

**Isotope effect in impure high- $T_c$  superconductors**

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The influence of various kinds of impurities on the isotope shift exponent  $\alpha$  of high-temperature superconductors has been studied. In these materials the dopant impurities, like Sr in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ , play different roles and usually occupy different sites than impurities like Zn, Fe, Ni, etc., intentionally introduced into this system to study its superconducting properties. In this paper the in-plane and out-of-plane impurities present in layered superconductors have been considered. They differently affect the superconducting transition temperature  $T_c$ . The relative change of isotope shift coefficient, however, is a universal function of  $T_c/T_{c0}$  ( $T_{c0}$  refers to an impurity-free system), i.e., for angle independent scattering rate and density of states function it does not depend on whether the change of  $T_c$  is due to in- or out-of-plane impurities. The role of the anisotropic impurity scattering in changing oxygen isotope coefficient of superconductors with various symmetries of the order parameter is elucidated. The comparison of the calculated and experimental dependence of  $\alpha/\alpha_0$ , where  $\alpha_0$  is the clean system isotope shift coefficient, on  $T_c/T_{c0}$  is presented for a number of cases studied. The changes of  $\alpha$  calculated within the stripe model of superconductivity in copper oxides reasonably well describe the data on  $\text{La}_{1.8}\text{Sr}_{0.2}\text{Cu}_{1-x}(\text{Fe,Ni})_x\text{O}_4$ , without any fitting parameters.

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**I. INTRODUCTION**

It is hard to overestimate the role played by the impurities introduced into otherwise clean superconductor. In response to impurities the superconducting properties of the material change. The changes include superconducting transition temperature, slope and jump of the specific heat, upper critical field, superfluid density, and other thermodynamic and electromagnetic characteristics.<sup>1,2</sup>

One of the parameters of great experimental and theoretical importance is the isotope coefficient  $\alpha$  defined by the power-law dependence of superconducting transition temperature  $T_c$  on the isotope mass  $M$  of the element:  $T_c \propto M^{-\alpha}$  or  $\alpha = -\partial \ln T_c / \partial \ln M$ . In the BCS model of superconductivity it has been predicted to take on the universal value  $\alpha_{BCS} = \frac{1}{2}$  and verified experimentally for a number of superconducting elements and simple compounds. In chemically complex multicomponent systems one usually defines the partial coefficients  $\alpha_i = -\partial \ln T_c / \partial \ln M_i$ , where  $M_i$  is the isotope mass of the  $i$ th component. In high-temperature superconductors (HTS's) typically  $\text{O}^{18}$  is replaced<sup>3-5</sup> by  $\text{O}^{16}$ . This defines the so-called oxygen isotope coefficient  $\alpha^{\text{O}}$ . Limited data are available on the copper isotope shift  $\alpha^{\text{Cu}}$  in these materials.<sup>6,7</sup>

The effect of impurities introduced into the superconductor on its  $T_c$  strongly depends on the symmetry of the order parameter. It is known that nonmagnetic impurities hardly change the  $T_c$  of  $s$ -wave superconductors (Anderson theorem). On the other hand non magnetic impurities are effective pair breakers in spin singlet  $d$ -wave and spin-triplet  $p$ - or  $f$ -wave superconductors. On the contrary, magnetic impurities break time-reversal symmetry and strongly affect the  $T_c$  of all superconductors including  $s$ -wave ones. Changing the  $T_c$  of the material, impurities indirectly influence all its parameters. In particular this is true for isotope coefficient  $\alpha$ . If one finds the change of the superconducting transition

temperature due to impurities as  $T_c/T_{c0} = f(T_{c0}, \gamma)$ , where  $\gamma$  symbolizes all relevant parameters other than  $T_{c0}$  itself, than  $\alpha/\alpha_0 = \partial \ln T_c / \partial \ln M / \partial \ln T_{c0} / \partial \ln M$  can easily be calculated from the explicit knowledge of function  $f(T_{c0}, \gamma)$ .

It is the purpose of this work to systematically study the effect of disorder on the isotope effect of superconductors by *assuming* that dependence of  $\alpha/\alpha_0$  on  $T_c/T_{c0}$  can be solely attributed to the effect of impurities. The impurities introduced into the superconductor modify the quasiparticle spectrum, interaction parameters, and induce pair breaking. This results in a change of the superconducting transition temperature and the isotope coefficient.

The motivation for the present analysis partially comes from the recent experiments which suggest a strong effect of electron-phonon coupling on the dynamics of electrons in high-temperature superconductors.<sup>8,9</sup>

The shift of  $T_c$  with ionic mass was a crucial experiment to confirm the electron-phonon mechanism of superconductivity in BCS superconductors. Similarly the systematic studies of various isotopic substitutions in HTS's are important to understand the role of electron-phonon interaction in these materials. After early experiments with contradictory conclusions<sup>3-5,10</sup> it has later been unequivocally established that the oxygen isotope shift  $\alpha$  is nonzero, and takes smallest value for optimally doped materials. It increases when one moves into the underdoped region.

Our paper extends the recent work of Openov *et al.*,<sup>11</sup> who considered the effect of magnetic and nonmagnetic impurities in  $s$ -wave and  $d$ -wave superconductors and that of Kresin *et al.*<sup>12</sup> who study the isotope effects in  $s$ -wave superconductors doped with magnetic impurities and those showing the dynamic Jahn-Teller and proximity effects. Our aim here is to elucidate the role (in changing  $\alpha$ ) of the out-of-plane impurities in layered systems and the effect of impurity anisotropy. We also analyze the change of the isotope effect due to Zn impurities in the striped phase model of high- $T_c$  superconductors. In view of the recent interest in supercon-

ductivity and the critical role of impurities played in Sr<sub>2</sub>RuO<sub>4</sub> possibly spin-triplet superconductors<sup>13</sup> we shall consider isotope coefficient for the  $p$ -wave order parameter.

