Impurity effects on nano-structured dirty superconductors: violation of Anderson’s Theorem

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Abstract
It is shown that in nano-structured s-wave superconductor, transition temperature \( T_c \) depends on random impurity potentials. This means violation of the Anderson’s theorem, which states that non-magnetic impurity does not affect the \( T_c \) of s-wave superconductor. We determine the impurity effects on \( T_c \) for nano-structured superconductor, using the finite element method to solve the Bogoliubov-de Gennes equations under spatially a random impurity potential. We show that some impurity potentials increase \( T_c \), but other impurity potentials decrease \( T_c \). We find that the superconductor with localized order parameter shows increased \( T_c \), which is contrary to expectation. Our results show that a dirty superconductor does not always mean weak superconductivity.

1. Introduction: file preparation and submission

Superconducting transition temperature \( T_c \) is important for applications of superconductors. Bulk superconductors have their own \( T_c \). However, for a nano-structured superconductor, \( T_c \) depends on the size of the superconductor. Recently, Nishizaki et al found that a bulk nano-structured Nb, which is made by high-pressure torsion and contains ultrafine grains [1–4], shows enhanced \( T_c \) [5]. However, a bulk nano-structured V shows decrease of \( T_c \) [6]. They discussed that Oxygen, which is included in V, decreases \( T_c \).

There are two mechanisms for size dependences of \( T_c \). The first mechanism is due to surface effects. Surface effects come from phonon softening [7, 8]. This mechanism can explain enhancement of \( T_c \) for some nano-size superconductors, such as Al [9, 10].

The second mechanism comes from quantum size effects. Anderson showed that superconductivity ceases when the size of superconductor becomes small and the electron discrete energy gap becomes larger than a superconducting energy gap [11]. However, Parmenter found that smaller granular superconductor shows higher \( T_c \) [12]. Also, investigating parity effects on \( T_c \) for superconducting particles, von Delft showed that \( T_c \) is enhanced just before superconductivity ceases with increasing the electron discrete energy gap [13]. Shanenko et al showed that \( T_c \)’s of atomic scale nano-films oscillate with decreasing thickness, and found that the oscillation has a relation with the Fermi level and the Debye energy of phonons, using the Bogoliubov-de Gennes (BdG) equations [14]. Also, Suematsu et al showed that \( T_c \)’s of nano-scaled superconducting square plates become higher than those of bulk superconductors, using the BdG equations [15]. In these two studies [14, 15], the spatial dependence of superconducting order parameter is taken into account, and therefore \( T_c \) is much enhanced than that of previous study [13]. In our previous study [16], we investigated that smaller superconductor shows higher \( T_c \), because density of superconducting order parameter increases with decreasing superconductor size.

Effects of impurities on nano-structured superconductors have not been well investigated. For a bulk superconductor, Anderson [11], and Abrikosov and Gor’kov [17] showed that non-magnetic impurities do not affect on s-wave superconductivity, because time-reversal pairing in the s-wave superconductivity is not affected by non-magnetic impurities. Also, Abrikosov and Gor’kov [18] showed that magnetic impurities decrease \( T_c \), because magnetic impurities lift degeneracy of energy levels of electron pairs, which have up and
down spins, and break Cooper pairs. Xiang et al [19] showed that a weak impurity potential that is concentrated at the center of a square s-wave superconductor weakly decreases superconducting energy gap, using the BdG equations on a tight binding model. Therefore, how impurities affect \( T_c \) enhancement in the nano-structured superconductor is still unclear. This is important for searching high \( T_c \) superconductor in nano-size.

In this paper, we numerically investigate non-magnetic impurity effects on \( T_c \) for a nano-structured superconductor. In order to take into account spatial variation of the superconducting order parameter, we use the BdG equations, with the finite element method (FEM) [15]. We introduce a random potential as non-magnetic impurities.

