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SMR/455 - 5

EXPERIMENTAL WORKSHOP ON HIGH TEMPERATURE SUPERCONDUCTORS & RELATED MATERIALS (BASIC ACTIVITIES)

12 - 30 MARCH 1990

METAL OXIDES: NORMAL-STATE PROPERTIES

LECTURE III

THE HIGH-Tc COPPER OXIDES

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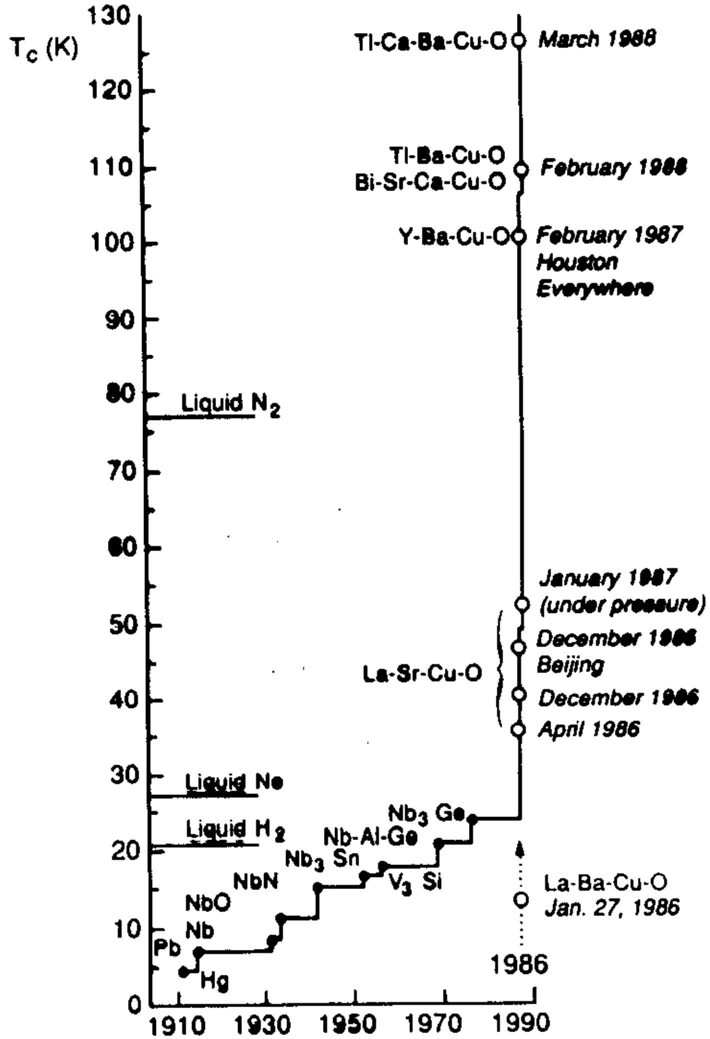
These are preliminary lecture notes, intended only for distribution to participants.

METAL OXIDES: NORMAL-STATE PROPERTIES

LECTURE III

THE HIGH-Tc COPPER OXIDES



Distinctive Features of High-T_c Copper-Oxide Superconductors

Structures

Intergrowth of
superconductor $CuO_2 \cdots CuO_2$ layers
and
"inactive" layers of variable oxygen

Normal-State Properties

- Supercond. in narrow mixed-valent range:

$$AF \rightleftarrows \text{Supercond.} \rightleftarrows \text{Normal Metal}$$

$$W < U \qquad W \approx U > E_p \qquad W > U$$

within one solid-solution field.

- Massive O-2p, Cu-3d covalent mixing

$$Cu^{3+} + O^{2-} \rightleftharpoons Cu^{2+} + O^{-} \qquad (E_M \approx E_I)$$

- Strong electron-phonon interactions

small polaron $\rightleftarrows$ itinerant electron $(W \approx \hbar\omega_0)$

Superconductive Properties

$$\xi_{\parallel} \approx 3\ \text{Å}, \quad \xi_{\perp} \approx 20\ \text{Å} \qquad \text{vs} \quad \xi(\text{conventional}) \approx 10^3\ \text{Å}$$

$$2\Delta_0 / kT_c \approx 7 \quad (\text{in } CuO_2 \text{ plane})$$

Intergrowth Structures

- Anisotropic
- Internal electric field $\mathcal{E}_{\parallel}$
- Bond-length mismatch

Examples

- $BaFe_{12-x}Mn_xO_{19} = \underbrace{(BaFe^{3+}_{1-x}Fe^{4+}_xO_{11})}_{(2-x)-} \cdot \underbrace{(Fe^{3+}_{1-x}Mn^{2+}_xO_8)}_{(2-x)+}$