In Sec. II we explain the approach and apply it to the layered systems in which carriers mainly reside in active layers (CuO in HTS's), while impurities are placed either in the active or in the passive layer. It turns out that due to low angle scattering these out-of-plane impurities have small effect on superconducting transition temperature. However, their effect on the isotope coefficient is universal in a sense that  $\alpha/\alpha_0$  depends only on  $T_c/T_{c0}$ . In Sec. III we analyze the role of in plane anisotropic scatterers in changing transition temperature and the isotope coefficient. Sec. IV contains discussion of the results and comparison with experimental data. The predictions of the change of  $T_c$  by Zn impurities obtained recently by the stripe theory of superconductivity lead to the isotope coefficient, which is calculated in Sec. V. We end with conclusions.

## II. IN-PLANE AND OUT-OF-PLANE IMPURITIES IN LAYERED SUPERCONDUCTORS

In this section we shall compare the effect of in-plane and out-of-plane impurities in high-temperature superconductors on  $T_c$  and  $\alpha$ . The Hamiltonian of the superconductor containing both kinds of impurities takes the form

$$H = \sum_{\vec{k}\sigma} (\varepsilon_{\vec{k}} - \mu) c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} + \sum_{\vec{k}\vec{k}'\sigma} V_{\text{in}}(\vec{k}, \vec{k}') c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}'\sigma} + \sum_{\vec{k}\vec{k}'\sigma} V_{\text{out}}(\vec{k}, \vec{k}') c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}'\sigma} + \sum_{\vec{k}\vec{q}} V_{\vec{k},\vec{q}} c_{\vec{k}\uparrow}^{\dagger} c_{-\vec{k}\downarrow}^{\dagger} c_{\vec{q}\downarrow} c_{\vec{q}\uparrow}, \quad (1)$$

where  $\varepsilon_{\vec{k}}$  is the single-particle energy,  $\mu$  chemical potential  $c_{\vec{k}\sigma}^{\dagger}$  ( $c_{\vec{k}\sigma}$ ) denotes the creation (annihilation) operator for a spin  $\sigma$  electron in a state  $\vec{k}$ . The second term describes the scattering of carriers by in-plane while the third by out-of-plane impurities. The pair potential  $V_{\vec{k}\vec{q}}$  is assumed to take on the separable form  $V_{\vec{k}\vec{q}} = -V_0 \phi(\hat{k}) \phi(\hat{q})$  dependent on the wave vector direction  $\hat{k} = \vec{k}/|\vec{k}|$ . The superconducting order parameter is defined by

$$\Delta(\vec{k}) = \sum_{\vec{k}} V_{\vec{k}\vec{q}} \langle c_{-\vec{q}\downarrow} c_{\vec{q}\uparrow} \rangle \quad (2)$$

and the self-consistent equation for it, easily derived by the Green's-function technique, reads<sup>14</sup>

$$\Delta(\vec{k}) = \sum_q V_{kq} \frac{1}{\beta} \sum_{\omega_n} \frac{\tilde{\Delta}(q)}{\tilde{\omega}_n^2 + (\varepsilon_q - \mu)^2 + |\tilde{\Delta}(q)|^2}, \quad (3)$$

where  $\tilde{\omega}_n$  and  $\tilde{\Delta}(q)$  are the renormalized frequency and order parameter in an impure system.

The correction to the self-energy due to impurity scattering  $\Sigma_{\vec{k}}(i\tilde{\omega}_n) = G_{0\vec{k}}^{-1} - G_{\vec{k}}^{-1}$ , where  $\omega_n = (2n+1)\pi k_B T_c$  is

the Matsubara frequency,  $G_{0\vec{k}}$  and  $G_{\vec{k}}$  are the Nambu-Gorkov (imaginary time) Green's functions, is calculated here in the Born approximation,<sup>14,15</sup>

$$\Sigma(\vec{k}, i\tilde{\omega}_n) = n_{\text{in}} \sum_q |V_{\text{in}}(\vec{k} - \vec{q})|^2 \hat{\tau}_3 G_q(i\tilde{\omega}_n) \hat{\tau}_3 + n_{\text{out}} \sum_q |V_{\text{out}}(\vec{k} - \vec{q})|^2 \hat{\tau}_3 G_q(i\tilde{\omega}_n) \hat{\tau}_3, \quad (4)$$

where  $V_{\text{in}}$  and  $V_{\text{out}}$  represent in-plane and out-of-plane impurity potentials while  $n_{\text{in}}$  and  $n_{\text{out}}$  their concentrations. After Kee<sup>16</sup> we assume the out-of-plane impurity potential to be of short-range type  $V(\vec{r}) = u_0/(r^2 + d^2)$ , where  $d$  is the distance of the impurity from the conducting plane and  $u_0$  its scattering amplitude. Fourier transform of this potential is expressed in terms of modified Bessel function of the second kind  $K_0(d|\vec{k} - \vec{k}'|)$ , which is a strongly decreasing function of its argument. Therefore we approximate it by constant  $K_0$  for  $d|\vec{k} - \vec{k}'| > 1$  and zero otherwise. This means that the momentum transfer  $|\vec{k} - \vec{k}'|$  in the scattering process by the out-of-plane impurities is limited to small values. In two dimensions this translates into small-angle scattering. There is no such limitation on the momentum transfer in the scattering by the in-plane impurities. Therefore we take<sup>16,17</sup>

$$V_{\text{out}}(\vec{q}) = \begin{cases} V_{\text{out}} & \text{for } \phi - \phi' < \theta_c \\ 0 & \text{otherwise} \end{cases}$$

and

$$V_{\text{in}}(\vec{q}) = V_{\text{in}}.$$

In the following we shall calculate the changes of  $T_c$  and  $\alpha$  due to both kinds of impurities in superconductors.

