A two-band electron-phonon model for superconductivity in graphite intercalation compounds

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A two-band electron-phonon model for superconductivity in graphite intercalation compounds has been developed. The new mechanism for the relaxation times for a superconductor with two-component order parameter caused by interband scattering of intraband pairs are proposed. The two distinct relaxation times $\tau_{1,2}$ of order parameters are predicted for C_6K and C_8K.

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Intercalation under high pressure, up to 50 kbar, has been used to synthesize alkali-metal graphite intercalation compounds (GIC's), such as C_6K, C_3K, C_4Na, C_3Na, C_2Na, and C_2Li with a relatively high metal concentration. It has been established that T_c increases with the metal concentration and reaches 5 K for C_2Na. Explaining superconductivity in alkali-metal GIC's it is important to take into account the nature of the electronic bands in these compounds. An alkali metal in GIC's acts as a donor and hence there is a charge transfer from the intercalate layer to host carbon layers, resulting in partially filled overlapping intercalate s-band and graphite π-bands. The fractional part of this electron transfer per intercalant atom, f, plays an important role in the electronic properties of GIC's.

A few years ago Jishi [1] proposed a two-band model for superconductivity in C_8K to explain experimental data available at that time. It was shown that superconductivity is caused by the electron-phonon interaction between s-band and π-band. In this report, we develop further the interband electron-phonon model of superconductivity [2,3]. The superconducting transition temperature equals

$$k_B T_c = 1.14\hbar\omega_D \exp\left\{\frac{-1}{|W|\sqrt{\rho_s \rho_\pi}}\right\}, \qquad (1)$$

where ρ_s and ρ_π are the densities of states at the Fermi surface for the s-band and π-band, ω_D is the Debye frequency, W is the effective interband electron-phonon interaction. In case the values of f for C_4Na, C_3Na and C_2Na are equal to 0.615, 0.60 and 0.54, respectively (in C_8K $f \approx 0.6$), $\rho = \sqrt{\rho_\sigma \rho_\pi}$ will have the values 1.067 and 1.16 G for C_3Na and C_2Na, respectively (G is the effective density of states at E_F for C_4Na). Choosing the Debye temperature $\Theta_D \approx 300$ K and using the experimental value of $T_c = 2.8$ K for C_4Na, we obtain $|W|G \approx 0.208$. Supposing that the values of $|W|$ are the same for C_xNa ($x = 2, 3, 4$), the transition temperature T_c equals to 5.4 K for C_2Na and 3.7 for C_3Na in good agreement with the experimental values 5, 3.5 and 2.8 K for C_2Na, C_3Na and C_4Na.

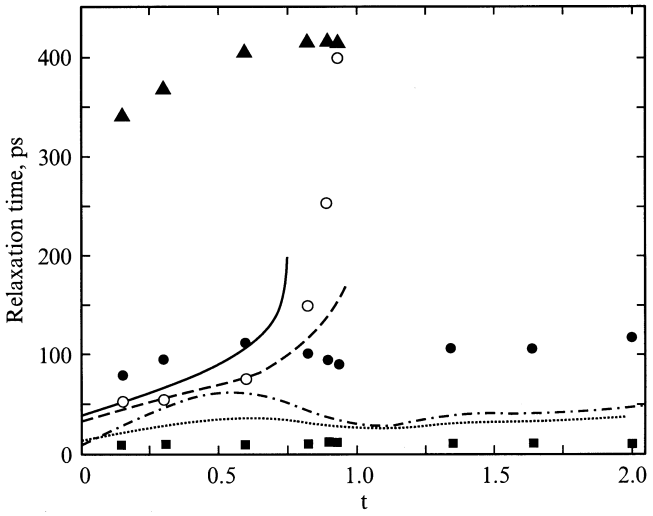
We have also derived the time-dependent Ginzburg–Landau (GL) equations and obtained the relaxation times $\tau_{1,2}$ for the order parameters (gaps)

$$\frac{1}{\tau_{1,2}(\mathbf{k})} = \frac{1}{2}\left(\frac{r_s + \gamma_s'^2 k^2}{\gamma_s} + \frac{r_\pi + \gamma_\pi'^2 k^2}{\gamma_\pi}\right) \mp \left[\frac{1}{4}\left(\frac{r_s + \gamma_s'^2 k^2}{\gamma_s} - \frac{r_\pi + \gamma_\pi'^2 k^2}{\gamma_\pi}\right) + \frac{R_s R_\pi}{\gamma_s \gamma_\pi}\right]^{1/2}, \qquad (2)$$

$$\gamma_s'^2 = \frac{\hbar\beta_1}{4m_s\eta_s(0,T)}, \quad \gamma_\pi'^2 = \frac{\hbar\beta_3}{4m_\pi\eta_\pi(0,T)},$$

$$\gamma_{s,\pi} = 4m_{s,\pi}\gamma_{s,\pi}'^2, \qquad (3)$$

$$\eta_{s,\pi}(0,T) = \sum_{\mathbf{k}} \frac{\tanh(\tilde{\varepsilon}_{s,\pi}(\mathbf{k})/2k_BT)}{\tilde{\varepsilon}_{s,\pi}(\mathbf{k})}, \qquad (4)$$



