

Theoretical aspect on solid state device by ionic C_{60} superconductors

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Abstract

For ionic superconductors (C_{60}^{3-} , C_{60}^{3+}) in a field-effect transistor (FET), an extended BCS-like equation is presented in order to make clear the mechanism of such exotic superconductivity, and to apply to solid state device. Within the theory of phonon-mediated superconductivity, the possibility of higher transition temperature T_c and the role of various inter- and intramolecular phonons are discussed in comparison with bulk superconductivity in alkali-doped A_3C_{60} . Although ionic C_{60}^{3-} and C_{60}^{3+} superconductors have two-dimensional structure in FET-device, it is indicated that the mechanism of superconductivity can be explained in a unified picture with three-dimensional bulk C_{60} superconductors (A_3C_{60}).

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1. Introduction

Recently, ionic superconductors (C_{60}^{3-} [1], C_{60}^{3+} [2]) are observed by the technique of gate-induced doping in a field-effect transistor (FET) with C_{60} single crystals. This gate-induced superconductivity shows n - and p -channel activity, and allows switching between insulating and superconducting states. In order to apply to solid state device, it is necessary to make clear the mechanism of these ionic C_{60} superconductors.

C_{60} -based compounds are known as fullerenes. Crystalline C_{60} is normally an insulator, but can be made metallic by electron doping or hole doping. The

filling of the energy bands is tried to control by the applied gate voltage [1,2]. On the other hand, this charge transfer can be made easily by chemical doping. Alkali metal-doped compounds A_3C_{60} ($A=K, Rb$, etc.) are already known as metallic, and at low temperatures, become to be superconductors [3]. By recent experimental efforts, the superconductivity in a C_{60} field-effect device is considered as the same type as in A_3C_{60} .

Superconductivity observed in A_3C_{60} is a well-known subject with high transition temperature T_c , surpassed only by the copper oxides, and seems to be explained by Schlüter et al. [4] and Varma et al. [5] in standard terms using McMillan's formula for T_c :

- (1) T_c values exceeding 30 K result from the coupling between conduction electrons in C_{60}

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π -orbitals and intramolecular vibrations with high frequencies.

- (2) T_c shows the linear relation to the lattice constant a_0 in FCC- A_3C_{60} , causing by the linear dependence of T_c on electron density of states (DOS) at the Fermi level $N(0)$.

However, a_0 dependence of T_c deviates from the linear relation and T_c goes down rapidly with decreasing a_0 in ternary fullerenes $Na_2A'C_{60}$ ($A'=K, Rb, Cs$) with smaller lattice constant [6]. Furthermore, the addition of NH_3 ions to A_3C_{60} compounds so as to expand a_0 mostly fails in the enhancement of T_c in spite of much experimental effort [7].

In this paper, therefore, we present a theory of phonon-mediated superconductivity, which leads to an extended BCS-like formula for T_c different from the conventional McMillan's equation, and explain the various experimental results including recent data on C_{60}^{3-} , C_{60}^{3+} and $Na_2A'C_{60}$. The unusual lattice dependence of T_c derived theoretically is in good agreement with the experimental data in Na-containing compounds. The most noticeable point of this theory is that each role of intermolecular acoustic, optical and intramolecular phonons can be discussed with the contribution of light alkali ions. Basing on this theoretical approach, the mechanism of ionic superconductors C_{60}^{3-} and C_{60}^{3+} without including alkali metals would be analyzed in order to extend not only to field-effect device but also to anion or cation conductor.

2. Theory

Since the recent discovery of MgB_2 superconductor with $T_c=39$ K [8], phonon-mediated superconductivity becomes an attractive problem going abreast of exotic superconductivity of high- T_c cuprates. Because the possibility of a maximum T_c for phonon-driven superconductors might be open to question, contrary to the limit $T_c=30$ – 40 K predicted by BCS theory, it will be useful to reconstruct the equation of T_c for C_{60} -based superconductors.