### A. Impurities in $d$ -wave superconductors

Now we specialize the calculations to specific symmetries of the order parameter starting with the  $d$ -wave one with the order parameter  $\Delta(\vec{k}) = \Delta_0 \cos 2\phi$ . To proceed we introduce angle dependent density of states (DOS) function  $N_F(\phi)$ , normalized to its average value, and assume it to be energy independent in the energy window near the Fermi energy. The integrals over  $(\varepsilon - \mu)$  can be easily performed and we find

$$\begin{aligned} \Sigma(\vec{k}, i\tilde{\omega}_n) = & -n_{\text{in}} V_{\text{in}}^2 \int_0^{2\pi} \frac{d\phi'}{2} N_F(\phi') \frac{i\tilde{\omega}_n - \tilde{\Delta}(\phi') \hat{\tau}_1}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}^2(\phi')}} \\ & - n_{\text{out}} V_{\text{out}}^2 \int_{\phi}^{\phi + \theta_c} \frac{d\phi'}{2} N_F(\phi') \frac{i\tilde{\omega}_n - \tilde{\Delta}(\phi') \hat{\tau}_1}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}^2(\phi')}}. \end{aligned} \quad (5)$$

We are interested in the change of the superconducting transition temperature and simplify the equations by neglecting powers of  $\tilde{\Delta}(\phi)$  higher than the first.

Even though it is possible to continue calculation for general  $N_F(\phi)$ , let us for a moment take  $N_F(\phi) = N_F$  independent of  $\phi$ , as is appropriate for the circular Fermi surface, to

underline the effect of small-angle scattering only. Assuming that  $u_n = \tilde{\Delta}/|\tilde{\omega}_n|$  is independent of the angle  $\phi$  we get

$$\begin{aligned} \tilde{\omega}_n - \omega_n &= \left( \frac{1}{2\tau_{in}} + \frac{\theta_c}{2\tau_{out}} \right) \text{sgn} \tilde{\omega}_n, \\ (\tilde{\Delta} - \Delta_0) \cos 2\phi &= \frac{\tilde{\Delta}}{|\tilde{\omega}_n|} \left( \frac{1}{\tau_{in}} \int_0^{2\pi} d\phi' \cos 2\phi' \right. \\ &\quad \left. + \frac{1}{2\tau_{out}} \int_{\phi}^{\phi+\theta_c} d\phi' \cos 2\phi' \right). \end{aligned} \quad (6)$$

In writing this equation we made use of the fact that  $\tilde{\Delta}(\phi) = \tilde{\Delta} \cos 2\phi$  and  $\tilde{\Delta}$  does not depend on  $\phi$  for the considered DOS. Vanishing of the integral multiplying  $1/\tau_{in}$  in Eq. (6)

for  $\tilde{\Delta}$  means that the in-plane impurities are strong pair breakers in  $d$ -wave superconductors. By the same token non-zero value of the integral multiplying  $1/\tau_{out}$  means that the out-of-plane impurities are much weaker pair breakers. This explains<sup>16</sup> the long-standing puzzle of why dopant impurities do not kill the  $d$ -wave superconductivity in HTS's.

Performing the integral over  $\phi'$  in the last equation and projecting the result onto  $\cos 2\phi$  function we get the equation

$$\tilde{\Delta}(\theta_c) - \Delta_0 = \frac{\tilde{\Delta}(\theta_c)}{|\tilde{\omega}_n|} \frac{1}{2\tau_{out}} \left( \frac{\sin 2\theta_c}{2} - tg 2\phi \sin^2 \theta_c \right), \quad (7)$$

which together with that for  $\tilde{\omega}_n$  allows us to solve for  $u_n(\theta_c) = \tilde{\Delta}(\theta_c)/|\tilde{\omega}_n|$ . The result reads

$$u_n = \frac{\Delta_0}{|\omega_n + \left( \frac{\theta_c}{2\tau_{out}} + \frac{1}{2\tau_{in}} \right) \text{sgn} \omega_n| - \frac{1}{2\tau_{out}} \left( \frac{\sin 2\theta_c}{2} - tg 2\phi \sin^2 \theta_c \right)}. \quad (8)$$

Gap equation (3) is linearized near  $T_c$  and standard manipulations allow us to find the  $T_c$  changes due to the simultaneous presence of both in-plane and out-of-plane impurities,

$$\ln \frac{T_c}{T_{c0}} = -\gamma(\theta_c) \sum_{n=0}^{\infty} \frac{1}{\left( n + \frac{1}{2} \right) \left[ n + \frac{1}{2} + \gamma(\theta_c) \right]}, \quad (9)$$

where to the lowest nonvanishing order in  $\theta_c$

$$\gamma(\theta_c) = \frac{1}{2\tau_{in} \pi k_B T_c} + \frac{1}{2\tau_{out} \pi k_B T_c} \left( \frac{2\theta_c^3}{3} \right)$$

plays the role of pair-breaking parameter. Note that the first and second order (in  $\theta_c$ ) contributions due to out-of-plane impurities vanish. This has previously been derived in Ref. 16, where the change of the  $T_c$  due to the out-of-plane impurities has been calculated. Equation (9) is valid to all orders in  $1/\tau_{in}$  and  $1/\tau_{out}$  but to the lowest nonvanishing order in  $\theta_c$ . It slightly generalizes the previous result<sup>16</sup> to the simultaneous presence of in- and out-of-plane impurities.

