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Numerical Simulation on Self-heating for Interlayer Tunneling Spectroscopy in $Bi_2Sr_2CaCu_2O_{8+x}$

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Abstract

For interlayer tunneling spectroscopy using a small stack of $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212) intrinsic junctions in a high-bias range, large self-heating takes place due to the poor thermal conductivity of Bi-2212. In this study, we numerically estimate the self-heating around a Bi-2212 sample stack for *I-V* or *dI/dV-V* measurements. Our results show that the temperature discrepancy between the Bi-2212 sample stack and top Au electrodes due to bias-induced self-heating is small enough along the *c*-axis direction of Bi-2212. On the other hand, the lateral temperature discrepancy between the sample stack and the Bi-2212 on-chip thermometer stack can be as large as ~20 K for the highest bias required to observe the pseudogap hump structure. We thus suggest a new *in-situ* ac thermometry, employing the Au current-bias electrode itself deposited on top of the sample stack as the resistive thermometer layer, which is supposed to allow safe temperature measurements for the interlayer tunneling spectroscopy.

Keywords : interlayer tunneling spectroscopy, $Bi_2Sr_2CaCu_2O_{8+x}$, self-heating

I. Introduction

Since the discovery of high-critical-temperature (T_c) superconductivity in cuprates, various anomalous behaviors have been discovered beyond the BCS theory. The appearance of the pseudogap (PG) is one of such anomalies, which is signified by the depletion of the zero-bias electronic density of states in the normal state of the materials. The PG is also accompanied by the broad hump in the background of the superconducting gap (SG). However, the relationship between the SG and the PG is still controversial [1]. The PG is claimed to be a precursor to the superconducting state [2]. On the other hand, it is also suggested that the PG is an order competing or coexisting with the superconducting state [3].

Recently, a variety of powerful measurement tools are developed to study the PG, such as angle-resolved photoemission spectroscopy, scanning-tunneling spectroscopy, etc. The interlayer tunneling spectroscopy (ITS) has become one of essential tools to examine the details of the electronic state distribution of cuprate materials, including the development of both the SG and the PG [4]. The ITS is accomplished by the tunneling-conductance measurements along the *c* axis of a stack of junctions that are naturally grown in a single crystal [known as intrinsic junctions (IJs)] of highly anisotropic cuprate materials such as $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212). An advantage of ITS, in comparison with other tools mentioned above, lies in the fact that one obtains the

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bulk information, rather the surface-sensitive information, of the quasiparticle density of states in cuprate materials. One should note that the *c*-axis electronic tunneling properties in Bi-2212, for instance, is dominated by the quasiparticle excitation around the (π, 0) or the M point in the first Brillouin zone, at which the van Hove singularity is present [5]. Thus, in comparison with other techniques, the ITS may be more sensitive information on opening of the PG, because the PG opens up, starting at the M point [1].

In spite of above-mentioned advantages of ITS, however, a serious problem arises in the ITS by self-heating in a high bias, due to the poor thermal conductivity of Bi-2212 material. Although reducing the junction size or using pulsed-bias measurements has been adopted to reduce the self-heating, one cannot totally avoid it [6]. Recently, we developed the "heating-compensation" technique using an IJs thermometer stack laid down a sub-micrometer apart from the sample stack, to reduce the bias-induced self-heating and thus obtaining the interlayer tunneling spectroscopic data at approximately a constant temperature irrespective of the bias level of interest. To this end, the proportional-integral-derivative (PID) control of the sample temperature using a substrate heater coil, based on the in-situ measured sample temperature, was employed. Details of the operation principle of this technique are described elsewhere [7].

Our calculation shows that the lateral temperature discrepancy between the sample stack and the thermometer stack turns out to be about 20 K, which is too large to accurately examine the PG in a high current bias. Reducing the *c*-axis bias voltage, by reducing the number of intrinsic junctions involved in the conductance measurements, may allow accurate-enough thermometry. The examination of the PG behavior in high temperatures (>100 K) can also be safe enough, because the self-heating is reduced in this temperature range owing to the reduced PG [8]. On the other hand, the temperature discrepancy in the vertical direction between the sample stack and the Au current-bias electrodes deposited on top of the sample stack can be reduced as small as 2 K. This suggests that the thermometry using the resistance change of the top Au electrodes, if it is realizable, may provide a convenient and safe thermometry in the presence of the self-heating. In this report, we thus suggest a new *in-situ* ac thermometry by measuring the resistance of the Au electrode at a fixed frequency.

II. Experiments

We numerically estimate the self-heating around a Bi-2212 sample stack for usual *I-V* or *dI/dV-V* measurements condition. The COMSOL multiphysics program is used to calculate the temperature profiles of a sample [9].