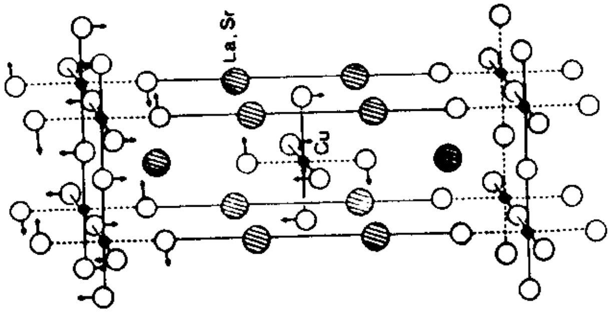
- La_2CuO_4

$$-LaO \mid \underset{2-}{CuO_2} \mid \underset{2+}{LaO-LaO} \mid \underset{2-}{CuO_2} \mid LaO-$$

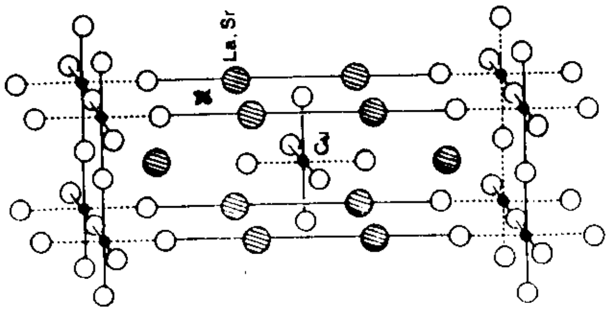
- $YBa_2Cu_3O_{6+x}$

$$-CuO_2 \mid \underset{\delta+}{BaO-CuO_x-BaO} \mid \underset{\delta-}{CuO_2-Y-CuO_2} \mid BaO-$$

$$t = \frac{A-O}{\sqrt{2}\,(B-O)}$$



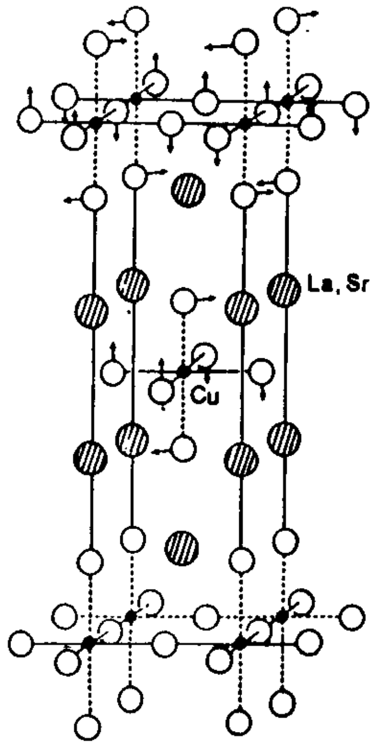
(b)



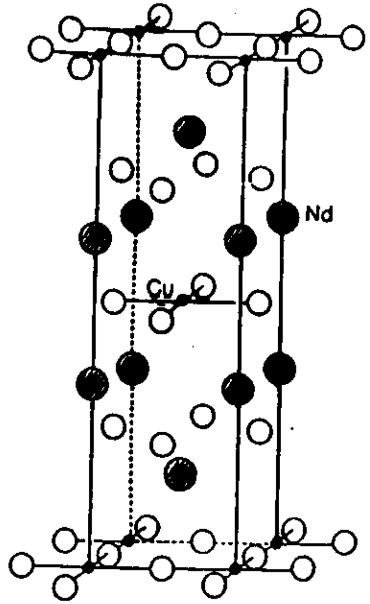
(a)

$t < 1$; p-type

$$t = \frac{(r_{La} + r_O)}{\sqrt{2}\,(r_{Cu} + r_O)}$$



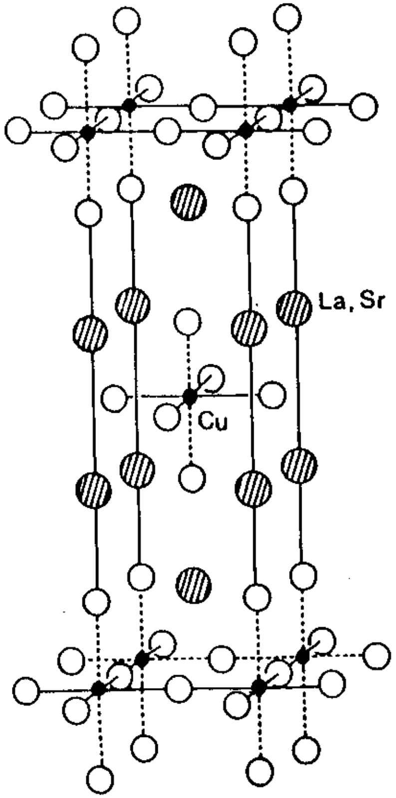
$La_{2-x}Sr_xCuO_4$ - p-type
Cu-O-Cu angle < 180°



$Nd_{2-x}Ce_xCuO_4$ - n-type
Cu-O-Cu angle = 180°

- ~~Large polarisability~~
- ~~Orbital hybridization adjusts readily into bond changes associated with lattice vibrations~~.
- ~~Strong electron-lattice coupling~~.