The sum on the right-hand side of Eq. (9) is expressed via digamma function  $\psi(z)$  as

$$\ln \frac{T_c}{T_{c0}} = \psi \left( \frac{1}{2} \right) - \psi \left( \frac{1}{2} + \gamma(\theta_c) \right). \quad (10)$$

Figure 1 shows large changes of superconducting transition temperature due to in-plane (thick solid line) and much weaker for out-of-plane impurities for two values of  $\theta_c$  (thin lines).

For small values of  $\theta_c$  even strong impurities have a negligible effect on  $T_c$ . The change of the isotope shift exponent can be easily calculated and found to read

where  $\psi'$  denotes the derivative of the di-gamma function.

This solution of the impurity problem has been obtained under the assumption of constant (i.e., angle independent) density of states function  $N_F(\phi)$  and scattering rate.

The solution of Eqs. (6) with  $\phi$  dependent density of states can also be easily obtained by assuming that  $u_n(\phi')$

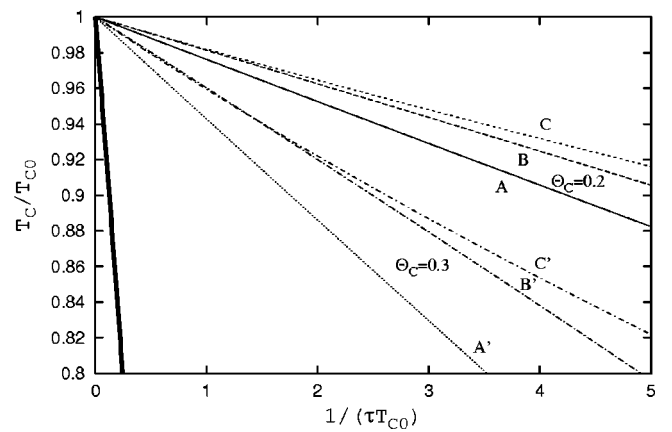


FIG. 1. Effect of in-plane (thick solid line) and out-of-plane impurities (thin lines) in  $d$ -wave HTS's on  $T_c$  for different values of  $\theta_c$  and for  $1/2\tau_{in}=0$ . The two groups of curves correspond to two values of  $\theta_c=0.2, 0.3$ , while different labels refer to different angle dependent density of states functions: A and A' are calculated with  $N(\phi)=1$ , B and B' with  $N(\phi)=\pi/2|\cos 2\phi|$ , C and C' with  $N(\phi)=\pi/2|\cos 4\phi|$ . Note the much weaker influence of out-of-plane impurities on  $T_c$ .

$=\tilde{\Delta}(\phi')/|\tilde{\omega}_n|$  is a slowly varying function of the angle for angles  $\phi' \in \langle \phi, \phi + \theta_c \rangle$  and we obtain

$$\ln \frac{T_c}{T_{c0}} = \frac{1}{a_0} \int_0^{\pi/4} d\phi N(\phi) \cos^2 2\phi \left[ \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \rho_c(\phi, \theta_c)\right) \right] \quad (12)$$

with the pair breaking parameter

$$\rho_c(\phi, \theta_c) = \frac{1}{2\pi k_B T_c \tau(\phi, \theta_c)} \quad (13)$$

and angle dependent relaxation time  $\tau(\phi, \theta_c)$

$$\frac{1}{\tau(\phi, \theta_c)} = \frac{1}{\tau_{in}} + \frac{1}{\tau_{out}} \int_{\phi}^{\phi + \theta_c} d\phi' N(\phi') \left( 1 - \frac{\cos 2\phi'}{\cos 2\phi} \right). \quad (14)$$

The parameter  $a_0$  is given by

$$a_0 = \int_0^{\pi/4} d\phi N(\phi) \cos^2 2\phi. \quad (15)$$

The first and second terms contributing to  $1/\tau(\phi, \theta_c)$  come from frequency renormalization by the in- and out-of-plane impurities, respectively, while the third one is due to gap renormalization by out-of-plane impurities. In-plane impurities do not renormalize the gap, as is seen from Eq. (6).

The effect of the angle dependent density of states on the suppression of  $T_c$  is also illustrated in Fig. 1. To facilitate comparisons we have properly normalized all the densities of states. The observed dependences are easy to understand. Strong changes, with  $\phi$ , of the functions appearing in Eq. (12) diminish the integral on its right-hand side and this results in a weaker decrease of  $T_c$ . Physically it means that due to the angular dependence of spectrum the phase space is reduced and scatterers are effectively weaker pair breakers.

