from the cubic to tetragonal phase at a temperature $T_M$[1-8]. The principal mechanism of this structural transition is known to be the coupling between the degenerate d electrons and the tetragonal strain mode. It is very interesting that all these compounds also show a superconducting transition at a lower temperature. Ghatak[10] et al and others[9] studied the effect of the superconductivity on the structural transition for a half filled two-fold degenerate band. Chen[11] examined the effects of different fillings of the two-fold degenerate eg-band on $T_c$ and $T_M$. Chen and Lo[12] considered the case where the Fermi energy passes through the three-fold degenerate $T_{2g}$-band and investigated the effect of cubic to tetragonal transformation in intermetallic compounds on superconductivity. However, the structural phase transition of the cubic to tetragonal superconductors has not been discussed. In this paper we examine this, problem for a half-filled doubly degenerate eg-band using the BCS mean field theory.

## II. MATHEMATICAL DESCRIPTION OF THE MODEL

The total Hamiltonian of the system is given as:

$$H = H_e + H_{int} + H_s + H_{BCS} \tag{1}$$

The Hamiltonian for the non-interacting d electrons is"

$$H_e = \sum_{\ell k \sigma} \epsilon_{\ell k \sigma} N_{\ell k \sigma} \tag{2}$$

where

$$N_{\ell k \sigma} = C^{+}_{\ell k \sigma} C_{\ell k \sigma}$$

$C^{+}_{\ell k \sigma}, C_{\ell k \sigma}$ are the creation and annihilation operators for the electrons in the $\ell^{Th}$ band of energy $\epsilon_{\ell k_\sigma}$ momentum k and spin $\sigma$. The usual Fermi commutation relations give

$$\left\{ C^{+}_{\ell k \sigma}, C_{\ell' k' \sigma'} \right\} = \delta_{\ell \ell'} \delta_{kk'} \delta_{\sigma \sigma'} \tag{3}$$

$H_{int}$ represents the coupling between the d electrons and the static elastic strains"

$$H_{int} = \sum_{\substack{\ell m ij \\ k\sigma}} G_{ij\ \ell m}\ e_{ij} C^{+}_{\ell k \sigma} C_{m k \sigma} \tag{4}$$

where $e_{ij}$ is ' the static strain tensor and $G_{ij\,\ell m}$ is the coupling constant. This interaction lifts the degeneracy of the eg-band

$$\begin{aligned} \epsilon_{1k} &= \epsilon_k + \delta \\ \epsilon_{2k} &= \epsilon_k - \delta \end{aligned} \tag{5}$$

where

$$\delta = Ge, \quad G = \frac{1}{2}(G_{12} - G_{11}) \ \text{and} \ e = \langle e_{33} \rangle$$

is the tetragonal strain.

The elastic energy for the tetragonal strain is proportional to $e^2$ and is given by[11]

$$H_s = \frac{3}{4} ce^2 \tag{6}$$

where $C = C^0_{11} - C^0_{12}$ is the cubic phase elastic constant.

The phonon-mediated electron-electron interaction Hamiltonian leading to the superconductivity is given by

$$H_{BCS} = -\sum_{kk'\ell m} V_{\ell mkk'} C^{+}_{\ell k\downarrow} C^{+}_{\ell -k\uparrow} C_{m-k'\downarrow} C_{mk'\uparrow} \tag{7}$$

where $V_{\ell mkk'}$ is the coupling constant.

Let us assume

$$< V_{Pmkk'} >= \begin{cases} V_B & \text{for } |\epsilon| \leqslant \hbar\omega_0 \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

where $\omega_0$ is of the order of the Debye frequency.