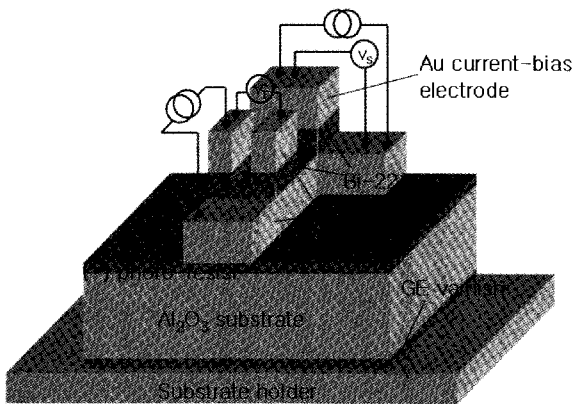

Fig. 1. The simplified model system adopted to calculate the temperature profiles in a sample. The thermometer stack is assumed to be 0.5 μm apart laterally from the sample stack.

In this estimation, we set up a simplified model for a sample consisting of a stack of Bi-2212 IJs, an Au-film electrode, a negative photo-resist layer used to attach a Bi-2212 single crystal to a sapphire substrate, the sapphire substrate itself, and a GE varnish layer used to fix the whole sample to the Cu substrate holder. We assumed that the thermometer stack is separated by 0.5 μm from the sample stack. The sample and the thermometer stacks have the lateral dimension of 3x3 and 3x2 μm^2, respectively.

The thickness of stacks, which contain 20 junctions, is set to be 30 nm. Both of the stacks are sandwiched by the top and the bottom Au-film electrodes (~100 nm thick), connected by a thinner Bi-2212 layer and an Au-film electrode underneath the stacks [refer to Fig. 1].

All Au-film electrodes are thermally and electrically connected by thin (<0.3 mm) indium wires at the end of electrodes. The thicknesses of the negative photo-resist layer, the sapphire substrate, and the GE varnish layer are set to be 1, 40, and 1 μm, respectively. The thermal conductivities of all materials used are adjustable variables, with different temperature dependences. The thermal conductivities of Bi-2212 and the Au-film electrodes play crucial roles in the heat flow through the sample. On the other hand, the thermal conductivities of negative photoresist, sapphire substrate, and GE varnish have comparatively minor effects on the heat flow. Thus, in the calculation the thermal conductivities of these materials are assumed to be temperature independent. The sample stack is considered to be a heat source. The heating power is selected to be 0.27, 1.35, and 2.7 mW. The last value, which is determined from our earlier work [10], corresponds to the one where the PG emerges.

III. Results and Discussion

The temperature discrepancy between the sample stack and the thermometer stack due to the bias-induced self-heating at the sample stack is sensitive to the temperature dependence of the thermal conductivities of Bi-2212 and the Au-film electrode. At room temperature, we adopt the official value for the *c*-axis thermal conductivity κ_c=0.87 W/mK of Bi-2212, which is approximately a factor of 10 smaller than that of the *ab*-plane, κ_{ab} [11]. Inset of Fig. 2(b) shows the thermal conductivities of Bi-2212 and the Au-film electrode as functions of temperature [12].

In Fig. 2(a), the temperature discrepancy between the sample stack and the thermometer stack, ΔT_{ab}, is lower than 20 K at high temperature (>100 K) for the highest heating power (2.7 mW) assumed. From 100 K to 200 K, ΔT_{ab} is almost temperature independent, because the temperature dependencies of the thermal conductivities of Bi-2212 and the Au-film electrode saturate in this temperature range [refer to the inset of Fig. 2(b)]. For temperature-independent thermal conductivity of the Au-film electrode, temperature profiles in the *b*-axis direction, along which the sample