In this section, therefore, a simplified weak-coupling theory is presented in order to understand the phonon-mediated superconductivity with the isotope

effect $T_c \propto M^{-\alpha}$ ($\alpha \sim 0.3$) for the substitution $^{12}C \rightarrow ^{13}C$ in Rb_3C_{60} . Due to the large mass difference between C_{60} and $A(A')$, the vibrations of A_3C_{60} solid are well separated into acoustic branches of mostly C_{60} character at low frequencies ($\omega_a \sim 50$ cm^{-1}) and optical branches of mostly alkali character at higher frequencies ($\omega_o \sim 100$ cm^{-1}). Therefore, it is useful to adopt the site representation formalism developed by Appel and Kohn [9]. Within the framework of BCS theory, Appel and Kohn gave a homogeneous integral equation in site representation for the vertex part Γ , from which the critical temperature T_c is calculated. Denoting the irreducible effective electron–electron interaction vertex by I , electron Green's function by G and Matsubara frequency by ω , Appel–Kohn equation is expressed in a schematic diagram form such as

$$\begin{array}{c} n_1', \omega' \quad n_1, \omega \\ \boxed{\Gamma} \\ n_2', -\omega' \quad n_2, -\omega \end{array} = \begin{array}{c} n_1', \omega' \quad n_1'', \omega'' \quad n_1'', \omega'' \quad n_1, \omega \\ \boxed{\Gamma} \quad \boxed{G} \quad \boxed{I} \\ n_2', -\omega' \quad n_2'', -\omega'' \quad n_2'', -\omega'' \quad n_2, -\omega \end{array}$$

The site representation is referred to as an orthonormal set of the Wannier functions $W_I(r-n_I)$ at C_{60} sites n_I on FCC lattice and $W_{II}(r-n_{II})$ at the tetrahedral A(T) sites n_{II} . A(T) site is the center of the tetrahedron consisting of four nearest-neighboring C_{60} molecules that are independent with each other in the FCC lattice. The final form for the equation is expressed as

$$\Gamma(n, \omega) = \beta^{-1} \sum_{n', \omega'} \Gamma(n', \omega') K(n', \omega'; n, \omega), \quad (1)$$

with

$$\begin{aligned} K(n', \omega'; n, \omega) = & - \sum_{n''} F(n'', \omega') \\ & \times I(n' - n'', \omega'; n, \omega), \end{aligned} \quad (2)$$

where the function

$$F(n, \omega) = \sum_{m_2} G(m_2 + n, \omega) G(m_2, -\omega) \quad (3)$$

describes the propagation of an electron pair. The contracted interaction vertex I is divided into phonon part and Coulomb part:

$$I(n'\omega'; n\omega) = I_{\text{ph}}(n'\omega'; n\omega) + I_{\text{C}}(n'\omega'; n\omega). \quad (4)$$

The Coulomb part may be assumed to be of short range, and it is put as

$$I_{\text{C}}(n', n; \omega) = \delta_{n',0} \delta_{n,0} U. \quad (5)$$

A merit of site representation formalism in the present problem is that the phonon part of the interaction vertex $I_{\text{ph}}(\omega', \omega)$ takes on a form such that the roles played by acoustic and optical phonons may be separated:

$$I_{\text{ph}} = I_{\text{a}} + I_{\text{o}}. \quad (6)$$

Thus the eigenvectors of acoustic phonon and intramolecular higher phonon have large amplitudes on C_{60} sites whereas those of optical phonon at $A(T)$ sites. This is reflected to the site- and mode-dependence of phonon Green's function.

