Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Field-induced Superconductivity

Hidemi Nagao [a], Hiroaki Saito [a], Ryoichi Suzuki [a], Yasutaka Kitagawa [b], Takashi Kawakami [b] & Kizashi Yamaguchi [b]

[a] Department of Computational Science, Faculty of Science, Kanazawa University, Kakuma, Kanazawa, 920-1192, Japan

[b] Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka, 560-0043, Japan

Version of record first published: 18 Oct 2010

To cite this article: Hidemi Nagao, Hiroaki Saito, Ryoichi Suzuki, Yasutaka Kitagawa, Takashi Kawakami & Kizashi Yamaguchi (2003): Field-induced Superconductivity, Molecular Crystals and Liquid Crystals, 379:1, 495-500

To link to this article: http://dx.doi.org/10.1080/713738601

Mol. Cryst. Liq. Cryst., Vol. 379, pp. 495-500

1058-725X/02 $12.00 + .00
DOI: 10.1080/10587250290090949

Field-induced Superconductivity

HIDEMI NAGAO[a], HIROAKI SAITO[a], RYOICHI SUZUKI[a], YASUTAKA KITAGAWA[b], TAKASHI KAWAKAMI[b] and KIZASHI YAMAGUCHI[b]

[a]*Department of Computational Science, Faculty of Science, Kanazawa University, Kakuma, Kanazawa 920-1192, Japan and* [b]*Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan*

Phase diagrams of theoretical models for CuO_2 plane and CuO chains are presented by using a two-band model.

Keywords Field-induced superconductivity; Two-band model; High-Tc superconductivity

INTRODUCTION

The discovery of high-Tc copper oxide suggested the idea that doping in antiferro- or ferromagnetic system may provide several exotic electronic phases, which are (1) ferromagnetic metal or insulator; (2) spin glass: (3) paramagnetic metal; (4) antiferromagnetic metal; (5) ferrimagnetic metal or insulator; and (6) charge- or spin-mediated superconductor[1,2]. Recently, we have therefore started our theoretical attempt to search possible models for charge- or spin-mediated superconductivity from these

works and have presented the hypotheses about the possibilities of the superconductivity in the intermediated region of metal-insulator transition in the previous papers[1-3]. Since 1960, many scientists made an effeort to modulate the superconducting properties by using transverse static electric fields. The investigations of field-induced superconductivity were extended to copper oxides with the high-Tc superconductivity. After many investigations of field effects of copper oxides, Schön et al.[4-6] have discovered superconductivity in molecular crystals of C_{60}, anthracene and so on with field-effect transistor (FET) configuration by charge (electron) injection. They have reported the high-Tc superconductivity (Tc=52K) of C_{60} induced by hole-doping, which has been conducted by using the field-effect transistor (FET) technique. Recently, field-induced superconductivity in a spin-ladder cuprate ($Sr_{1-x}Ca_xCu_2O_3$ and $(Sr_{1-x}Ca_x)_{14}Cu_{24}O_{41}$) has been also reported by using the FET technique by Schön et al. [7].

In this study, we theoretically investigate field-induced superconductivity in CuO_2 plane and CuO chains with the FET configuration by using a two-band model[3,8,9]. We present phase diagrams of themodel crystals obtained from the two-band model.

THEORETICAL BACKGROUND

For the theoretical work, Konsin and Sorkin [10] proposed a two-band model including the field effect on the superconductivity, providing a theoretical rationalization of the observation in the Y-123 copper oxide. Recently we have extended their theory for high-*Tc* superconductor of copper oxide to more general formalism. In our two-band model, we consider a Hamiltonian with four effective electron-electron interactions; intraband two-particle normal scattering g_1, intraband umklap scattering g_2, interband umklap scattering g_3, and interband normal scattering g_4, in the case of the Fermi enregy level crossing two bands. In the framework of a mean-field approximation, we proposed a theoretical formula for analytically expressing the transition temperature for superconductivity induced by external electric filed [3,8].

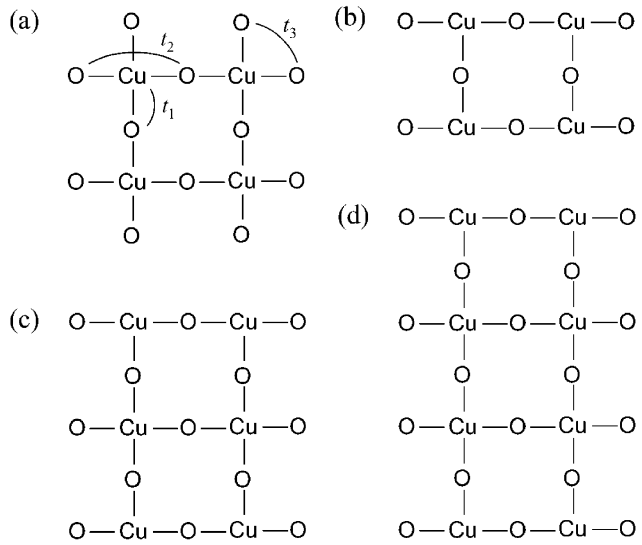

FIGURE 1. Model crystals. (a) CuO_2 plane. (b) 2-leg ladder. (c) 3-leg ladder. (d) 4-leg ladder.