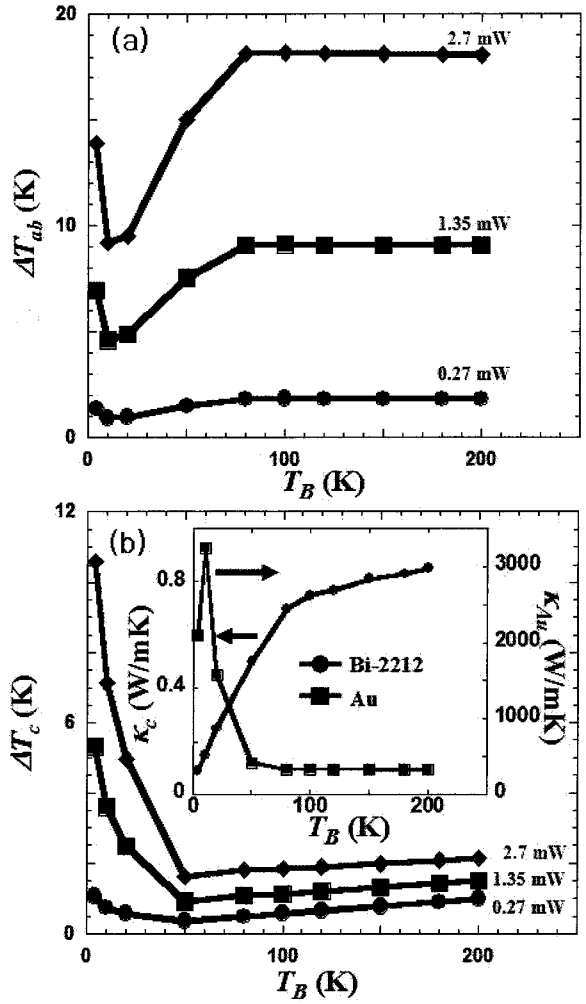

Fig. 2. The temperature discrepancies as a function of the temperature for various heating powers (a) between the sample stack and the thermometer stack and (b) between the sample stack and the Au current-bias electrode deposited on top of the sample stack. Inset of (b): The thermal conductivities of Bi-2212 along the *c*-axis direction and the Au-film electrode as a function of temperature.

stack and the thermometer stack are aligned, show a similar behavior and also ΔT_{ab} has few variations at different substrate holder temperatures for a given heating power (not shown). In Fig. 2, at a given fixed substrate holder temperature, ΔT_{ab} and ΔT_c are linearly proportional to the heating power, which is consistent with the general expectation [13].

At low temperatures (<100 K), ΔT_{ab} linearly increases with temperature due to the decreased thermal conductivity of the bottom Au-film electrode. Surprisingly, for T<10 K, the slope of ΔT_{ab} gradually deviates from that in the temperature range of 20 K ~ 80 K. In addition, at 4 K, ΔT_{ab} is abruptly increases. The heat flow in the *ab*-plane is dominated by the Au-film electrode whose thermal conductivity is 30~300 times larger than the one of Bi-2212. Although the heat flow in the *ab*-plane is dominated by the Au-film electrode, the heat flow in the *ab*-plane of Bi-2212 contributes little to the heat flow in *ab*-plane of the sample unless the substrate holder temperature falls below 20 K. However, since the thermal conductivity of Bi-2212 at 4 and 10 K is significantly smaller the heat flow through the *ab*-plane of Bi-2212 is negligible. Thus, the heat generated from the sample stack flows down to the bottom of the thermometer stack just through the Au-film electrode underneath the stacks. This transferred heat flows up to the thermometer stack along the *c*-axis direction, which is indeed much lower than that through the *ab*-plane of Bi-2212. This explains the anomaly of ΔT_{ab}'s below 10 K.

For laterally arranged sample and thermometer stacks, the computerized proportional-integral-derivative (PID) temperature control [7] does not allow the exact heating compensation, because *in-situ* measurement of the temperature using the thermometer stack does not provide accurate-enough temperature reading of the sample stack. The proportionality of ΔT_{ab} to the heating power suggests that reducing the number of junctions in a sample down to a few is required to obtain accurate-enough temperature reading to examine the SG and the PG. Under this condition, estimation of the PG, whose size shrinks with increasing temperature, can be still valid in a high temperature range (>100 K).

The temperature discrepancy along the *c*-axis (or vertical) direction between the sample stack and the Au current-bias electrode deposited on top of the sample stack, ΔT_c, is shown in Fig. 2(b). Very thin (<30 nm) sample stack allows a negligible temperature difference along the *c*-axis direction. However, at 4, 10, and 20 K, the slope of ΔT_c changes rapidly and ΔT_c increases much. As shown in the inset of Fig. 2(b), ΔT_c seems to vary in inversely proportion to the thermal conductivity of Bi-2212. This fact indicates that ΔT_c is caused by the heat flow through the sample stack along the *c*-axis direction. The decrease of the thermal conductivity of Au-film electrode causes an upturn variation of ΔT_c in the temperature range of 50 K~200 K.

Using the Au current-bias electrode deposited on top of the sample stack, accurate thermometry can be accomplished by measuring the resistance of the electrode itself, because the temperature discrepancy between the sample stack and the Au current-bias electrode is less than 2 K as shown in Fig. 2(b). One can obtain the resistance of the Au current-bias electrode itself separately from the *c*-axis tunneling measurement in a finite bias through the electrode. It is accomplished by adopting an ac measurement for the electrode resistance with its frequency different from that for the tunneling measurement. For this *in-situ* ac thermometry, two current biases through the common Au current-bias electrode are required. Once the sample temperature is accurately obtained the computerized PID temperature control can lead to ideal heating compensation, enabling the genuine tunneling spectroscopic measurement.

In conclusion, the thermometry using a lateral arrangement of the thermometer stack does not allow accurate-enough temperature reading, which hampers the genuine tunneling spectroscopic measurement. However, the temperature discrepancy, in the vertical direction, between the sample stack and the Au current-bias electrode deposited on top of the sample stack is less than 2 K for the temperature ranges of 50 K~200 K. A new *in-situ* ac thermometry using the Au current-bias electrode deposited on top of the sample

stack, utilizing the resistance reading of the Au electrode, may allow the accurate-enough temperature reading for heating-free tunneling spectroscopic measurements.

Acknowledgments

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