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An evaluation of Temperature Dependent Energy Gap Parameter for Organic Superconductor

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Abstract: Using BCS- theory, we have evaluated the temperature dependent energy gapparameter Δ(T) of organic superconductors having TC between 10K to 12K. Our theoretically evaluated results are in good agreement with the experimental data and also with other theoretical workers.

Key words: Organic superconductors, Temperature dependent energy gap parameter,BCS-theory, Vacuum tunneling device, Scanning microscopy, Intermolecular modes, Piezoelectric crystal

INTRODUCTION

A point contact tunneling experiment provides the first measurement of a superconducting energy gap parameter Δ(T) in an organic superconductor[1]. The organic superconductor is s-based $\beta-(BEDT-TTF)_2 AuI_2$ with T_C=3.8K at ambient pressure. By assembling chains or rings of Carbon atoms chemists have fabricated more than two millions organic substances, which serve as fibers, coatings, adhesives, pharmaceuticals, synthetic rubbers, structural plastics and so on. It seems an organic molecule can be constructed to have almost any physical property. Establishing superconductivity in an organic solid seems more remarkable because the great majority of synthetic organic materials are electrical insulator. It was observed that several of the $(TMTSF)_2$ X charge-transfer salts super conduct under pressure where TMTSF is an electron donor and X^- can be AsF_6^-, Clo_4^-, PF_6^- and TaF_6^- etc. At present, we have organic superconductors[2-6] having transition temperature

T_C from 1.2K to (10.4± 0.3) K. These materials are based on sulphur contain organic donor BEDT-TTF.

In this paper, we have determined the temperature dependent energy gap parameter Δ(T) for three organic superconductor $[BEDT\text{-}TTF]_2$ $Cu(NCS)_2$ (T_C=10.4K) , $[BEDT\text{-}TTF]_2$ $Cu[N(CN)]_2Br$ (T_C=11.6K) and $[BEDT\text{-}TTF]_2Cu[N(CN)]_2$ Al (T_C=12.8K). We have used BCS-theory in this evaluation[7]. The magnitude of the energy gap parameter obtained from the experimental analysis[8] is found higher than the weak coupling limit 1.76 $K_\beta T_C$ at T=0. This experiment also indicates that energy gap parameter Δ(T) depends on the magnetic field and temperature T. The energy gap parameter Δ(T) decreases with magnetic field. This decrease in small magnetic field is consistent with the inductive measurement of critical fields in the material[9]. This energy gap measurement is due to potential difference between organic superconductors and standard metal-coating systems. The conduction electrons exhibit a reduced dimensionality leading to anisotropic band structure[10] and the electron-phonon coupling induce intermolecular modes[11]. Morse etal.[12] have suggested a gap value about 12 times the BCS weak coupling value for $(TMTSF)_2PF_6$ under pressure on the basis of Schottky tunneling[12]. On the other hand other tunneling studies[13,14] of the ambient pressure organic superconductor $(TMTSF)_2\,ClO_4$ have not confirmed this observation. However, only one study[8] at the temperature well below T_C have determined the variation of energy gap parameter Δ(T) for organic materials. No variation of energy gap with magnetic field has been reported. Vacuum-tunneling device for scanning microscopy and for spectroscopic analysis of superconductors were preferred. An electrochemically polished gold tip is moved along a direction perpendicular to the sample surface by the combined action of a differential micrometer and a stack of piezoelectric crystals. These are placed in a suitable rigid assembly mounted in a liquid-helium cryostat which is isolated from external vibration by use of a sandbox mounted on an air-suspension system. The unit is operated in an acoustic screened room in the laboratory.

MATHEMATICAL FORMULAE USED IN THE EVALUATION

For the evaluation of temperature dependent energy gap parameter, one takes the self-consistent equation[15] which is written as

$$\Delta = \frac{g}{\beta\hbar}\Sigma_n \int \frac{d^3k\hbar\Delta}{(2\pi)^3(\hbar\omega_n)^2 + E^2{}_k} \qquad (1)$$

The inter particle potential has been approximated by an attractive delta function with strength g>0.

$$\xi_k = \frac{\hbar^2 k^2}{2m} - \mu \qquad (2)$$

$$E_k = (\xi^2{}_k + \Delta^2)^{\frac{1}{2}} \qquad (3)$$

Where $\xi_k, E_k and \mu$ are single particle energy, energy of superconductor and the chemical potential. Now using the density of states at the Fermi surface N(0) where N(0) is given by

$$N(0) = \frac{mk_F}{2\pi^2\hbar^2} \qquad (4)$$

where k_F is the Fermi wave-vector. Now using the cut off $|\xi_k| = \hbar\omega_D \le \varepsilon_F$ and the symmetry of the integrand allows one to write

$$1 = gN(0)\int_0^{\hbar\omega_D} \frac{d\xi}{(\xi^2+\Delta^2)^{\frac{1}{2}}} \tanh\frac{(\xi^2+\Delta^2)^{\frac{1}{2}}}{2K_\beta T} \qquad (5)$$

When T $\rightarrow$ T_C the gap vanishes identically and the above equation reduces to the following equation

$$1 = gN(0) \int_0^{\hbar\omega_D} \frac{d\xi}{\xi} \tanh \frac{\xi}{2K_\beta T_C} \qquad (6)$$

To solve this implicit equation for T_C, it is convenient to introduce a dimensionless integration variable

$$\frac{1}{gN(0)} = \int_0^z \frac{dz}{z} \tanh z \qquad (7)$$

Where the cut off Z= $\frac{\hbar\omega_D}{2K_\beta T_C}$ is essential because the integral diverges logrith-mecally for Z $\rightarrow\infty$.