$$T_c^{SSC} = 1.13\left(E_c - \zeta\right)^{1/2}\left[\zeta\left(\zeta - E_j\right)\right]^{1/4} \times \exp\left[-\left(\left(\frac{1}{4}\log\frac{\zeta}{\zeta - E_j} + \frac{k_i - k_j}{2K}\right)^2 + \frac{1}{K} + \frac{k_i k_j}{K^2}\right)^{1/2} + \frac{k_i + k_j}{2K}\right] \quad (1)$$

where $k_i = g_1\rho_i$, $k_j = g_1\rho_j$, $K = (g_2^2 - g_1^2)\rho_i\rho_j$. In this equation, E_c is the cut-off energy value, ζ is the chemical potential, E_j is the top energy of the lower band, ρ_i and ρ_j are respectively densities of states (DOS) of the higher and lower bands, and g_1 and g_2 are respectively the intraband two-particle normal and umklapp scatterings. In this theoretical framework, electron- or hole-doping in the FET configuration is modeled with the change in the Fermi level (ζ) due to the applied electric field. We have already applied this model to the molecular crystals of anthrathane and obtained a phase diagram which well reproduces the superconducting transition behavior experimentally observed by the electron-doping [9].

In this study, we consider model crystals of copper oxides as shown in FIGURE 1 and estimate phase diagram of their crystals by us-

ing eq.(1) in the two-band model. We used the transfer integrals in FIGURE 1, t_1=1, t_2=0.2, t_3=-0.6, and $\Delta=v_o-v_{Cu}$=3 (eV) to obtain band structure of these crystals, and assumed that the crystal structures are not affected by applying the external electric field, or by hole- or electron-doping. Thus we obtained the parameters necessary for evaluating *Tc* in eq.(1) from the band structure, and examined the superconducting transition behavior. Effective elecron-electron interactions were estimated according to the procedure in the previous papers [8,9].

RESULT AND DISCUSSION

FIGURE 2 shows band structure of crystals in FIGURE 1. We summarize

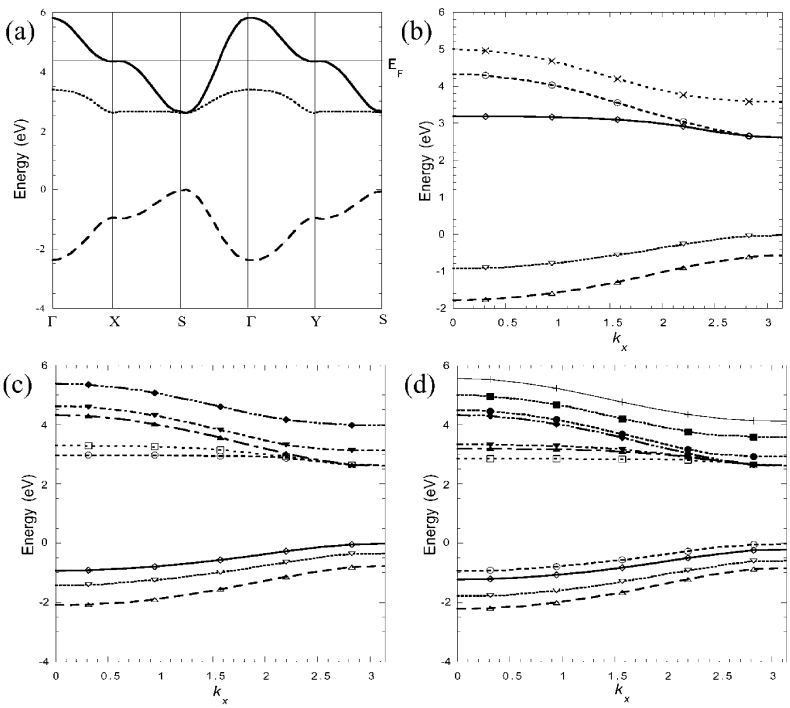

FIGURE 2. Band structure. (a) CuO_2 plane. (b) 2-leg ladder. (c) 3-leg ladder. (d) 4-leg ladder.