Using the BCS mean field approximation, we obtain the following equations for the energy gap and the tetragonal strain.

$$\frac{V_B}{2}\int_{-\hbar\omega_0}^{\hbar\omega_0} [\frac{1-2f_1(\epsilon)}{E_1(\epsilon)} + \frac{1-2f_2(\epsilon)}{E_2(\epsilon)}] \rho(\epsilon)\, de = 1 \tag{9}$$

$$e = \frac{4G}{3C} [\int_{-B}^{B} (\frac{1}{1+e^{\epsilon_2\beta}} - \frac{1}{1+e^{\epsilon_1\beta}}) \rho(\epsilon)\, d\epsilon$$

$$+ \int_{-\hbar\omega_0}^{\hbar\omega_0} [\frac{\epsilon_1}{2E_1(\epsilon)} (1-2f_1(\epsilon)) - \frac{\epsilon_2}{2E_2(\epsilon)} (1-2f_2(\epsilon)) + \frac{-1}{1+e^{\epsilon_2\beta}}$$

$$+ \frac{1}{1+e^{\epsilon_1\beta}}] \rho(\epsilon)\, d\epsilon \tag{10}$$

where

$$\begin{aligned} E_1(\epsilon) &= \sqrt{\epsilon_1^2 + \Delta^2} \\ E_2(\epsilon) &= \sqrt{\epsilon_2^2 + \Delta^2} \\ f_1(e) &= \frac{1}{1+e^{\beta E_1(\epsilon)}} \\ f_2(\epsilon) &= \frac{1}{1+e^{\beta E_2(\epsilon)}} \end{aligned} \tag{11}$$

and

$$\Delta_k = A , \qquad \epsilon_1 = \epsilon + \delta , \qquad \epsilon_2 = \epsilon - \delta$$

B is the band width and $\rho(\epsilon)$ is the state density. The free energy for the tetragonal superconductor is given by

$$F_t = \int_{-\hbar\omega_0}^{\hbar\omega_0} \rho(\epsilon)\, [2\epsilon - \frac{\epsilon_1^2}{E_1(\epsilon)}(1 - 2f_1(\epsilon)) - \frac{\epsilon_2^2}{E_2(\epsilon)}(1 - 2f_2(\epsilon))]\, de$$

$$+ \frac{-1}{4}\int_{-\hbar\omega_0}^{\hbar\omega_0}\int_{-\hbar\omega_0}^{\hbar\omega_0} V_B\, [\frac{\Delta^2}{E_1(\epsilon)E_1(\epsilon')}(1 - 2f_1(\epsilon))(1 - 2f_1(\epsilon'))$$

$$+ \frac{\Delta^2}{E_2(\epsilon)E_2(\epsilon')}(1 - 2f_2(\epsilon))(1 - 2f_2(\epsilon'))$$

$$+ 2\frac{\Delta^2}{E_1(\epsilon)E_2(\epsilon')}(1 - 2f_1(\epsilon))(1 - 2f_2(\epsilon'))\rho(\epsilon)\rho(\epsilon')d\epsilon d\epsilon'$$

$$+ \frac{2}{\beta}\int_{-\hbar\omega_0}^{\hbar\omega_0}\sum_{i=1}^{2} [f_i(\epsilon)\ln f_i(\epsilon) + (1 - f_i(\epsilon))\ln(1 - f_i(\epsilon)) + \ln(1 + e^{-\epsilon_i\beta})]\,\rho(\epsilon)d\epsilon$$

$$- \frac{2}{\beta}\int_{-B}^{B} [\ln(1 + e^{\epsilon_2\beta}) + \ln(1 + e^{-\epsilon_1\beta})]\,\rho(\epsilon)d\epsilon + \frac{3}{4}c\,e^2 \tag{12}$$

where we have assumed that the Fermi energy is zero.

The structural phase transition between the cubic superconducting phase and the tetragonal superconducting phase can be obtained as follows.