Straightforward differentiation leads to the following expression for the isotope coefficient  $\alpha$ :

$$\frac{\alpha_0}{\alpha} = 1 - \frac{1}{a_0} \int_0^{\pi/4} d\phi N(\phi) \cos^2 2\phi \rho_c(\phi, \theta_c) \times \psi' \left( \frac{1}{2} + \rho_c(\phi, \theta_c) \right). \quad (16)$$

The effect of angle dependence in  $N_F(\phi)$  on isotope coefficient is illustrated in Fig. 2. It is very small in relatively clean samples (large  $T_c/T_{c0}$ ) and increases for smaller  $T_c/T_{c0}$ . In order to see the simultaneous effect of both types of impurities on the isotope coefficient we have assumed that fraction  $x$  of impurities goes into planes while the rest into out-of-plane positions. Assuming that both types of impurities can be characterized by the same value of relaxation rate parameter, i.e.,  $1/\tau_{in} = 1/\tau_{out} = 1/\tau$ , we rewrite Eq. (14) as

$$\frac{1}{\tau(\phi, \theta_c)} = \frac{1}{\tau} \left[ x + (1-x) \int_{\phi}^{\phi + \theta_c} d\phi' N(\phi') \left( 1 - \frac{\cos 2\phi'}{\cos 2\phi} \right) \right]. \quad (17)$$

Figure 3 illustrates the changes of  $\alpha/\alpha_0$  with  $x$ . The bottom

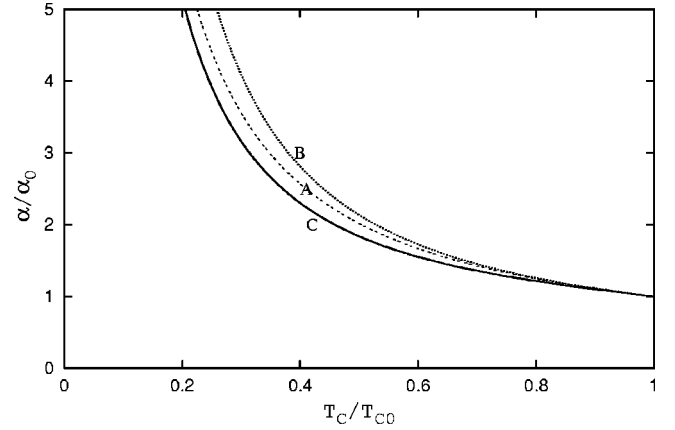


FIG. 2. Effect of the density of states on relative isotope effect. The curve labeled A refers to constant density of states  $N(\phi) = 1$ , B to  $N(\phi) = \pi/2 |\cos 2\phi|$ , and C to  $N(\phi) = \pi/2 |\cos 4\phi|$ .

curve in the figure corresponds to  $x=0$  and thus to the changes induced by the out-of-plane impurities while the top one corresponds to the case with all impurities occupying in-plane positions. The assumption  $\tau_{in} = \tau_{out}$  is not a realistic one. In fact to get the whole curve for  $x=0$  one has to take unphysically large values of  $1/\tau_{out} T_{c0}$ .

Figure 4 shows the changes of the normalized isotope coefficient with disorder characterized by the ratio  $T_c/T_{c0}$  (solid curve) together with experimental data<sup>18,19</sup> on  $\text{La}_{1.85}\text{Sr}_{0.15}\text{Cu}_{1-x}\text{M}_x\text{O}_4$  (points). A theoretical line has been calculated for  $d$ -wave superconductor with  $N_F(\phi) = 1$  and an angle independent scattering rate. As discussed above angle dependence adds a new degree of freedom.

## B. Impurity effects in $s$ -wave layered superconductor

In the  $s$ -wave superconductor the order parameter  $\Delta(\vec{k}) = \Delta_0$ , and nonmagnetic isotropic impurities change neither  $T_c$  nor the isotope coefficient  $\alpha$ . This is true for both in-plane and out-of-plane impurities.

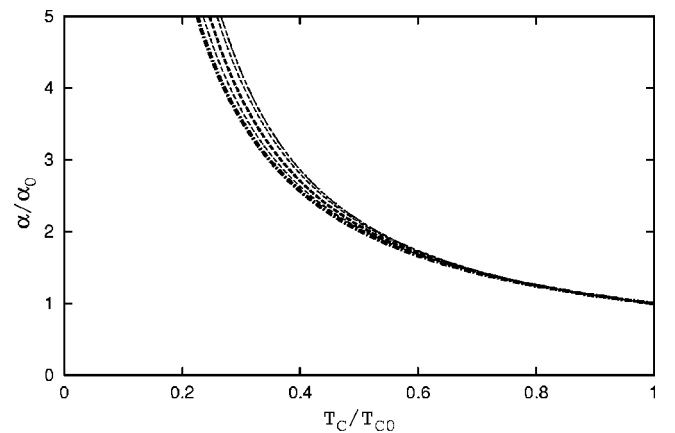


FIG. 3. Simultaneous effect of in-plane and out-of-plane impurities on the isotope coefficient for various values of  $x$  (from the bottom curve  $x=0.0, 0.01, 0.03, 0.1, 1.0$ ) which measure the relative contribution of in-plane impurities to the total scattering rate [c.f. Eq. (17)].