~~Hybridization (or polarisation) fluctuation mechanism~~.



(a)

La_2CuO_4

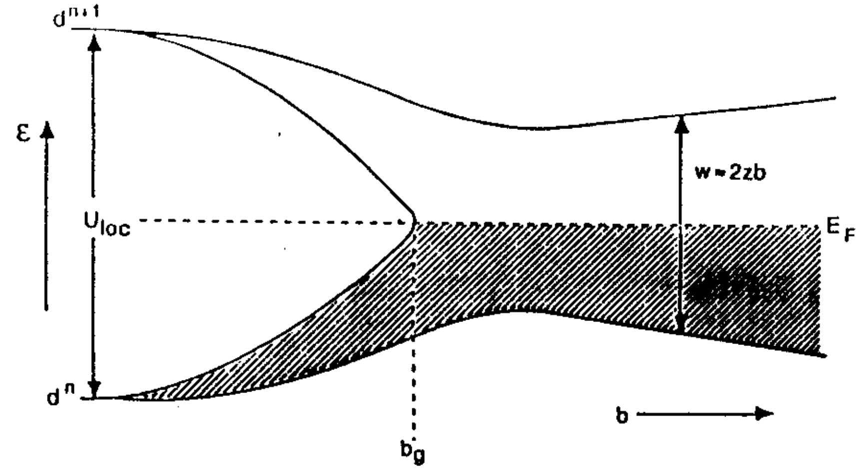
Cu-O-Cu interactions

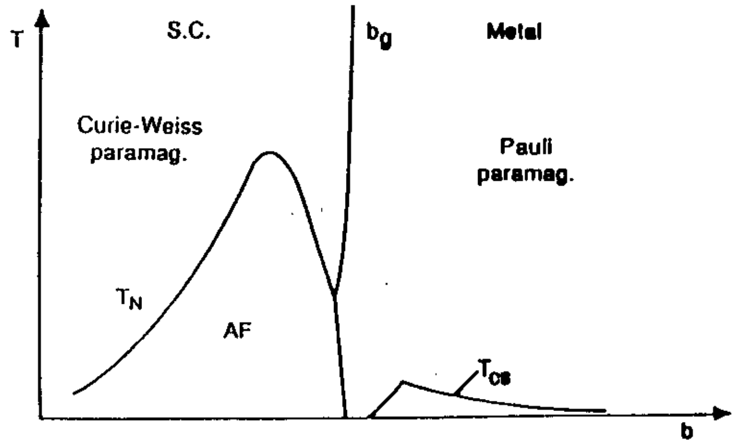
$$\psi_{x^2-y^2} = N_\sigma\,(f_{x^2-y^2} - \lambda_\sigma\phi_\sigma - \lambda_s\phi_s)$$

$$b = (\psi_i, H'\psi_j) \approx \varepsilon_{ij} N_\sigma^2 (\lambda_\sigma^2 + \lambda_s^2)$$