Another noticeable point is that the phonon due to C_{60} intramolecular vibration exists with the highest frequency: $\omega_{\text{t}} \sim 1500 \text{ cm}^{-1}$ modes are mostly tangential in character (Ag(2), Hg(5)–Hg(8) modes) and $\omega_{\text{r}} \sim 1000 \text{ cm}^{-1}$ modes have mostly radical character (Ag(1), Hg(1)–Hg(4) modes) [4]. Therefore, the cutoff frequency below which the effective interelectron interaction becomes attractive is different for various phonon modes:

$$\omega_{\text{a}} < \omega_{\text{o}} \ll \omega_{\text{r}} < \omega_{\text{t}}. \quad (7)$$

Hereafter, the main cutoff frequencies ω_{a} , ω_{o} , ω_{t} are used for acoustic, optical and tangential high-frequency phonons, respectively. It is guessed that the highest phonon will give rise to attractive interaction I_{H} for wider range of electron pair energy, and to yield higher T_{c} .

By adopting the contact approximation on Eqs. (1) and (4), a homogeneous integral equation is set up for the vertex part Γ from which the critical temperature T_{c} is calculated [10];

$$\Gamma(\omega) = -\beta^{-1} \sum_{\omega'} \Gamma(\omega') F(\omega') [I_{\text{ph}}(\omega', \omega) + U]. \quad (8)$$

In the weak coupling theory, we take I_{ph} constants (I_{a} , I_{o} , I_{H}) according to the effective energy range for acoustic, optical and highest phonons respectively:

$$I_{\text{ph}}(\omega', \omega) = \begin{cases} -(I_{\text{a}} + I_{\text{o}} + I_{\text{H}}), & 0 < |\omega|, |\omega'| \leq \omega_{\text{a}}, \\ -(I_{\text{o}} + I_{\text{H}}), & \omega_{\text{a}} < |\omega|, |\omega'| \leq \omega_{\text{o}}, \\ -I_{\text{H}}, & \omega_{\text{o}} < |\omega|, |\omega'| \leq \omega_{\text{t}}, \\ 0, & \text{otherwise.} \end{cases} \quad (9)$$

Then, the solution of Eq. (8) should have a form

$$\Gamma(\omega) = \begin{cases} \Gamma_{\text{C}} + \Gamma_{\text{o}} + \Gamma_{\text{a}}, & 0 < |\omega| \leq \omega_{\text{a}}, \\ \Gamma_{\text{C}} + \Gamma_{\text{o}}, & \omega_{\text{a}} < |\omega| \leq \omega_{\text{o}}, \\ \Gamma_{\text{C}}, & \omega_{\text{o}} < |\omega| \leq \omega_{\text{F}}, \\ 0, & \text{otherwise,} \end{cases} \quad (10)$$

where Γ_{a} , Γ_{o} and Γ_{C} are contributed by acoustic phonon, optical phonon and Coulomb force, respectively, and the cutoff frequency for electron–electron Coulomb interaction is denoted by ω_{F} . The vertex part Γ corresponding to I_{H} is also made at the C_{60} site, and should be renormalized to Γ_{a} by using the different phonon frequency ω_{t} .

Now, it is convenient to define for acoustic phonon

$$\beta^{-1} \sum_{|\omega| \leq \omega_{\text{a}}} F(\omega) = N(0) \ln \alpha \beta \omega_{\text{a}} \equiv f_{\text{a}} \quad (11)$$

with $\alpha = 2e^{\gamma}/\pi = 1.13$ (γ =Euler's constant) for C_{60} -site intermolecular mode ω_{a} , and similarly f_{o} for optical phonon, f_{H} for high-frequency phonon and f_{F} for Coulomb part are defined by replacing ω_{a} in f_{a} by $A(A')$ -site mode ω_{o} , C_{60} -site intramolecular tangential mode ω_{t} and Coulomb cutoff frequency ω_{F} , respectively. It should be noticed that f_{H} is renormalized to f_{a} made at C_{60} site with ω_{t} in spite of ω_{a} .