Integrating by parts, we have

$$\frac{1}{gN(0)} = [\ln z \tanh z]^z{}_0 - \int_0^z dz \ln z \sec h^2 z \qquad (8)$$

In all cases of interest, the upper limit is very large the above equation can be approximated as

$$\frac{1}{gN(0)} = \ln \frac{\hbar\omega_D}{2K_\beta T_C} - \int_0^\infty dz \ln z \sec h^2 z \qquad (9)$$

where the definite integral is known. A simple rearrangement yields

$$K_\beta T_C = 1.13\hbar\omega_D \exp(-\frac{1}{N(0)g}) \qquad (10)$$

One sees that T_C and the zero –temperature gap Δ(T=0) =Δ_0 both depend sensitively on the parameter N(0)g. This dependence cancels in forming the ratio

$$\frac{\Delta_0}{K_\beta T_C} = \pi e^{-\gamma} = 1.76 \qquad (11)$$

which is universal constant independent of the particular material. The temperature dependence of the gap parameter may be derived from equation (5). The limiting behavior is written as[16]

$$\Delta(T) = \Delta_0 - (2\pi\Delta_0 K_\beta T)^{\frac{1}{2}} e^{\frac{-\Delta_0}{K_\beta T}} for T \ll T_C \qquad (12)$$

$$\Delta(T) = 3.06 K_\beta T_C (1 - \frac{T}{T_C})^{\frac{1}{2}} for T_C - T \ll T_C \qquad (13)$$

DISCUSSION OF RESULTS

In this paper, using the BCS-theory[7], we have evaluated the temperature dependent energy gap parameter Δ(T) for three organic superconductors whose transition temperatures are 10.4K, 11.6K and 12.8K. These are the highest known Transition temperature (T_C) organic superconductors. Experimentally point contact tunneling experiments were used to measure Δ(T). We have performed an evaluation of $\frac{\Delta(T)}{K_\beta T_C}$ as a function of (T/T_C). Our theoretically evaluated results are in good agreement with the experimental data[3]. The theoretically evaluated results of $\frac{\Delta(T)}{K_\beta T_C}$ as a function of (T/T_C) are shown in table T1, table T2 and table T3. The theoretical results of Δ(T) as a function of T is shown in table T4, table T5 and table T6. Both calculations have been performed using BCS-theory. There are some recent works[17-28] which also reveal the similar behavior.

Table- T1: $(BEDT\text{-}TTF)_2\ Cu(NCS)_2$ T_C =10.4K

T/Tc	$\frac{\Delta(T)}{K_\beta T_C}$
0.0	3.06
0.5	2.91
1.0	2.76
1.5	2.62
2.0	2.47
2.5	2.32
3.0	2.18
3.5	2.03
4.0	1.88
4.5	1.74
5.0	1.59
5.5	1.45
6.0	1.33
6.5	1.23
7.0	1.15
7.5	1.05
8.0	0.72
9.0	0.41
10.0	0.12

Table T2 : $(BEDT\text{-}TTF)_2\ Cu\ (NCS)_2\ Br$ T_C =11.6K

T/T_C	$\frac{\Delta(T)}{K_\beta T_C}$
0.0	3.06
1.0	2.80
2.0	2.53
3.0	2.27
4.0	2.00
5.0	1.74
6.0	1.48
7.0	1.21
8.0	0.95
9.0	0.68
10.0	0.43
11.0	0.16
12.0	0.10

Table T3: $(BDT\text{-}TTF)_2\ Cu(NCS)_2\ T_C$ =Al2.8K

T/T_C	$\frac{\Delta(T)}{K_\beta T_C}$
0.0	3.06
1.0	2.82
2.0	2.58
3.0	2.34
4.0	2.10
5.0	1.86
6.0	1.62
7.0	1.39
8.0	1.15
9.0	0.91
10.0	0.67
11.0	0.43
12.0	0.19
13.0	0.11

Table T4: $(BEDT\text{-}TTF)_2\ Cu\ (NCS)_2$ (T_C =10.4K)

T(K)	Δ(T) (meV)
1.0	2.647
2.0	2.218
3.0	1.954
4.0	1.690
5.0	1.426
6.0	1.162
7.0	0.898
8.0	0.634
9.0	0.370
10.0	0.106
11.0	0.987

Table T5: $(BEDT\text{-}TTF)_2$ Cu($NCS)_2$ Br (T_C =11.6K)

T(K)	Δ(T) (meV)
1.0	2.798
2.0	2.534
3.0	2.270
4.0	2.201
5.0	1.742
6.0	1.478
7.0	1.214
8.0	0.950
9.0	0.686
10.0	0.422
11.0	0.158

Table T6 :($BEDT\text{-}TTF)_2$ Cu($NCS)_2$ Al (T_C =12.8K)

T(K)	Δ(T) (meV)
1.0	3.115
2.0	2.851
3.0	2.587
4.0	2.323
5.0	2.059
6.0	1.795
7.0	1.531
8.0	1.267
9.0	1.003
10.0	0.739
11.0	0.475
12.0	0.211

CONCLUSION

From the above evaluation, we conclude that energy gap and its temperature dependence of these organic superconductors can be studied quite satisfactorily with BCS-theory.

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