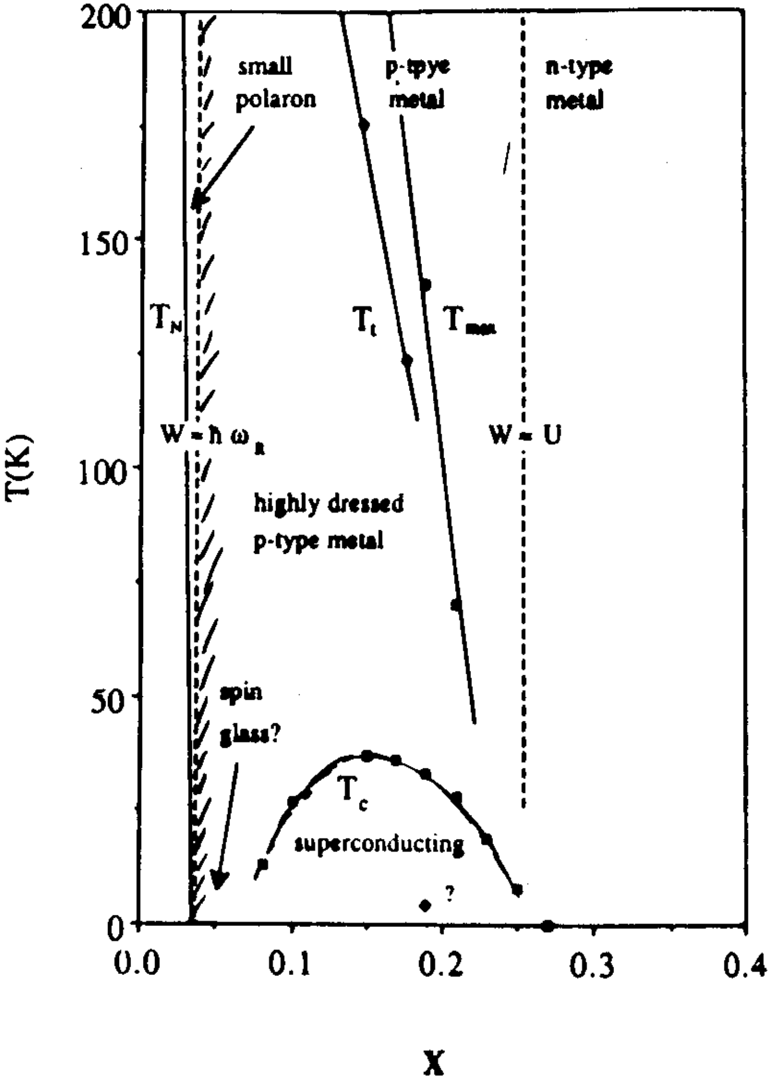
$$T_N \sim b^2/U \sim \lambda_\sigma^4/U$$