Hence, Eq. (8) is transcribed into coupled three linear equations for three quantities Γ_s (s=a, o, C):

$$\Gamma_C = -U(f_a\Gamma_a + f_o\Gamma_o + f_F\Gamma_C), \quad (12)$$

$$\Gamma_o = I_o(f_a\Gamma_a + f_o\Gamma_o + f_o\Gamma_C), \quad (13)$$

$$\Gamma_a = (I_a + I_H)f_a(\Gamma_a + \Gamma_o + \Gamma_C). \quad (14)$$

It is evident that T_c should be determined from the solubility condition for the homogeneous linear Eqs. (12)–(14) and it needs only short algebra to have a condition

$$f_a I_{\text{eff}} = 1, \quad (15)$$

with

$$I_{\text{eff}} = (I_a + I_H) + \frac{I_o - U^*}{1 - (I_o - U^*)N(0)\ln(\omega_o/\omega_t)}, \quad (16)$$

and

$$U^* = \frac{U}{1 + N(0)U\ln(\omega_F/\omega_t)}. \quad (17)$$

Here, to eliminate f_F and f_o in terms of f_a , use has been made of the relations

$$f_F = f_o + N(0)\ln(\omega_F/\omega_o), \quad (18)$$

and

$$f_o = f_a + N(0)\ln(\omega_o/\omega_a). \quad (19)$$

Thus, by solving conditions (15) and (16) for T_c , the transition temperature is given as

$$k_B T_c = 1.13\omega_a \exp[-1/N(0)I_{\text{eff}}], \quad (20)$$

which is the same form with the generalized BCS theory. I_{eff} in Eq. (20) varies from $I_a + I_H$ substantially because of the presence of the last term in Eq. (16). When intramolecular phonon propagation part I_H is playing a primary role in maintaining the electron pair correlation, most strong effect of the lattice distortions will be received by an electron pair which is located at C_{60} site. The cutoff frequency (ω_a , ω_t) below which

the effective interelectron interaction becomes attractive is different for inter- and intramolecular phonons on C_{60} site. It is guessed that the contribution of optical phonon to T_c is enhanced by I_o and reduced by a factor $\ln(\omega_o/\omega_t)$ in the last term of Eq. (16). The role of doped alkali ions except for introducing electron density would be worth to examine on the appearance of superconductivity in the next section.

3. Numerical results

In the previous section, an equation for T_c is presented for C_{60} -based superconductors in spite of whether alkali ions are doped in the three-dimensional (3D) bulk C_{60} (A_3C_{60} , $A_2A'C_{60}$) or not as quasi-two-dimensional (2D) FET C_{60} (C_{60}^{3-} , C_{60}^{3+}). Here using Eqs. (16), (17) and (20), we show numerical results on unusual lattice dependence of T_c in these electron-doped or hole-doped C_{60} superconductors, and discuss the difference between bulk and FET C_{60} .

3.1. Role of optical phonon

Within the framework of weak-coupling theory, we observe in Eqs. (16) and (20) that the optical phonon part I_o contributes to enhance T_c by the addition to the dominant interaction part $I_a + I_H$ ($I_a \ll I_H$). I_H is given by 37.2 meV as the electron-phonon coupling constant [4] due to intramolecular higher phonon frequencies (Hg(1–8) and Ag(1–2) modes) at C_{60} site, whereas I_o is the optical phonon–electron coupling constant at the A(A') site to give rise to the attractive interaction for ω between ω_a and ω_o . Approximating as $I_a + I_H \sim I_H$ in Eq. (16), I_{eff}/I_H is indicated as the function of I_o/I_H in Fig. 1. It is guessed that $I_o/I_H=0.6$ is a reasonable value to fit to $T_c=29$ K for a typical example Rb_3C_{60} ($N(0)=22$ states/eV). When I_o/I_H exceeds 0.18, I_{eff} becomes larger than I_H , which means that the optical phonon assists the appearance of superconductivity, and that T_c has the higher value than that explained by noticeable intramolecular phonon modes in conventional McMillan's equation. If I_o/I_H becomes smaller than 0.18, the existence of optical phonon disturbs the superconductivity. The boundary line, $I_o/I_H=0.18$, is the value of no contribution of phonon by doped alkali ions on superconductivity. The expected value