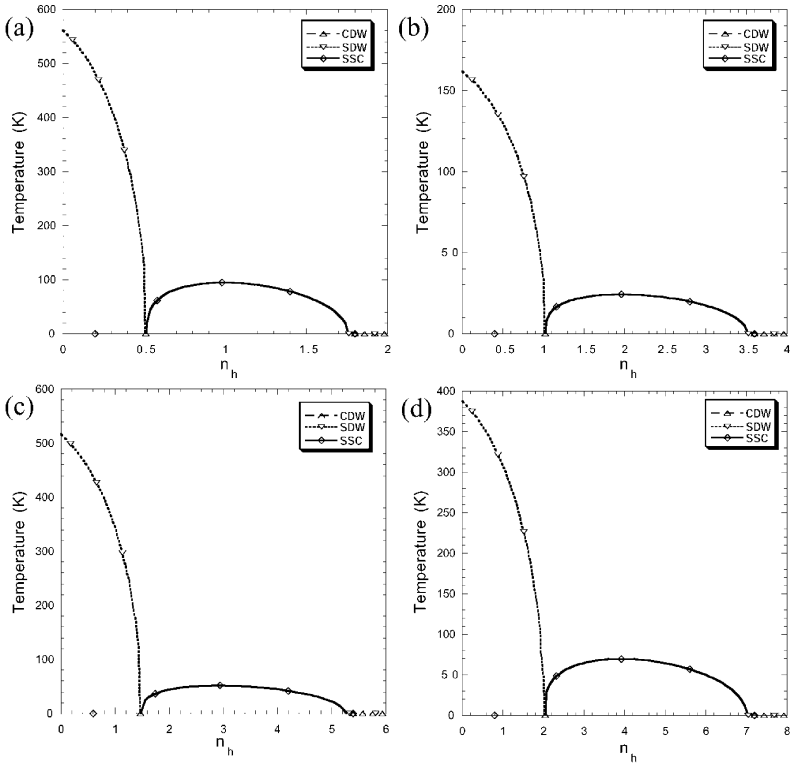

FIGURE 3. Phase diagram. (a) CuO_2 plane. (b) 2-leg ladder. (c) 3-leg ladder. (d) 4-leg ladder.

parameters used in this study in TABLE 1. Using these parameters and eq.(1), we obtain phase diagrams of these crystals as shown in FIGURE 3. The maximal transition temperature for each system is (a) 94.4 K around

TABLE 1 Parameters for each crystal.

System	E_c	E_j	E_i^w	ρ_i	ρ_j	g_1	g_2	g_3	g_4
(a)	2.81	2.43	3.20	0.63	2.59	0.00	0.21	0.00	0.30
(b)	2.11	1.82	2.40	0.83	3.43	0.00	0.12	0.00	0.17
(c)	2.45	2.10	2.80	0.71	2.85	0.00	0.16	0.00	0.29
(d)	2.60	2.23	2.96	0.67	2.72	0.00	0.18	0.00	0.25

1 hole, (b) 24.2 K around 2 holes, (c) 51.4 K around 3 holes, and (d) 69.5 K around 4 holes per unit cell. The transition temperature of a spin-ladder system obtained from experimental results is 14 K [7]. The present results qualitatively agree with the experimental result. We can find that as increase of the number of chain, the maximal transition temperature becomes higher. However, it may be necessary to estimate the effective electron-electron interaction for 3-leg ladder more strictly, because the band structure is different from other even-leg ladder systems. We will present the studies for problems such as mechanism of phase transition elsewhere.

ACKNOWLEDGMENT

H.N and K.Y. are grateful for a financial support of the Ministry of Education, Science and Culture of Japan (Research No.12020234, No. 13740328, No.10146101, No.10149105).

REFERENCES

[1] K.Yamaguchi, Int. J. Quantum Chem., **37**, 167 (1990).
[2] H. Nagao, M. Nishino, M. Mitani, Y. Yoshioka, and K. Yamaguchi, Int. J. Quantum Chem., **65**, 947 (1997).
[3] H. Nagao, M. Mitani, M. Nishino, Y. Shigeta, Y. Yoshioka and K. Yamaguchi, Int. J. Quantum Chem., **75**, 549 (1999).
[4] J. H. Schön, Ch. Kloc, R. C. Haddon, B. Battlog, Science, **288**, 656 (2000).
[5] J. H. Schön, Ch. Kloc, B. Battlog, Nature, **406**, 702 (2000).
[6] J. H. Schön, Ch. Kloc, B. Battlog, Nature, **408**, 549 (2000).
[7] J. H. Schön, M. Dorget, F. C. Beuran, X. Z. Xu, E. Arushanov, M. Laguës, C. Deville Cavellin, Science, **293**, 2430 (2001).
[8] H. Nagao, M. Nishino, Y. Shigeta, Y. Yoshioka and K. Yamaguchi, J. Chem. Phys., **113**, 11237 (2000).
[9] H. Nagao, Y. Kitagawa, T. Kawakami, T. Yoshimoto, H. Saito, and K. Yamaguchi, Int. J. Quantum Chem., **85**, 608 (2001).
[10] P. Konsin, B. Sorkin, Phys. Rev. B **58**, 5795 (1998) .