$$W \approx 2zb \sim \lambda_\sigma^2$$

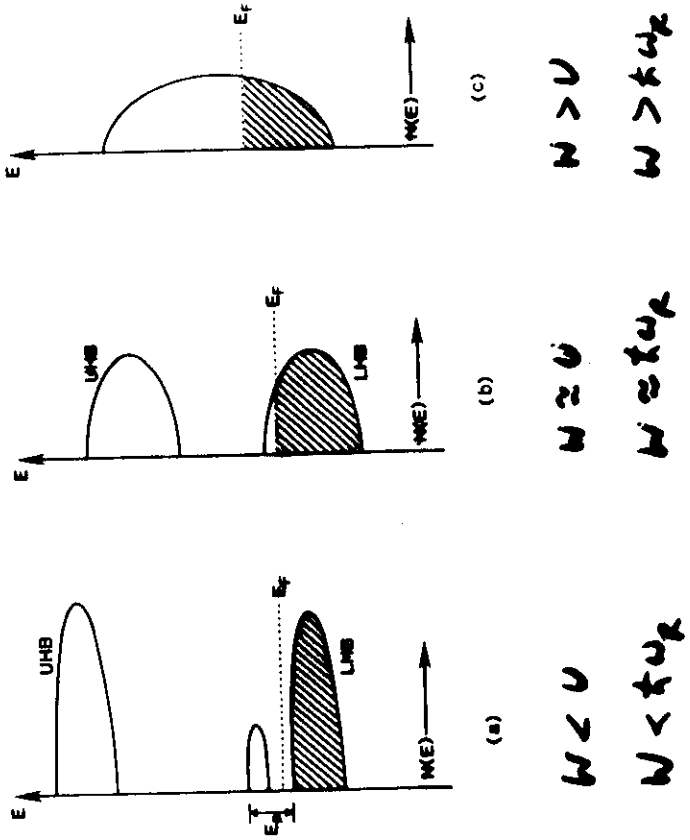




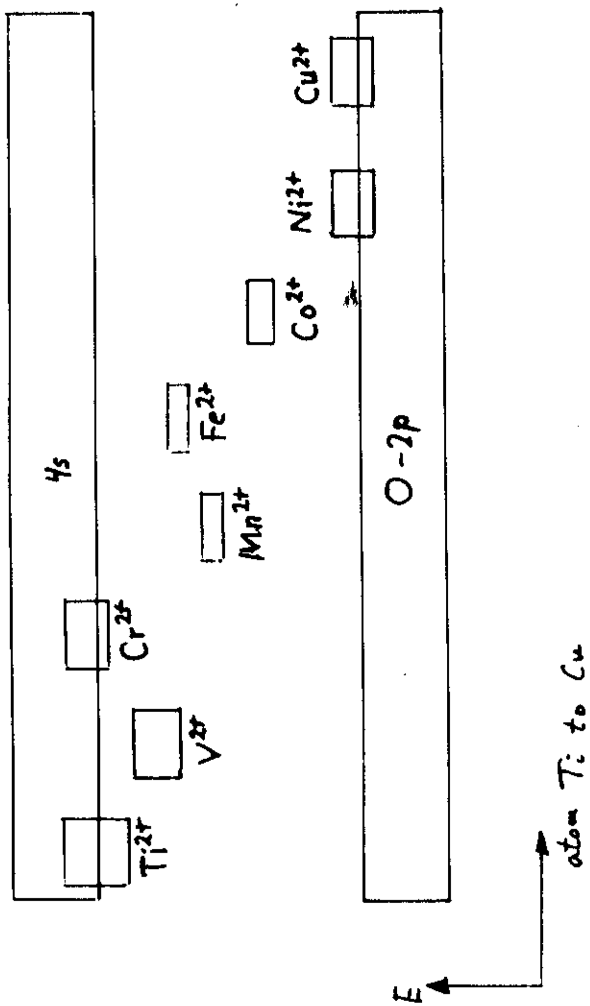
At $b = b_g$, $W \approx U > E_F$

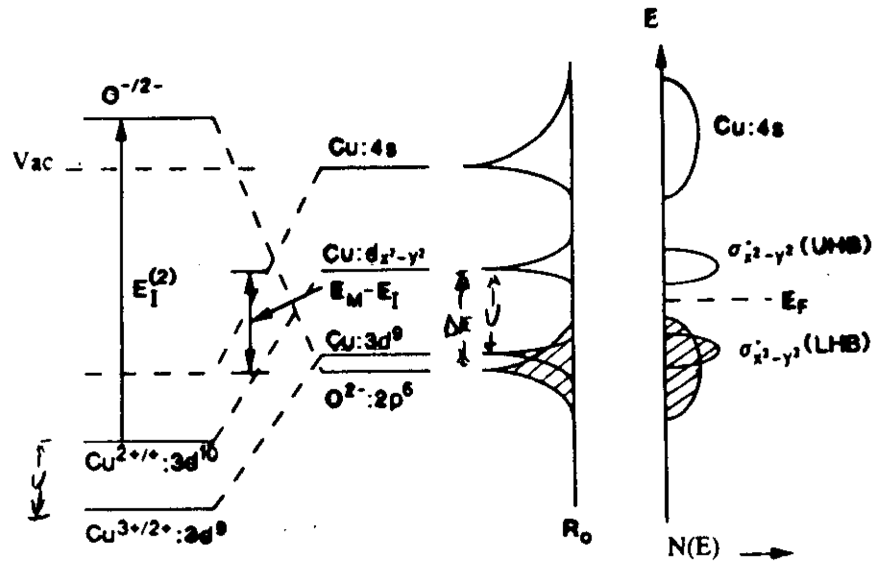


200
150
100
50
0
0.0
0.1
0.2
0.3
0.4
T(K)
X
small
polaron
p-tpye
metal
n-type
metal
T_N
T_t
T_{max}
$W \approx \hbar\,\omega_R$
$W \approx U$
highly dressed
p-type metal
spin
glass?
T_c
superconducting
?



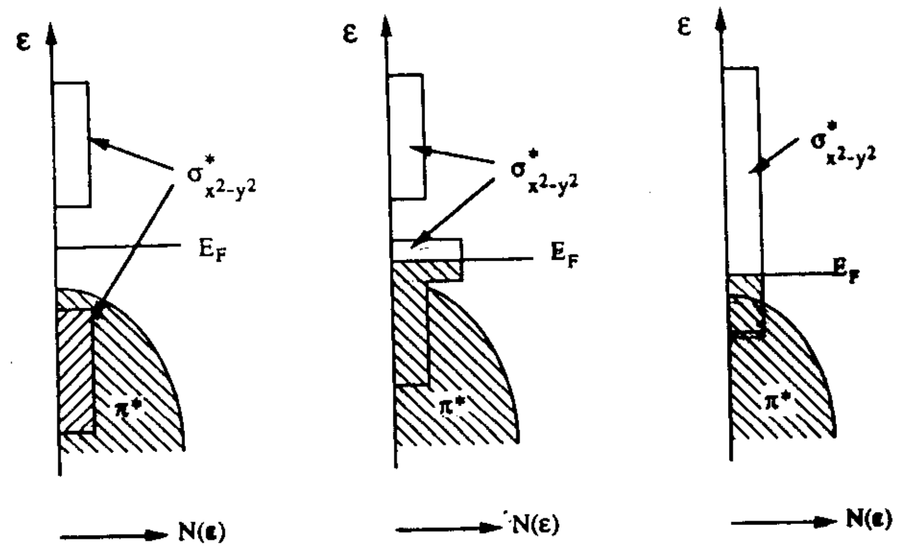
E_F
E
N(E)
(c)
$W > U$
$W > \hbar\omega_R$
UHB
LHB
(b)
$W \approx U$
$W \approx \hbar\omega_R$
(a)
$W < U$
$W < \hbar\omega_R$





(a) (b) (c)

$$\lambda_\sigma = b^{ca} / \Delta E$$



(a) (b) (c)