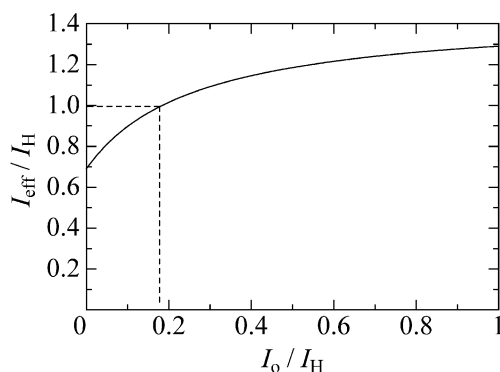


Fig. 1. I_0/I_H dependence of I_{eff}/I_H in Eq. (16).

for A_3C_{60} system, $I_0/I_H=0.6$, makes $I_{\text{eff}}/I_H \sim 1.2$, which means about 20% enhancement of T_c by the existence of alkali ions.

In Fig. 2(a), the result of T_c-a_0 relation is shown as a solid curve for $\omega_a \sim 50 \text{ cm}^{-1}$ and a parameter $I_0/I_H=0.6$ in good agreement with experimental data in the almost a_0 region. By the conventional equation, it is impossible to fit to the experimental T_c-a_0 relation for so long a_0 region. In the present calculation, $T_c-N(0)$ curve in Fig. 2(b) and $N(0)-a_0$ relation in Fig. 2(c) are used to make the systematic T_c-a_0 relation. The monotonic behavior shown by the solid curve comes from the linear dependence of T_c on density of states at the Fermi level $N(0)$, which can be understood as the case with large Coulomb interaction $\mu^*=N(0)U^*$ (~ 0.2 , which will be discussed in detail in the next paragraph) in BCS-like formula for T_c . On the calculation of a_0 dependence of $N(0)$, NMR data for K_3C_{60} and Rb_3C_{60} [11] is interpolated to adjust to $N(0)-a_0$ relation by the band calculation [12].

Here assuming that the acoustic phonon shows a kind of softening due to C_{60} intermolecular orientation ordering at smaller a_0 ($\omega_a \rightarrow 0$), we obtain the dotted curve going down to $T=0$ at $a_0=14.06 \text{ \AA}$. In the

smaller a_0 region, the strong intermolecular interaction among four nearest neighboring C_{60} molecules changes the monotonic T_c-a_0 relation to correlating with FCC \rightarrow SC structural phase transition due to the ordering of C_{60} orientation [13].