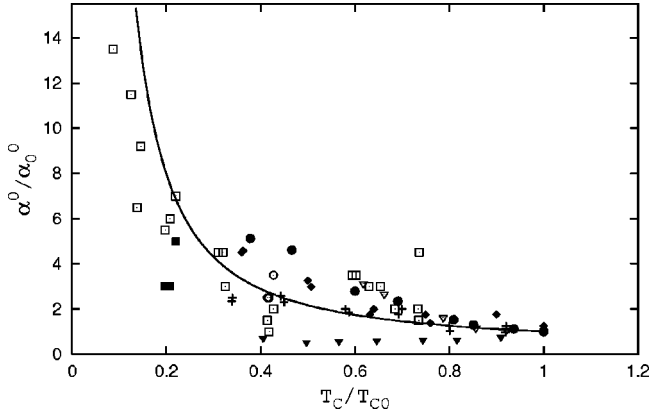


FIG. 4. The solid curve shows the universal dependence of the normalized isotope coefficient versus normalized transition temperature calculated for the  $d$ -wave impure superconductor with constant  $N_F$ . The data points are experimental values for a number of materials. Optimally doped  $\text{La}_{1.85}\text{Sr}_{0.15}\text{Cu}_{1-x}\text{M}_x\text{O}_4$  with  $M=\text{Co}$  (opened triangles),  $\text{Zn}$  (filled diamonds), and  $\text{Ni}$  (crosses); overdoped  $\text{La}_{1.80}\text{Sr}_{0.20}\text{Cu}_{1-x}\text{M}_x\text{O}_4$  with  $M=\text{Ni}$  (filled triangles),  $\text{Fe}$  (filled circles) (Ref. 18);  $\text{Y}_{1-x-y}\text{Pr}_x\text{Ca}_y\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$  with  $x=0.2$  and for  $y=0.15$  (opened circles),  $0.25$  (filled squares);  $\text{YBa}_2(\text{Cu}_{1-z}\text{Zn}_z)_3\text{O}_{7-\delta}$  (open squares) (Ref. 19).

Contrarily, the magnetic (in-plane) impurities are pair breakers in  $s$ -wave superconductors and do change  $T_c$ ,<sup>14,15</sup>

$$\ln \frac{T_c}{T_{c0}} = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \rho_c\right), \quad (18)$$

where  $\rho_c = 1/2\pi k_B T_c \tau_m$ ,  $\tau_m$  is the corresponding magnetic relaxation time. This leads to the changes of the isotope effect

$$\frac{\alpha_0}{\alpha} = 1 - \rho_c \psi'\left(\frac{1}{2} + \rho_c\right). \quad (19)$$

### C. Impurity effects of $p$ -wave layered superconductor

The order parameter of the  $p$ -wave superconductor is taken here as

$$\Delta(\phi) = \Delta_0 \cos \phi. \quad (20)$$

Repeating the calculations for the in-plane and out-of-plane impurities in the  $p$ -wave superconductor with constant density of states we get Eqs. (9)–(11) with

$$\gamma(\theta_c) = \frac{1}{2\tau_{\text{in}}\pi k_B T_c} + \frac{1}{2\tau_{\text{out}}\pi k_B T_c} \left(\frac{\theta_c^2}{6}\right).$$

It is important to note that for a constant density-of-states function the calculated changes of the isotope coefficient follow the universal curve independently which is the cause of the changing superconducting transition temperature. The universal  $\alpha/\alpha_0$  vs  $T_c/T_{c0}$  dependence is presented by curve A in Fig. 2. Note that numerically this dependence for the  $d$ -wave superconductor is the same as that obtained for magnetic impurities in the  $s$ -wave material.

### III. ANISOTROPIC MAGNETIC AND NONMAGNETIC IMPURITY POTENTIALS

High-temperature superconductors are strongly anisotropic systems with relatively low carrier concentration and layered structure. This means that the screening is not very effective and the impurity-quasiparticle interaction is anisotropic. This motivates the study of anisotropic impurities<sup>20</sup> in HTS's. The effect of anisotropic magnetic and nonmagnetic impurities on  $T_c$  of superconductors with the general form of the order parameter  $\Delta(\vec{k}) = \Delta e(\vec{k})$  have been considered in Ref. 20. These authors have taken the momentum-dependent impurity potential  $u(\vec{k}, \vec{k}') = v(\vec{k}, \vec{k}') + J(\vec{k}, \vec{k}') \vec{S} \cdot \vec{\sigma}$ , (where  $\vec{S}$  is a classical spin of the impurity and  $\vec{\sigma}$  the electron spin density) and assumed a separable form of scattering probabilities,

$$v^2(\vec{k}, \vec{k}') = v_0^2 + v_1^2 f(\vec{k}) f(\vec{k}'), \quad (21)$$

$$J^2(\vec{k}, \vec{k}') = J_0^2 + J_1^2 g(\vec{k}) g(\vec{k}'), \quad (22)$$

where  $v_0(v_1)$ ,  $J_0(J_1)$  are isotropic (anisotropic) scattering amplitudes for nonmagnetic and magnetic potentials.  $f(\vec{k})$ ,  $g(\vec{k})$  are the momentum-dependent anisotropy functions in the nonmagnetic and magnetic scattering channel, respectively. The averages over the Fermi surface of  $f(\vec{k})$  and  $g(\vec{k})$  vanish  $\langle f(\vec{k}) \rangle_{\text{FS}} = 0$  and are normalized as  $\langle f^2(\vec{k}) \rangle_{\text{FS}} = 1$ . The change of transition temperature calculated in the Born approximation is given in Ref. 20 and the isotope effect is found to be

$$\begin{aligned} \frac{\alpha_0}{\alpha} = & 1 - (1 - \langle e \rangle^2 - \langle ef \rangle^2) \cdot \left( \frac{\Gamma_0 + G_0}{2\pi k_B T_c} \right) \psi' \left[ \frac{1}{2} + \left( \frac{\Gamma_0 + G_0}{2\pi k_B T_c} \right) \right] \\ & - \langle ef \rangle^2 \left( \frac{\Gamma_0 + G_0 + G_1 - \Gamma_1}{2\pi k_B T_c} \right) \cdot \psi' \\ & \times \left( \frac{1}{2} + \frac{\Gamma_0 + G_0 + G_1 - \Gamma_1}{2\pi k_B T_c} \right) - \langle e \rangle^2 \left( \frac{2G_0}{2\pi k_B T_c} \right) \\ & \times \psi' \left( \frac{1}{2} + \frac{2G_0}{2\pi k_B T_c} \right), \end{aligned} \quad (23)$$

where  $\Gamma_0 = \pi n_i N_0 v_0^2$ ,  $\Gamma_1 = \pi n_i N_0 v_1^2$ ,  $G_0 = \pi n_i N_0 J_0^2 S(S+1)$ , and  $G_1 = \pi n_i N_0 J_1^2 S(S+1)$  are the respective scattering rates.