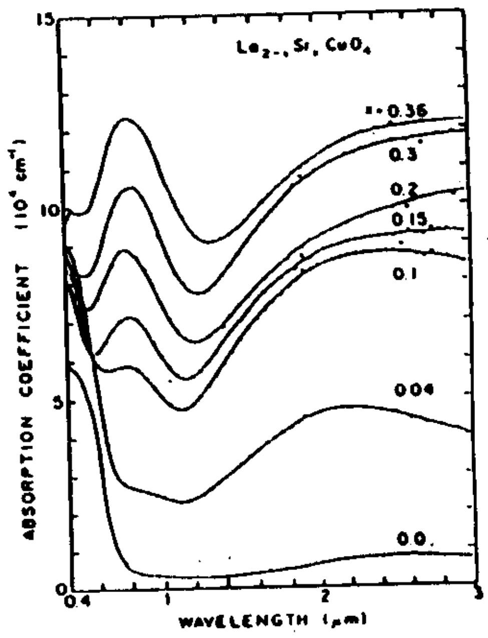


Fig. 1 Optical absorption coefficient for $La_{2-x}Sr_xCuO_4$. (Ref. 9)

COVALENT MIXING

$$W \sim \varepsilon_\sigma (\lambda_\sigma^2 + \lambda_s^2)$$

$$\lambda_i \equiv b_i^{ca} / \Delta E_i$$

An $E_M \approx E_I$ means that ΔE is small for

$$Cu^{3+} + O^{2-} \longrightarrow Cu^{2+} + O^-$$

and

ΔE decreases with increasing hole conc. p in LHB

b^{ca} increases with decreasing Cu–O bond length

$\therefore$ (1) <u>W increases sensitively with p</u>

(2) <u>For fixed p, W increases if Cu–O shortened</u>

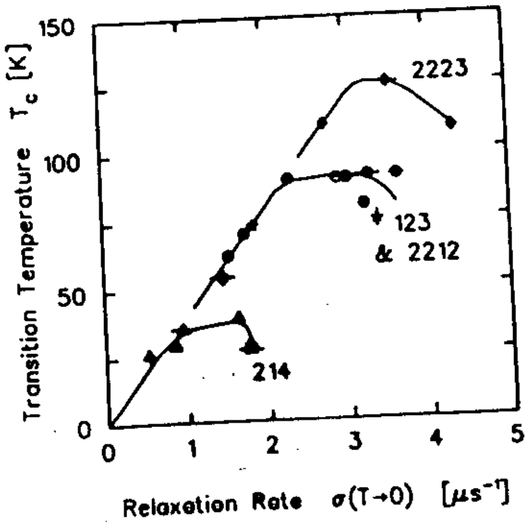
<u>NOTE</u>: For $W \lesssim U$,

$$\underline{dU/dW < 0 \quad \text{and} \quad dV_c/dW < 0}$$

where

U = intraatomic correlation energy

V_c = near-neighbor " "



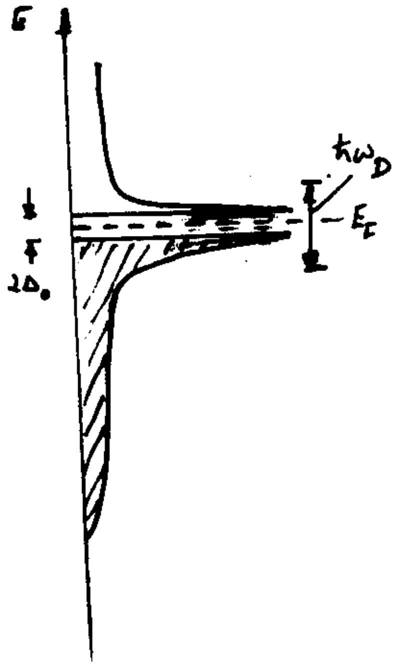
Uemura et al.