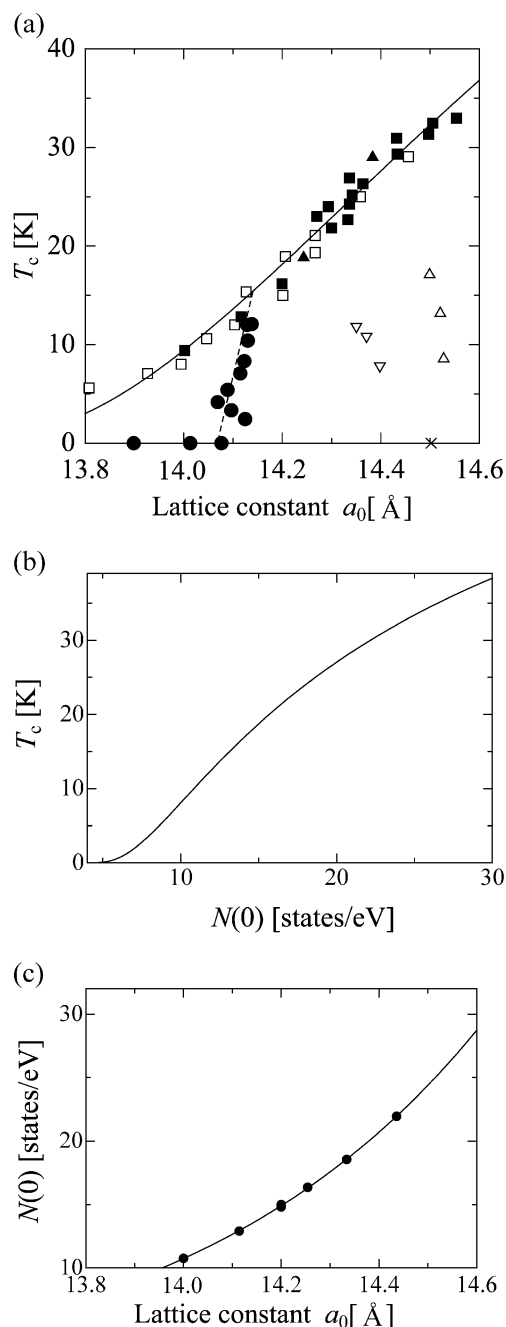


Fig. 2. (a) Calculated results of T_c-a_0 relation for various C_{60} -based superconductors. $I_0/I_H=0.6$ is adopted to lead $T_c \sim 30 \text{ K}$ in Rb_3C_{60} for $N(0)=22 \text{ states/eV}$ and $I_H=37.2 \text{ meV}$. $\mu^*=N(0)U^*=0.15$ is used by the estimation in Section 3.2; solid line: $\omega_a=50 \text{ cm}^{-1}$, broken line: Na-included A_3C_{60} type by taking into account the softening of ω_a . Experimental data are plotted as the symbols \blacksquare , \square , \blacktriangle , \bullet , \triangle , ∇ , \times in the figure, where \square : Na_2A' C_{60} ; \triangle , ∇ , \times : NH_3 -included compounds. (b) $N(0)$ dependence of T_c calculated from Eqs. (16) and (20). (c) $N(0)-a_0$ relation adopted in the calculation of (a), which is referred to band calculation [12] and NMR data [11] to make a smooth curve.

Thus, although rough estimation of T_c might be decided by intramolecular tangential mode ω_t , various kinds of phonons play each important role in the equation of T_c as in Eqs. (16), (17) and (20), and contribute to make the interesting physical properties.

3.2. Coulomb repulsion

In the previous section, Coulomb repulsion is given in a dimensionless form by $\mu^*=N(0)U^*$ derived from Eq. (17), where the effective Coulomb interaction U^* becomes smaller than the original U by the reason that Coulomb cutoff frequency is ought to be larger than the highest phonon frequency, that is, $\omega_F \gg \omega_t$. Eq. (17) is, therefore, a right expression with physical meaning. However, in the process of the derivation of Eq. (16), $\ln(\omega_F/\omega_t)$ in the denominator of Eq. (17) was $\ln(\omega_F/\omega_0)$ primarily. This might be the origin of the fact that μ^* in C_{60} -based superconductors is observed as about 0.2 [11], which is a fairly large value different from $\mu^*=0.1$ in most of typical superconductors.

Hence, let us estimate the value of μ^* within the present theory.

Assuming the regular value as

$$\frac{N(0)U}{1 + N(0)U \ln(\omega_F/\omega_0)} = 0.1, \quad (21)$$

we obtain the value of $\mu^*=N(0)U^*$ with Eq. (17) as about 0.15, where the simple calculation is performed by taking into account $\ln(\omega_F/\omega_t) = \ln(\omega_F/\omega_0) - \ln(\omega_t/\omega_0)$ with $\omega_0 = 100 \text{ cm}^{-1}$ and $\omega_t = 1500 \text{ cm}^{-1}$. In Fig. 2(a), $T_c - a_0$ curve is depicted for $\mu^*=0.15$, which describes naturally the best fit to most of experimental data for the wide region of a_0 .

Thus the observed Coulomb repulsion $\mu^*=0.2$ was proved to be reasonable value from the theoretical viewpoint. The monotonic $T_c - a_0$ relation can be mainly deduced from BCS-like equation with this large μ^* .