The temperature dependences of the relaxation times: τ_1, C_8K, $k = 0$ (solid line); τ_1, C_8K, $k = 1 \cdot 10^{-10}\,\mathrm{m}^{-1}$ (dashed line); τ_2, C_8K, $k = 0$ (dashed-dotted line); τ_2, C_8K, $k = 1 \cdot 10^{-10}\,\mathrm{m}^{-1}$ (dotted line); $\tau_1 \cdot 10^{-2}$, C_6K, $k = 0$ (open circles); τ_1, C_6K, $k = 1 \cdot 10^{-10}\,\mathrm{m}^{-1}$ (solid triangles); τ_2, C_6K, $k = 0$ (solid squares); $\tau_2 \cdot 10^{-1}$, C_6K, $k = 1 \cdot 10^{-10}\,\mathrm{m}^{-1}$ (solid circles).

where $\tilde{\varepsilon}_{s,\pi}$ are the electronic spectra,

$$\beta_1 = \frac{7\xi(3)\rho_s p_{sF}^2}{12 m_s \pi^2 k_B^2 T_c^2}\chi_{s0}, \quad \beta_3 = \frac{7\xi(3)\rho_\pi p_{\pi F}^2}{12 m_\pi \pi^2 k_B^2 T_c^2}\chi_{\pi 0},$$

$$\chi_{\sigma 0} = \frac{8}{7\xi(3)} \sum_{n=0}^{\infty} (2n+1)^{-2} \left(2n + 1 + \frac{\xi_{\sigma 0}}{l_\sigma}\right)^{-1},$$

$$\xi_{\sigma 0} = \frac{v_{\sigma F}\hbar}{2\pi k_B T_c},$$

$r_{s,\pi}$ and $R_{s,\pi}$ are the linearization coefficients of GL equations in the two-band model [2], the quantities l_σ are the $\sigma = s, \pi$ electron mean free paths, $v_{\sigma F}$ and $p_{\sigma F}$ are the Fermi velocities and momenta, respectively, k is the wave vector in spatial inhomogeneous case (in gradient term of GL equation), $\xi(3) = 1.202$. $\chi_{\sigma 0}$ takes into account the intraband impurity s-wave scattering of electrons. We obtain the following values of parameters for C_8K: $T_c = 0.134\,\mathrm{K}$, $l_s = 400\,\text{Å}$, $l_\pi = 5030\,\text{Å}$, $\xi_{s0} = 4.6 \cdot 10^4\,\text{Å}$, $\xi_{\pi 0} = 8 \cdot 10^4\,\text{Å}$, $m_s = 1.615 m_0$, $m_\pi = 0.25 m_0$. For C_6K, we obtain $T_c = 1.5\,\mathrm{K}$, $l_s = 340\,\text{Å}$, $l_\pi = 560\,\text{Å}$, $\xi_{s0} = 4000\,\text{Å}$, $\xi_{\pi 0} = 7000\,\text{Å}$, $m_s = m_0$, $m_\pi = 0.25 m_0$. The calculated relaxation times for C_8K and C_6K $\tau_{1,2}$ are given in Figure. As it is seen from the Figure, the relaxation time τ_2 as a function of $t = T/T_c$ has not the critical behavior on the temperature just as in cuprates (for K_3C_{60} and Rb_3C_{60} see [4]).

References

[1] R. Al-Jishi. Phys. Rev. **B28**, *1*, 112 (1983).
[2] P. Konsin. Phys. Stat. Sol. (*b*) **189**, *1*, 185 (1995).
[3] P. Konsin, B. Sorkin. Phys. Rev. **B58**, *9*, 5795 (1998).
[4] S.B. Fleisher, B. Pevzner, D.J. Dougherty, H. J. Zeiger, G. Dresselhaus, M.S. Dresselhaus, E.P. Ippen, A.F. Hebard. Phys. Rev. **B62**, *2*, 1366 (2000).