$$T_c \sim p/m^*$$

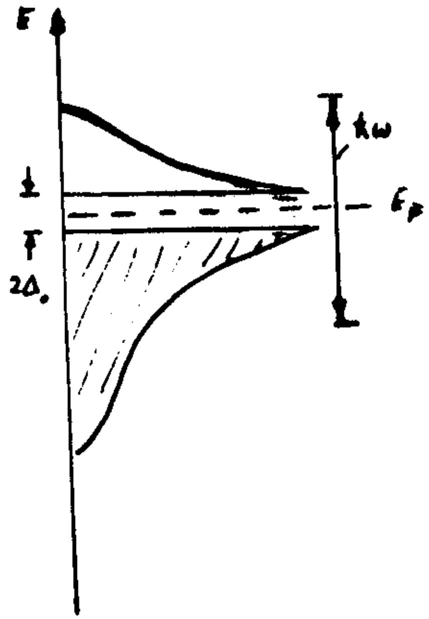
COHERENCE LENGTH

Experimental $\xi \approx 10$ Å

<u>Uncertainty Principle</u>: Small ξ, large $\Delta \underline{k}$



$\xi \approx 10^3$ Å, large W



$\xi \approx 10$ Å, small W

CORRELATION BAG MODEL

$$kT_c = 1.14\,\hbar\omega \exp(-1/\Lambda)$$

<u>BCS</u>: $\hbar\omega = \hbar\omega_D, \quad \Lambda = (E_p' - \mu^*)N(E_F)$

$[\hbar\omega_D \ll W,\ \xi \approx 10^3$ Å, retarded$]$

<u>Aleksandrov</u>: $\hbar\omega = W[n(2-n)]^{1/2}$

$$\Lambda = \left[(E_p^0 - U_0) + z(E_p' - U_1)(\Delta_F/W)^2\right]/W$$

$$E_p = -\frac{1}{2N}\sum_q g_q^2/\hbar\omega_q$$

$[\hbar\omega \sim W,\ \xi \approx 10$ Å, non-retarded, De Jongh$]$

<u>Spin bag</u>: (Schrieffer et al) $\hbar\omega = [\varepsilon_F \cdot 2\Delta_{SDW}]^{1/2}$ for $\varepsilon_F > 2\Delta_{SDW}$

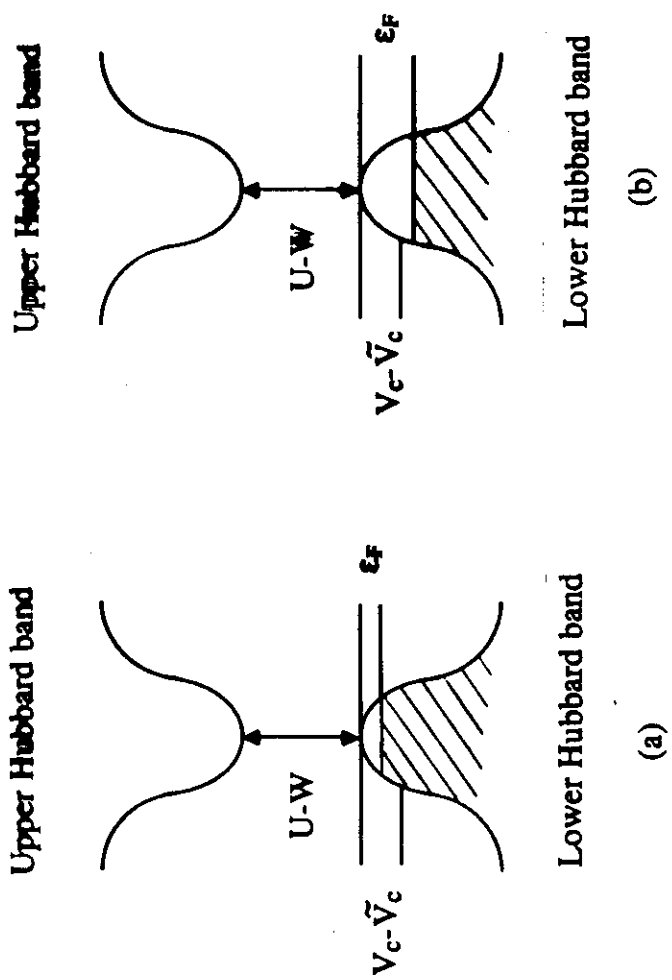
$$\Lambda = V^* N(E_F)$$

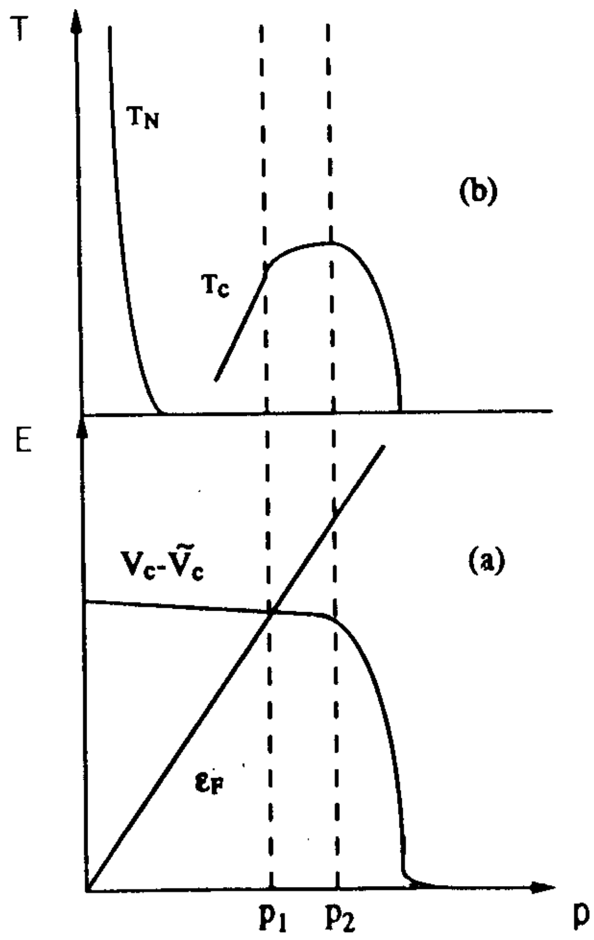
<u>Correlation bag</u>: $\hbar\omega = \varepsilon_F \sim p$ for $\varepsilon_F < \hbar\omega_{max}$