3.3. Ionic superconductor

In this section, the observed two kinds of transition temperature, $T_c(C_{60}^{3-}) = 11 \text{ K}$ and $T_c(C_{60}^{3+}) = 52 \text{ K}$ [1,2], will be analyzed basing on the present theory, and the possibility of $T_c > 50 \text{ K}$ will be discussed by the model calculation.

The most interesting point is whether the existence of alkali-ions promotes or disturbs the occurrence of superconductivity. To analyze the ionic C_{60} superconductors in FET device, it is worth showing the calculated results without phonons due to the doped alkali ions. In Fig. 3, the solid line is the curve described for a parameter $I_o/I_H = 0.6$ as the same as the solid line in Fig. 2(a), which is the case of best fit to experimental data. The broken line is the case for $I_o/I_H = 0.18$, which is a parameter corresponding to that where optical phonon plays no role, as mentioned in Section 3.1. By estimating the value of T_c on the broken line for the lattice constant in C_{60}^{3-} , $a_0 = 14.16 \text{ \AA}$, we can predict $T_c(C_{60}^{3-}) \sim 9 \text{ K}$, which is in fairly good agreement with the observed 11 K and is considerably lower than $T_c(A_3C_{60}) \sim 16 \text{ K}$ on the solid line. Thus the superconductivity by electron doping (C_{60}^{3-} , A_3C_{60}) can be explained in the same mechanism. Optical phonon due to the doped alkali ions contributes to the defense of direct $C_{60} - C_{60}$ interaction in order to disturb FCC \rightarrow SC phase transition, and to assist T_c . In 2D FET device, ionic C_{60} superconductors are composed of only a single layer of C_{60} molecules, and therefore, $C_{60} - C_{60}$ orientation ordering ought not to take place from the outset.

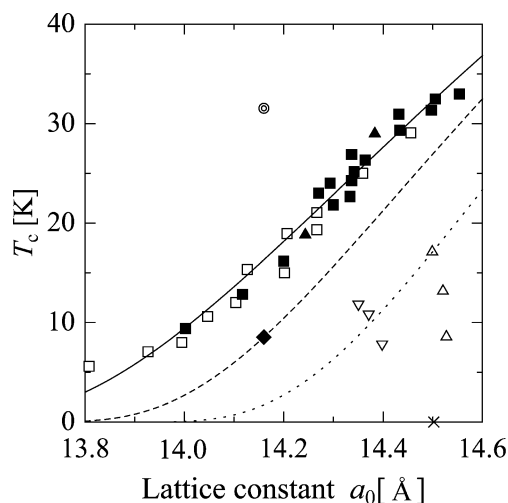


Fig. 3. $T_c - a_0$ relation curve for assuming the different contribution of I_o , I_o/I_H , without FCC \rightarrow SC phase transition; solid line: $I_o/I_H = 0.6$ for the case that optical phonon assists T_c ; broken line: $I_o/I_H = 0.18$ for no contribution of optical phonon; and dotted line: $I_o/I_H = 0$ for the case that optical phonon disturbs T_c extremely. \blacklozenge is the point predicted for C_{60}^{3-} , and \odot for C_{60}^{3+} .

