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Twin-boundary dynamics and properties of high-T_c superconductors

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We present evidence for collective twin-boundary oscillations in the high-T_c oxide superconductors and propose that their coupling with electrons enhances T_c. These special modes, which we call "dyadons," have a highly anisotropic and low-frequency spectrum, causing the specific heat to change from a T^3 temperature dependence to T^2 at lower temperatures, consistent with anomalies below ~ 12 K in doped La_2CuO_4 and in $YBa_2Cu_3O_7$. The low-frequency dyadons also account for the extended linear temperature dependence of the normal-state resistivity. Due to the unusual anisotropy of both dyadon and electron spectra, vertex corrections generate a strong electron-dyadon coupling at lower temperatures.

The recent discoveries of ceramic-type superconductors with a high transition temperature T_c led to intensive studies of these materials in search for a clue to the mechanism of high T_c.[1,2] In particular, a tetragonal-to-orthorhombic (TO) transition at a temperature T_d above or near T_c seems to be a key feature.[3-9] A positive correlation is found between T_c and the volume fraction of the orthorhombic phase of $YBa_2Cu_3O_{7-\delta}$.[5,6] Furthermore, in the $La_{2-x}Sr_xCuO_{4-\delta}$ compounds, T_d decreases from 533 K at $x=0$ to ~ 40 K at $x=0.19$ (Refs. 3 and 4) where T_c shows a maximum. A similar correlation of T_c with structural transitions is well known in the $A15$ and other compounds.[2]

We consider the formation of twin boundaries (TB's) as the most dramatic manifestation of the TO transition and its martenistic nature. TB's exist well below T_d and in a sense maintain the anisotropy and lattice softening which occur at T_d. In particular, $YBaCu_3O_{7-\delta}$ shows twinned orthorhombic bands with 10–100 parallel TB's in a grain and TB spacing of $l=10^2-10^3$ Å.[6-9]

A direct correlation of TB's and T_c was in fact demonstrated in Sn, In, Re, Tl, and Nb by mechanically generating TB's.[10,11] In particular, a single TB enhances $T_c=3.72$ K of Sn by 0.04 K, while a high density of TB's yields $T_c \simeq 7$ K.[10] These phenomena were analyzed[12] in terms of superconductivity localized and enhanced near a static TB by an unknown mechanism. The proximity effect can then considerably enhance the bulk T_c if $l \lesssim \xi_0$, where ξ_0 is the superconducting coherence length. However, this mechanism seems ineffective in the high-T_c compounds where $\xi_0 \simeq 30$ Å $\ll l$.[13]

We have recently reported[14] a study of the TB lattice dynamics with some unusual results. First, the detachment of very low-frequency collective modes from the transverse phonon branch; softening of the latter is associated with the martensitic transition at T_d. Second, due to the long-range nature of the elastic fields, these modes affect the entire transformed phase and therefore can couple to electrons in a bulk fashion. These modes might be called collective twin-boundary oscillations; we have chosen "dyadons" for short.

In the present work we first evaluate the contribution of dyadons to the specific heat and show that they can account for the anomalies observed[15] at ~ 12 K in $La_{1.85}Ba_{0.15}CuO_4$ and $La_{1.8}Sr_{0.2}CuO_4$ and[16,17] below ~ 10 K in $YBa_2Cu_3O_7$. Given the dyadon low frequencies, the electron-dyadon coupling also naturally explains the normal-state resistivity which is linear with temperature[4,17-19] to as low as ~ 40 K. Finally, we examine vertex corrections caused by the electron-dyadon coupling. Due to the unusual anisotropy of both dyadon and electron spectra, Migdal's theorem is not applicable and the vertex function is strongly enhanced.

Before proceeding, some disclaimers: First, dyadons are not proposed as the fundamental mechanism of high T_c, rather they enhance electron-phonon or electron-electron interactions.[1,2] Second, we do not rely on proximity effect[12] since dyadons couple to electrons in the bulk. Third, the effect is not a conventional soft-phonon mechanism[2] since vertex corrections arising from anisotropy are essential.