$$= [\varepsilon_F(V_c - \tilde{V}_c)]^{1/2} \equiv \hbar\omega_{max} \text{ for } \varepsilon_F > \hbar\omega_{max}$$

$[0.1 \leq \hbar\omega_{max}/W$ for $\xi \approx 10$ Å$]$

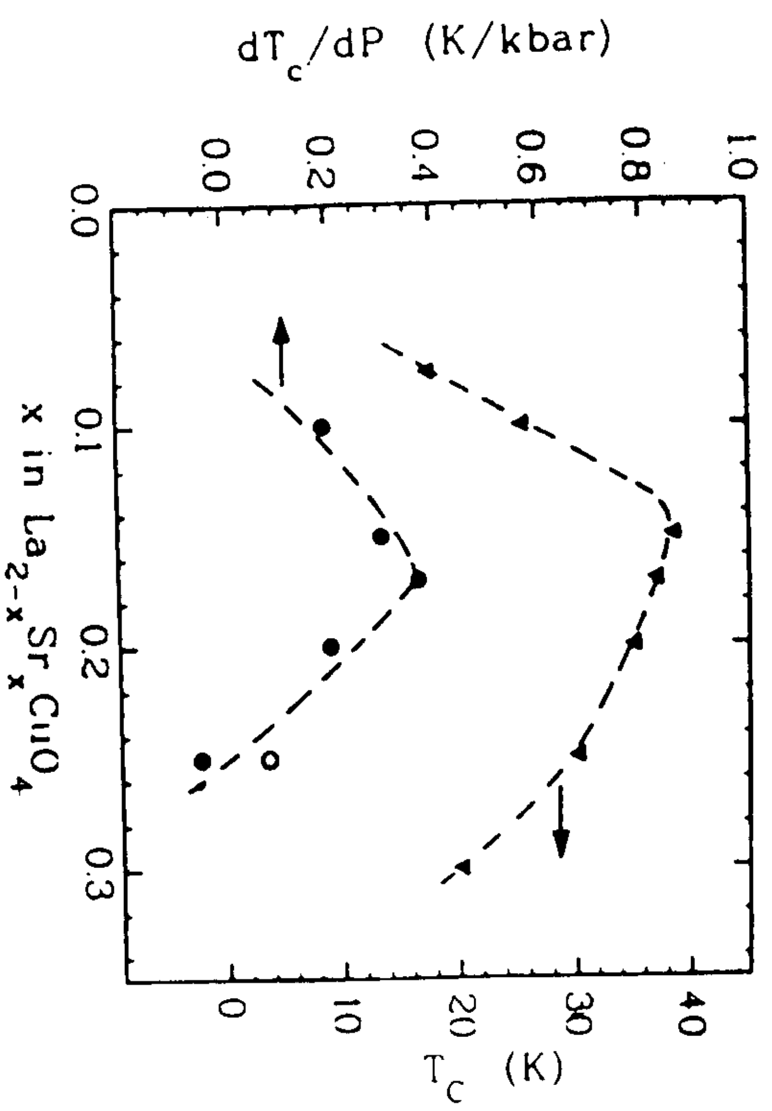
$$\Lambda = (E_p' - \tilde{V}_c)N(E_F)$$





NOTE: $\frac{d\varepsilon_F}{dP} > 0$, but $\frac{dp_1}{dP} \approx \frac{dp_2}{dP} \approx 0$

$\frac{d(V_c - \tilde{V}_c)}{dP} \approx 0$, but $\frac{dV_c}{dP} < 0$

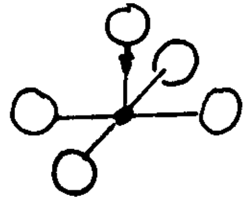


SHIRBER et al

POSSIBLE BAG DISPLACEMENTS

• p-type: reduce Cu-O

and



• n-type: increase Cu-O