Now, T_c can be varied by changing the band filling (doping level) or by changing the band width (lattice parameter). It is because T_c is decided as a function of electron (or hole) density. In FET C_{60} , the density of states at the Fermi level, $N(0)$, is controlled by the applied gate voltage. As C_{60} is strongly electronegative, adding holes to C_{60} (e.g. C_{60}^{3+}) is expected to be very difficult. However, if hole-doping in C_{60} would be performed, $T_c(C_{60}^{3+}) > T_c(C_{60}^{3-})$ might be predicted, because $N(0)$ for C_{60}^{3+} is larger than that for C_{60}^{3-} as shown in the band calculation [14]. Estimating $N(0)$ for C_{60}^{3+} as twice of $N(0)=14$ states/eV for C_{60}^{3-} with $a_0=14.16\text{\AA}$, and probably the maximum $N(0)$ value in the conduction band, T_c can be presented through Fig. 2(b),(c) to be $T_c(C_{60}^{3+}) \sim 32$ K. This is certainly larger than $T_c(C_{60}^{3-})$ and also than $T_c(A_3C_{60})$, but is exceptionally smaller than the observed $T_c=52$ K. The origin of this discrepancy will be elucidated in the near future. Within this calculation, we could get the optimum $T_c \sim 54$ K for hole-doped C_{60} with the limit $I_0/I_H=1$ at $a_0=14.6\text{\AA}$ just before Mott-Insulator transition.

Although the optimum condition of T_c is of course that the Fermi level lies at the maximum point in the density of states of the conduction band, whether optical phonon assists or disturbs T_c gives an interesting contribution in addition to the conventional mechanism of superconductivity.

4. Discussion and conclusions

In a C_{60} -based FET device, the channel becomes a superconductor depending both on the temperature and on the applied gate voltage. As mentioned in the previous section, the mechanism of these ionic superconductors can be explained within a phonon-mediated weak coupling theory. The two-dimensional nature of the channel is the same condition with the so-called high- T_c superconductors. These low interface density of states of FET will be useful to the application to solid state device and also to the next research on high- T_c superconductors.

The most interesting behavior of C_{60} -based molecular superconductors is (1) a rather high T_c and (2) the anomaly in T_c - a_0 relation. According to the previous section, (1) originates from the Cooper pairing mediated by intramolecular phonon with

C_{60} tangential high-frequency modes ω_t , and (2) from large μ^* and C_{60} molecular orientation ordering through the softening of the intermolecular acoustic phonon mode ω_a .

In the present formula, high T_c has two aspects: (i) The different phonon modes (ω_a , ω_t) are made at the same C_{60} site. If C_{60} molecule is treated as a huge atom without intramolecular phonons, $I_H=0$ and $\omega_t=\omega_a$ lead to $T_c=0$. (ii) The optical (or nonacoustic) phonon is mainly made at the A(A') site and possibly also at C_{60} site. The region of I_0/I_H larger than 0.18 exhibits the contribution of A(A') site optical phonon to enhance T_c .

Thus, light alkali ions play a role to create the competition between two transition points, T_c and $T_{FCC \rightarrow SC}$ in superconducting fullerenes. In this approach, low ω_a takes the lead in the equation for T_c , and therefore, Migdal theorem is conserved because of $\omega_a \ll \varepsilon_F$ (~ 0.2 eV). This weak-coupling theory is successful in analyzing explicitly the role of each phonon on T_c , from which it might be easy to explicit new molecular superconductors in the near future.¹

Furthermore, basing on this theory, the unusual isotope effect on T_c with $\alpha \neq 0.5$ ($T_c \propto M^{-\alpha}$ for the isotope mass M) by $^{12}\text{C} \rightarrow ^{13}\text{C}$ substitution will be predicted in another paper. The anomalous behavior by partial substitution (for example, the difference between atomically substitution and solid solution [15], $T_c(\text{Rb}_3[^{12}\text{C}_{0.5}^{13}\text{C}_{0.5}]_{60}) \neq T_c(\text{Rb}_3[^{12}\text{C}_{60}]_{0.5}[^{13}\text{C}_{60}]_{0.5})$) might be driven from the characteristic structure of the soccer-ball-shaped C_{60} molecule. By taking account of the several roles of various phonons, the isotope effect in ionic C_{60} superconductors should be explained as the different one from the anomaly of the isotope effect in alkali-doped C_{60} superconductors.

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¹ Before this study was published, $T_c=117$ K for hole-doped C_{60}/CHBr_3 was observed by Schön et al. [16], which would be explained by the additional mechanism in excess of phonon-mediated superconductivity.

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