2. Method

The BdG equations are given as follows,

\[
H_0 u_\alpha(r) + \Delta(r) v_\alpha(r) = E_n u_\alpha(r),
\]

\[
-H_0^* v_\alpha(r) + \Delta^*(r) u_\alpha(r) = E_n v_\alpha(r).
\]

Here \( u \) and \( v \) are wave functions of particle and hole components of a quasi-particle of the superconductivity, respectively. And Hamiltonian is

\[
H_0 \equiv \frac{1}{2m} \left( \frac{\hbar}{i} \nabla - \frac{eA}{c} \right)^2 + V_{\text{imp}}(r) - \mu,
\]

where \( \mu \) is the chemical potential and \( V_{\text{imp}}(r) \) is a random potential from impurities. The order parameter \( \Delta \) is determined by following the self-consistent equation,

\[
\Delta \equiv V \sum_{n} v_n^*(r) u_n(r)(1 - 2f(E_n)),
\]

where \( E_c \) is the cut-off energy of the BCS theory. \( \mu \) is determined by the electron number conservation law as follows.

\[
N_e = \int \sum_{n} |f(E_n)| u_n(r)|^2 + (1 - f(E_n)) |v_n(r)|^2 |dr.
\]

In the FEM, we divide a system into triangular elements, and we define area coordinates \( \zeta_i^e(r) \) in \( e \)-th element [15]. We expand \( u, v, V_{\text{imp}} \) and \( \Delta \) using the area coordinates.

\[
u(r) = \sum_{i,e} u_{i}^e \zeta_i^e(r),
\]

\[
v(r) = \sum_{i,e} v_{i}^e \zeta_i^e(r),
\]

\[
\Delta(r) = \sum_{i,e} \Delta_{i}^e \zeta_i^e(r),
\]

\[
V_{\text{imp}}(r) = \sum_{i,e} V_{\text{imp},i}^e \zeta_i^e(r),
\]

where \( i \) is a node number and \( e \) is an element number. Then the BdG equations and the self-consistent equation become

\[
\sum_{i} P_{i}^e u_i^e + \sum_{i} Q_{i}^e v_i^e = E \sum_{i} I_{i}^e u_i^e,
\]

\[
-\sum_{i} P_{i}^e v_i^e + \sum_{i} Q_{i}^e u_i^e = E \sum_{i} I_{i}^e v_i^e,
\]

\[
\sum_{i} \Delta_{i}^e I_{i}^e = g \sum_{n} \sum_{i,j} u_{i}^e v_{j}^e u_{n,i}^e (1 - 2f(E_n)) I_{i,j}^e,
\]

where

\[
I_{i,j}^e = \int \zeta_i^e(x) \zeta_j^e(x),
\]

\[
I_{i,j}^e = \int \zeta_i^e(x) \zeta_j^e(x) \zeta_i^e(x),
\]

\[
K_{i,j}^{\alpha} = \int \frac{\partial \zeta_i^e(x)}{\partial x_i} \frac{\partial \zeta_j^e(x)}{\partial x_j},
\]
In order to determine $T_c$, we set temperature $T$ tends to $T_c$, and $\Delta \to 0$. So we get the equation to determine $T_c$,

$$
\det \left[ I_{ij}^\epsilon - g \sum_{i_2, i_3} I_{i_2 i_3}^\epsilon \left[ \sum_{n} u_{n,i_2}^{\epsilon} v_{n,i_3}^{\epsilon \ast} (1 - 2f(E_n)) \right] \right] = 0
$$

We investigate impurity potentials dependences of $T_c$ and mechanism of the impurity dependencies.

### 3. Results and discussions

We consider a superconducting rectangular $(3.2\xi_0 \times 6.4\xi_0)$ plate, where $\xi_0$ is the coherence length at $T = 0$. Figure 1 shows the FEM model of the superconductor. We set boundary conditions that wave functions, $u$ and $v$, become zero at edges of the superconductor. Therefore, the order parameter becomes zero at edges of the superconducting plate. We set $k_F\xi_0 = 3.0, \Delta_0/E_c = 0.2$, where $k_F$ is the Fermi wave number and $\Delta_0$ is an amplitude of the order parameter for a bulk superconductor at $T = 0$. And total number of electrons $N_e$ and the interaction constant $g$ are fixed. We consider twenty patterns of impurity random potential named $(V1)$–$(V20)$. Examples of impurity potentials $(V1), (V3), (V4)$ and $(V5)$ are shown in figures 2. In the simulation on each
random potential, we change an upper bound of the impurity potential $V_{\text{impMax}}$. Figure 3 shows $V_{\text{impMax}}$ dependences of $T_c$ for impurity potentials ($V_1$)–($V_{20}$). From this figure, we can see that some impurity potentials increase $T_c$, and other impurity potentials decrease $T_c$. To clarify origins of this variation of impurity potential dependence of $T_c$, we investigate $V_{\text{imp}}(r)$ dependence of eigen-energies $E_n$.