Let

$$\Delta F = F_t - F_c \tag{13}$$

where $\Delta F$ is the difference between the free energies of the cubic and tetragonal superconducting phases in the limit as $e \to 0$. The transition temperature $T_M$ is determined by[10]

$$\left.\frac{\partial^2 \Delta F}{\partial e^2}\right|_{e=0} = \left.\frac{\partial^2 F_t}{\partial e^2}\right|_{e=0} = 0 \tag{14}$$

From equation (14), we obtain

$$-J\,[2\int_{-B}^{B}\rho(\epsilon)\frac{dF}{d\epsilon} - \int_{-\hbar\omega_0}^{\hbar\omega_0}\rho(\epsilon)\frac{d}{d\epsilon}[\frac{\epsilon}{E(\epsilon)}(1 - 2f(\epsilon)) + 2F(\epsilon)]\,d\epsilon = 1 \tag{15}$$

where

$$F(\epsilon) = \frac{1}{1 + e^{\beta\epsilon}}, \quad E(\epsilon) = \sqrt{\epsilon^2 + \Delta^2}$$

and

$$J = \frac{4}{3}\frac{G^2}{c}$$

Equation (15) implies that the structural phase transition in the absence of a superconductor is

$$-J\int_{-B}^{B} 2\rho(\epsilon)\frac{dF}{d\epsilon}\, d\epsilon = 1 \qquad (16)$$

Under the approximation that $B >> kT_M$ we obtain

$$k_B T_M \; \frac{0}{\pi} \,\bar{-}\, (1 - \frac{1}{J_1})^{1/2}\, \eta \qquad (17)$$

where

$$J_1 = J\rho_t(o),\ \rho_t(o) = 2\rho(o)$$

and

$$\eta = [\frac{\rho'(o)^2}{\rho(o)^2} - \frac{\rho''(o)}{\rho(o)}]^{-1/2}$$

which agrees with the result obtained by Ghatak[10] et al ( as it should). In the presence of superconductivity, namely $T_C > T_M$, equation (15) can be rewritten approximately as

$$k_B T_M = \frac{\sqrt{6}}{\pi}\,(\frac{J_1 - 1}{J_1} - \frac{\Delta^2}{2(\hbar\omega_0)^2})^{1/2}\, \eta \qquad (18)$$

To proceed, let us assume that the state density has the following form

$$\rho(\epsilon) = \frac{4}{\pi B}\,(1 - (\frac{\epsilon}{B})^2)^{1/2}$$

For weak coupling namely $K_B T_M << B$ and $K_B T_C << \hbar\omega_0$, if

$$\ln \chi_0 + \frac{\pi B}{4V_B} > 0$$

where

$$\chi_0 = \frac{B}{\hbar\omega_0}\,(\frac{J_1 - 1}{J_1})^{1/2}\,\frac{\sqrt{6}}{1.14\pi} \,.$$

a martensitic transition occurs first at $T_M$

$$K_B T_M = \frac{B\sqrt{6}}{\pi}\,(\frac{J_1 - 1}{J_1})^{1/2} \qquad (19)$$

On the other hand. if

$$\ln \chi_0 + \frac{\pi B}{4V_B} < 0 \quad ,$$

the superconductor occurs first at $T_c$

$$K_B T_c = 1.14\,\hbar\omega_0 \exp(-\frac{\pi B}{4V_B}) \quad . \tag{20}$$

Therefore the structural transition between the cubic and tetragonal phases occurs at the lower temperature $T_M$ given by

$$K_B T_M = \frac{\sqrt{6}}{\pi}\left(\frac{J_1 - 1}{J_1} - \frac{}{2(\hbar\omega_0)^2}\right)^{1/2} B \tag{21}$$

## III. CONCLUSION

In this paper we have shown for the first time that if $\ln\chi_0 + \frac{\pi B}{4V_B} < 0$, the superconductivity occurs first at $T_C$ and the structural transition occurs at the lower temperature $T_M$. We have demonstrated the results by performing the calculation for a special form of state density explicitly. Therefore, the statement that there is no structural transition if the superconductivity occurs first was not true". In our calculation we neglect the effect of phonon softening due to the electron-phonon interaction. It will be very interesting to extend our calculation to include the phonon softening effect, in order to have a better understanding of these A-l 5 compounds.

## IV. REFERENCES


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