Consider a periodic array of TB's parallel to the (110) plane; this structure can be described by an elastic displacement field $u(s)$ in the $[1\bar{1}0]$ direction with period $2l$ and s is in the [110] direction.[20,21] When the TB thickness is much smaller than l we can define a collective coordinate S_n for the position along [110] of the nth TB. The normal coordinates η_n for small oscillations, i.e., dyadons,[14] are given by the nonlocal transformation $\eta_n=2\times\sum_{j=1}^{n-1}(-)^j\delta_j+\delta_0-\delta u$, where $S_n=nl+\delta_n$ and δu is an overall shift of $u(s)$. The restoring force for the TB motion is a long-range elastic force mediated through the interface with another phase. The latter could be the tetragonal parent phase, a differently oriented twin band or an altogether difference phase. However, the kinetic mass is a *bulk* one, involving the motion of the whole twinned product phase. The resulting frequencies $\omega(q_1)$ for wave vectors q_1 in the [110] direction are, therefore, very low with the dispersion relation[14]

$$\omega^2(q_1)=\omega_d^2\sin^2(\tfrac{1}{2}q_1l)\sum_{p=-\infty}^{\infty}\left\{\left|\frac{q_1l}{2\pi}-p\right|^{-1}-\left|\frac{1}{2}-p\right|^{-1}\right\}. \quad (1)$$

Here $\omega_d=[4\alpha/\pi\rho lL_2]^{1/2}$ with α an effective elastic constant, ρ the mass density, and L_2 the width of the twin band in the $[1\bar{1}0]$ direction; $\omega_d\simeq\Theta_Da/\sqrt{lL_2}$ where Θ_D is the Debye temperature and a the lattice constant. For $\Theta_D\simeq400$ K,[15-17] $a=3.8$ Å, $l\simeq10^2$ Å, and $L_2\simeq10^4$ Å,[6-9] we estimate $\omega_d\simeq10^{11}\ \mathrm{s}^{-1}\simeq1$ K.

When the TB position δ_n depends on coordinates perpendicular to s, it describes a TB bending. We expect that now the elastic energies scale with the kinetic mass so that the transverse dispersion is linear. For wave vectors q_2,q_3 in the $[1\bar{1}0]$ and [001] directions respectively, the three-dimensional dyadon dispersion is then

$$\omega_q^2=\omega^2(q_1)+v_2^2q_2^2+v_3^2q_3^2\ , \quad (2)$$

where v_2,v_3 may be of the order of sound velocities.

Equation (1) yields $\omega(q_1)\sim\sqrt{q_1}$ as $q_1\to0$ which is a manifestation of the long-range force. As $q_1\to\pi/l$, $\omega(q_1)\sim|q_1-\pi/l|$ and $\omega(\pi/l)=0$ corresponds to the uniform translation mode of the twin lattice; impurities or discreteness effects for very sharp TB's may pin this mode and then $\omega(\pi/l)\neq0$. For example, for $YBa_2Cu_3O_{7-\delta}$ with $\delta=0$ oxygen ordering can be related to the TO transition and a TB separates distinct directions of oxygen ordering.[9,22] We note that thermal fluctuations of a TB are [using (2)] $\sim1\%$ of the lattice constant at room temperature.

The spectrum [(1) and (2)] implies an unusual specific heat. There are four distinct temperature regimes. (a) $T\lesssim v\pi/L_2\simeq\Theta_Da/L_2$ where v is a typical sound velocity. Since acoustic phonons with wave vectors $|q_1|\lesssim\pi/L_2$ cannot be confined in the product phase, we expect a normal specific heat $c_v\sim T^3$ for $T\lesssim0.1$ K. (b) $v\pi/L_2\lesssim T\ll\omega_d$ where the $(q_1)^{1/2}$ dispersion implies a $c_v\sim T^4$ contribution for $T\ll1$ K. (c) $\omega_d\lesssim T\lesssim v\pi/l\simeq\Theta_Da/l$ where all the frequencies $\omega(q_1)$ are excited and the specific heat is effectively two-dimensional. Thus, for 1 K $\lesssim T\lesssim10$ K we expect $c_v\sim T^2$. (d) $T\gtrsim v\pi/l$ where ordinary phonons dominate and $c_v\sim T^3$.

Numerical evaluation of the contribution of dyadons using Eqs. (1) and (2) to the specific heat is shown in Fig. 1. For comparison we also show the specific heat of isotropic acoustic phonons assuming a victory $v=v_2=v_3=(\alpha/\rho)^{1/2}$, and $L_2/l=100$ (dashed line). These two specific-heat terms are not simply additive; the dyadon de-

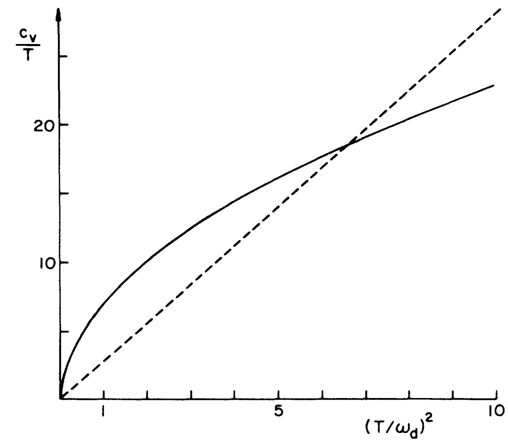

FIG. 1. Specific heat c_v due to dyadon excitations (full line) and due to normal acoustic modes (dashed line) with $v=v_2=v_3$ and $L_2/l=100$; c_v/T is in units of $\omega_d/(2\pi v_2v_3l)$.

grees of freedom are formed at the expense of low-frequency acoustic phonons; hence the two lines in Fig. 1 are limiting forms for either regimes *b* and *c* (full line) or regime *d* (dashed line).