The dependence of  $\alpha/\alpha_0$  on  $T_c/T_{c0}$  has been shown in Fig. 5. The value of anisotropy of the  $\langle ef \rangle^2$  and the scattering  $\Gamma_1$  present new degrees of freedom which can be used to fit experimental data. The universality seen for isotropic scattering is lost in this scenario.

### IV. COMPARISON WITH EXPERIMENTS

Let us start the comparison of the obtained results with existing experimental data with a word of caution. There may exist a number of factors which can affect the value of isotope coefficient of the impure system  $\alpha$ . In particular electron-phonon interaction and the phonon spectrum may

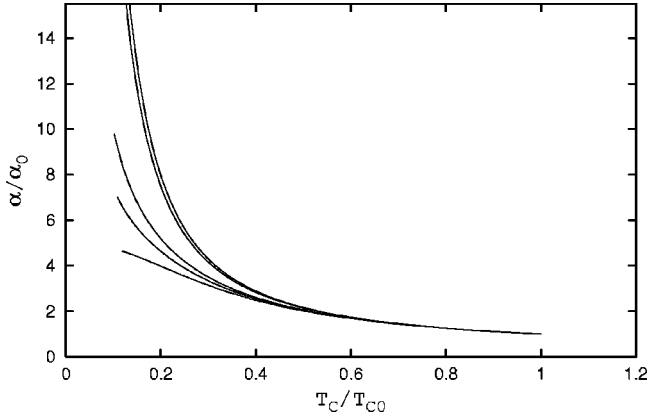


FIG. 5. The isotope coefficient of the  $d$  wave superconductor ( $\langle e \rangle = 0.0$ ), for different values of the normalized anisotropic scattering rate (from top):  $\Gamma_1/\Gamma_0 = 0.0, 0.5, 0.9, 0.95, 1.0$ . We have taken  $\langle ef \rangle^2 = 0.2$  and assumed nonmagnetic impurities.

change after the impurity doping. We do not take such effects into account.

We have also implicitly assumed that electron-phonon interaction does play a role in driving the superconducting instability of the system and makes the clean material coefficient  $\alpha_0$  nonzero albeit it may take on very small value. This, however, seems to be well established by various experimental techniques.<sup>21,22</sup>

Here we concentrate on the oxygen isotope effect, but it has to be noted that interesting results have also been obtained in the studies of copper isotope substitutions. The negative value of  $\alpha_{\text{Cu}}$  observed in some underdoped  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  samples,<sup>6,7</sup> have been recently explained<sup>23</sup> as due to scattering of electrons by low-frequency phonons with large momenta. It is to be checked whether the same mechanism is responsible for negative oxygen isotope effect in a very clean  $\text{Sr}_2\text{RuO}_4$   $p$ -wave superconductor.<sup>24</sup>

The oxygen isotope shift in high-temperature superconductors does depend on the concentration of carriers. The explanation of this dependence has been a subject of a number of papers.<sup>25–30</sup> The authors invoke such effects as: anharmonicity, zero-point motion, mass dependence of carrier concentration, energy dependence of the density of states, opening of the normal-state pseudogap, and the  $T_c$  changes due to impurities.

In the present work we contribute to the elucidation of the role played by various impurities in changing  $T_c$  and  $\alpha$  of superconductors. Because the  $T_c$  reduction due to dopant impurities like Sr in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  is small their influence on  $\alpha$  follows the standard curve like one presented in Fig. 4. The departures would be seen for a smaller ratio of  $T_c/T_{c0}$  as is evident from Fig. 3. Small values of  $\theta_c$  which reflect weaker pair breaking character of out-of-plane impurities do not influence the slope of the  $\alpha/\alpha_0$  vs  $T_c/T_{c0}$  curve. Isotope changes due to impurities in systems with the same bare scattering rate but with differing values of  $\theta_c$  follow the same universal curve.

On the other hand, the effect of anisotropic impurity scattering changes the universal dependence. Isotope coefficients of the systems with various degrees of anisotropy follow

slightly differing curves. This additional degree of freedom allows for a better fit to the experimental data. The fit, however, is ambiguous. The same changes can be induced by anisotropy of scattering and the anisotropy of the order parameter.

## V. ISOTOPE EFFECT IN IMPURE STRIPED CUPRATES

The strong sensitivity of  $T_c$  to in-plane impurities in high-temperature superconductors, independently on their magnetic nature, and the difficulties of the existing theories to fully describe the wealth of experimental data has resulted in new approaches to the problem. In a recent work Smith *et al.*<sup>31</sup> have developed the scenario of  $T_c$  suppression by Zn impurities, based on the stripe picture of high- $T_c$  oxides. Assuming that the doped Zn does not affect the superfluid density the authors considered the increase of local inertia of the stripe due to pinning forces and local slowing down of their dynamics. The calculations within this model give, in agreement with experimental findings, the suppression of  $T_c$  which is linear in the concentration of impurities  $z$ . It also gives the quadratic dependence of critical Zn concentration  $z_c$  ( $z_c$  is the concentration at which superconductivity disappears) on the superconducting transition temperature of Zn-free (“clean”) systems  $T_{c0}$ .