Figure 4 shows $V_{\text{impMax}}$ dependences of eigen-energies $E_n$ for impurity potentials, which increase $T_c$, the most ($V_4$), the second ($V_5$), the second worst ($V_1$) and the worst ($V_3$).

Figure 5 (figure 6) shows $\Delta E_n$ for each eigen-energy for the four impurity potentials, for which $T_c$ increases (decreases) the most, respectively. In order to clarify the effects of $\Delta E_n$ on $T_c$, we focus on the eigen-energies close to the Fermi energy ($-0.2 \leq E_n/E_c \leq 0.2$), which have strong effects on $T_c$. From figure 6, we can see that the electron eigen-energies of the superconductor, which shows lower $T_c$, become apart from the Fermi energy.

In the BCS theory, there is a relation between eigen-energies $E_k = \epsilon_k - \mu$ and $T_c$ as follows [20],

$$
\frac{1}{g} = \frac{1}{2} \sum_k \frac{1}{|\xi_{\epsilon_k}|} \tanh \left( \frac{|\xi_{\epsilon_k}|}{2T_c} \right),
$$

Figure 3. $V_{\text{impMax}}$ dependences of $T_c$ for impurity potentials ($V_1$)–($V_{20}$).

Figure 4. $V_{\text{impMax}}$ dependences of eigen-energies $E_n$ for impurity potentials, which increase $T_c$ the most ($V_4$), the second ($V_5$), the second worst ($V_1$) and the worst ($V_3$).
where $g$ is an interaction constant, $\xi_k = \epsilon_k - \mu$, and $\mu$ is a chemical potential. Then, we see that smaller $\xi_k$ has higher contribution to the superconductor. Therefore $T_c$ increases, when $|\xi_k|$ becomes smaller. However, in above cases, relation between $T_c$ and eigen-energies is opposite.
In order to understand these behaviors, we investigate distributions of the order parameter. Figure 7 shows distributions of the order parameter at \(V_{\text{impMax}} = 0.00\) (0) and 0.50 (for V1, V3, V4 and V5). From this result, each impurity potential distorts the distribution of the order parameter. In previous study [16], we discussed that the smaller superconductor shows higher \(T_c\) because of the confinement of the order parameter. So, the distortion of distribution of order parameter may lead to enhancement of \(T_c\). In order to evaluate the distortion, we calculate degree of the localization of the order parameter \(\alpha\) as follows,

\[\alpha = \frac{\langle \Delta^2 \rangle}{\langle \Delta \rangle^2},\]

where \(\langle \rangle\) is the average over all nodes in the FEM. Figure 8 shows \(V_{\text{impMax}}\) dependences of \(\alpha\), for four impurity potentials, which increase \(T_c\) the best (1) and the worst (2). From this result, we can see that the order parameter distribution for the impurity potential that shows higher \(T_c\), is more localized. This is because localized order parameter shows larger order parameter density, and leads to higher \(T_c\).

4. Conclusion

In summary, in order to investigate the impurity effects on \(T_c\), we have solved the Bogoliubov-de Gennes equations for superconducting rectangular \((3.2\xi_0 \times 6.4\xi_0)\) plates, with the FEM. We have introduced a random potential as non-magnetic impurities. We have obtained \(T_c\) for twenty random impurity potentials. We have found that some impurity potentials increase \(T_c\), but other impurity potentials decrease \(T_c\). To investigate this difference, we have determined eigen-energies and distribution of order parameters. We have found that some of eigen-energies become apart from the Fermi energy for impurity potentials that show higher \(T_c\). However, we have found that the distribution of the order parameter is distorted by the impurity potential and the localization of the order parameter leads to higher \(T_c\). We may expect impurities or localization of the order parameter lead to weakening of the superconductivity and lowering \(T_c\). Our results are contrary to this expectation. Therefore, a dirty superconductor does not always mean weak superconductivity.

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