Specific-heat data on $La_{1.85}Ba_{0.15}CuO_4$ and $La_{1.8}Sr_{0.2}CuO_4$ (Ref. 15) show a deviation from a T^3 law at ~12 K. We suggest that the bend at ~12 K is the crossover to a T^2 law at lower temperatures. Thus, the extrapolation to $T=0$ and the apparent large $c_v\sim T$ term[15] should be reexamined by experiments at lower temperatures. Data on $YBa_2Cu_3O_7$ shows[16,17] a peak of magnetic origin at ~2 K. A magnetic field H partially freezes the magnetic moments and the peak disappears; the data[16,17] are then consistent with Fig. 1 with $\omega_d\simeq1$ K. Sample dependence[16,17] of this anomaly indicates different distributions of TB arrays. Further experiments on the $c_v(H)$ dependence should clarify the relative roles of spins and TB's.

We turn now to address the electron-dyadon coupling, first via the normal-state resistivity and then its effects on T_c. The Fourier transforms of $u(s)$ and η_n are related by[14]

$$u(q_1)=\bar{u}(q_1)+i(q_1l)^{-1}[\exp(iq_1l)-1]\eta(q_1)+O(\eta^2)\ ,$$

where $\bar{u}(q_1)$ corresponds to the static TB lattice. Thus, $\eta(q_1)$ produces a significant modulation in $u(s)$ if $|q_1|\lesssim\pi/l$. Electrons, which would ordinarily couple to a phonon displacement $u(\mathbf{q})$ with a coupling constant $g_0(\mathbf{q})$, will then couple to dyadons with a coupling

$$g_d(\mathbf{q})=ig_0(\mathbf{q})(e^{iq_1l}-1)/(q_1l)\ . \quad (3)$$

We define a dimensionless coupling by a *two-dimensional* average

$$\lambda_d(q_1)=(2/\pi v_F)\sum_{q_2,q_3}|g_d(q)|^2/\omega_q\ ,$$

where v_F is a Fermi velocity in the q_1 direction. We are mainly interested in $|q_1|<\pi/l$, where $\lambda_d(q_1)\simeq\lambda_d(0)\equiv\lambda_d$ is weakly dependent on q_1 [Eq. (3)]. The shear displacement u is parallel to q_2 and $g_0(q) \sim q_2$; so although the very low-frequency modes precisely at $q_2 = q_3 = 0$ do not couple, those in the neighborhood can enhance λ_d to $\lambda_d > 1$, i.e., larger than the corresponding λ_0 (Ref. 23) for the coupling to the ordinary phonons.

The linear temperature dependence of the resistivity $\rho(T)$ (Refs. 4 and 7–19) is a natural outcome of the low-frequency dyadon spectrum. Note that $\rho(T) \sim T$ down to ~ 40 K (Refs. 4 and 19) in doped La_2CuO_4 for which a normal Debye spectrum with $\Theta_D \simeq 400$ K (Ref. 15–17) cannot account. Analogous to the electron-phonon formalism[23] the electron-dyadon contribution to $\rho(T)$ for $T \gtrsim \omega_q$ is $\rho(T) = 2\pi m^* f \lambda_d T/(e^2 n)$ where m^* and n are the electron effective mass and density, respectively. The factor f accounts for the reduced phase space $|q_1| < \pi/l$ in which λ_d is effective, i.e., $f \simeq a/l$. Using data[17–19] for samples with the lowest intercept ρ_0 of $\rho(T)$ at $T=0$ we estimate $f\lambda_d \simeq m/m^* < 1$. We can view the small coupling $f\lambda_d$ as a three-dimensional average; since $f \ll 1$ the two-dimensional average is large, $\lambda_d \gg 1$.

The slope $d\rho/dT$ exhibits large sample-dependent variations consistent with expected variations in $f \simeq a/l$. Curiously, $d\rho/dT$ increases with ρ_0 which may indicate that an increase in a/l implies an increased ρ_0 via static disorder in the TB lattice.