The resulting formula for  $T_c$  suppression in the regime of incompressible stripes is<sup>31</sup>

$$\frac{T_c}{T_{c0}} = 1 - \frac{\gamma z}{T_{c0}^2}, \quad (24)$$

where  $z$  is the concentration of Zn (or other in-plane impurities),  $\gamma$  is a factor depending *inter alia* on the stripe distance and lattice constant  $a$ . In the optimally doped and overdoped region, where charged stripes behave as a compressible quantum fluid, the  $T_c$  reduction has been found to be universal and given by

$$\frac{T_c}{T_{c0}} = 1 - \frac{z}{z_c}. \quad (25)$$

with constant  $z_c$ .

In the stripe scenario we find that the change of the isotope coefficient due to impurities reads

$$\alpha/\alpha_0 = \frac{2}{(T_c/T_{c0})} - 1 \quad (26)$$

in the incompressible region and

$$\alpha/\alpha_0 = 1 \quad (27)$$

in the compressible region (See Fig. 6).

Roughly inverse dependence of  $\alpha/\alpha_0$  on  $T_c/T_{c0}$  at low  $T_c$  is in good qualitative agreement with experimental data (cf. Fig. 4) and gives credit to the stripe picture of superconductivity in this material.

It is, however, hard to explain the difference between Fe and Ni substitution to the otherwise overdoped  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  sample. According to the theory<sup>31</sup> one ex-

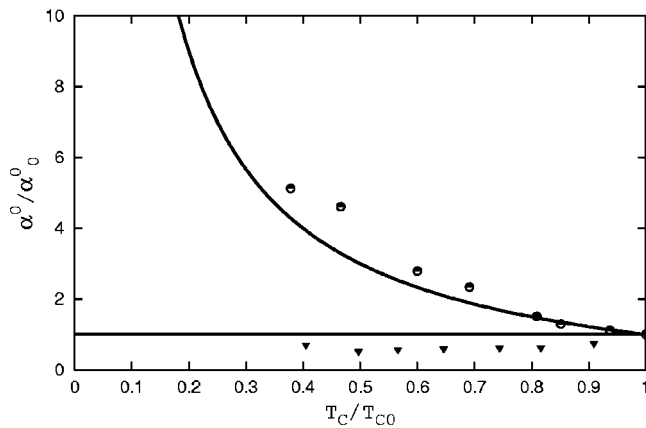


FIG. 6. The isotope effect in impure striped cuprates. The continuous line is given by Eqs. (26) and (27). The data points are experimental values for overdoped  $\text{La}_{1.80}\text{Sr}_{0.20}\text{Cu}_{1-x}\text{M}_x\text{O}_4$ , with Ni (filled triangles), Fe (circles) (Ref. 18).

pects in this material incommensurate stripes and thus no influence of impurities on both  $T_c$  and  $\alpha$ . The difficulty arises from the fact that both impurities (Ni and Fe) do change the transition temperature but the isotope shift is nearly constant for Ni substitution. One explanation is that concentration of carriers may change in the doping process. The divalent Ni does not change the concentration and the position of the Fermi level remains roughly constant while trivalent Fe ions change it driving the system effectively into an underdoped or optimally doped regime. If this is true the Fe doped system is thus expected, within the stripe scenario, to change both  $T_c$  and  $\alpha$ .

It is obvious that the isotope coefficient  $\alpha$  of the impure system can take nonzero values only for those systems for which  $T_{c0}$  depends on an isotope mass and  $\alpha_0 \neq 0$ . The question thus arises whether the formation of stripes and the driving mechanism of superconductivity in striped metal are of purely electronic origin or electron-phonon interaction plays

the role to make  $\alpha_0 \neq 0$ . These issues have been recently addressed.<sup>32</sup> The x-ray appearance near-edge structure experiments revealed a large oxygen isotope effect on the stripe formation temperature  $T^*$ , as also on effective supercarrier mass. This shows that electron-phonon interaction does play a role in a stripe model of superconductivity and validates the above analysis and conclusions.

## VI. CONCLUSIONS

We have studied the effect of various impurities on the isotope coefficient  $\alpha$ . While the in-plane and out-of-plane impurities affect the superconducting transition temperature quite differently (c.f. Fig. 1), their influence on  $\alpha$  is universal for the angle independent scattering relaxation rate and density-of-states function.

Experimental changes of  $\alpha/\alpha_0$  with  $T_c/T_{c0}$  for a number of high-temperature copper oxides can be well described solely by the effect of impurities on  $d$ -wave superconductors. The angle dependence of relaxation rate and  $N_F(\phi)$  or the simultaneous presence of anisotropic scatterers of magnetic and nonmagnetic nature adds new degrees of freedom which can be used to quantitatively describe the data.

These mechanisms of  $T_c$  and  $\alpha$  changes operate for both dopant (like Sr) and extra impurities (like Ni or Zn). However, they do not differentiate between underdoped and overdoped systems. On the other hand, the stripe model of superconductivity describes the detrimental effect of Ni or Zn on  $T_c$ . The stripe theory predicts an increase of  $\alpha$  with impurity concentration on the underdoped side of the phase diagram and no change of it in the overdoped region. This agrees with data<sup>18</sup> on Ni and Fe doped  $\text{La}_{1.80}\text{Sr}_{0.20}\text{Cu}_{1-x}\text{Ni(Fe)}_x\text{O}_4$ .

## ACKNOWLEDGMENT

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