The electron-dyadon coupling provides a long-range attractive coupling between electrons. It is well known that in both one-dimensional[24] and quasi-one-dimensional metals[25] a long-range attractive force favors superconductivity relative to other types of instabilities, provided the mediating phonons have a sufficiently high frequency. For isotropic soft phonons however the leading effect cancels,[26] so that scenario does not apply directly to dyadons.

The unusual feature in the present system is the anisotropy. Dyadons are highly two dimensional in the (110) plane while electrons are quasi two dimensional in the (001) plane, or even one dimensional since the Fermi surface may have flat regions[1] parallel to {110}. Furthermore, the static part of the TB lattice enhances this one dimensionality by folding the Fermi surface into a narrow slab of width $2\pi/l$ in the [110] direction. At temperatures below $\sim v_F/l$ we expect the electrons to become susceptible to the strong coupling λ_d.

To demonstrate the effect we assume a Fermi surface parallel to (110) and show that the vertex function $\Gamma(\mathbf{k},n;\mathbf{q}m)$ (Fig. 2) can diverge when $T \simeq v_F/l$, i.e., Migdal's theorem[27] is not applicable. Figure 2 represents an integral equation for the renormalization of *any* coupling g_e to electrons due to exchange of dyadons with coupling λ_d when $|k_1 - k_1'| < \pi/l$ or exchange of the rest of the acoustic branch with ordinary coupling λ_0 when $|k_1 - k_1'| > \pi/l$. Using the Matsubara representation[27] of Γ and keeping just the $n'=n$ terms we find a divergence for $q_1 = 0$; the highest temperature where this divergence can occur is for $\omega_n = -\omega_{n+m} = \pi T$, i.e., $n=0$, $m=-1$. The main k_1' dependence is in the electron propagators which for $|k_1'| < \pi/l$ yield

$$\sum_{k_1'} (\pi^2 T^2 + v_F^2 k_1'^2)^{-1} \sim \tan^{-1}(v_F/Tl),$$

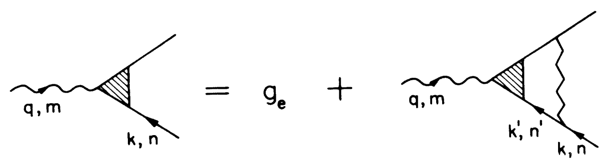

FIG. 2. Vertex renormalization of a coupling g_e due to any interaction (wavy line) with electrons (straight lines). The zigzag line is a dyadon or acoustic phonon propagator; $\mathbf{q},\mathbf{k},\mathbf{k}'$ are wave vectors and m,n,n' correspond to the frequencies $\nu_m, \omega_n, \omega_{n'}$, where $\nu_m = 2\pi T m$ and $\omega_n = \pi T(2n+1)$.

while the $k_2' k_3'$ summation yields the two-dimensional coupling λ_d. The $|k_1'| > \pi/l$ sum involves λ_0 with the final result

$$\Gamma = g_e/[1 - \lambda_0 - (2/\pi)(\lambda_d - \lambda_0)\tan^{-1}(v_F/Tl)] \ . \quad (4)$$

This result shows the crossover from the weak coupling λ_0 at $T \gtrsim v_F/l$ to the strong coupling λ_d at lower temperatures. In particular for $\lambda_d > 1 > \lambda_0$, (4) diverges at $T \equiv T_0 \simeq v_F/l$. Note that for $l \to \infty$, (4) shows a temperature-independent correction which is usually neglected in one-dimensional theories.[24] Thus, the divergence in (4) is specific to the dyadon anisotropy and the appearance of a new energy scale v_F/l.

Since λ_d depends on a/l there may be an optimal λ_d for which T_0 is maximal. If T_c is enhanced by dyadons, a distribution of grains with various a/l yields the T_c of the optimal grains, as long as they form a percolating cluster. Thus, small variations in the distribution [which *can* affect c_v and $\rho(T)$] do not change T_c; large variations do change T_c, as in the case with rapid quenching[5] where T_c drops by $\sim \frac{1}{2}$.

We note that the coupling g_e in Fig. 2 and Eq. (4) is not specified. At present, not having computed T_c, we do not know whether dyadons could be more effective in enhancing the conventional electron-phonon mechanism or other nonconventional mechanisms.[1,2]

In conclusion, we have shown that dyadons can account for the specific-heat anomaly at ~ 12 K, for the observed $\rho \sim T$ relation and lead to enhanced electron interactions. Further experiments on the low-temperature specific heat and on the effect of the twin-band geometry on T_c, $d\rho/dT$ and the specific heat are essential for illuminating the role of dyadons in the high-T_c superconductors.

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