Scanning tunnelling microscopy and spectroscopy of MgB₂

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Abstract. Experiments of the scanning tunnelling microscopy and spectroscopy (STM/STS) have been carried out on the layered superconductor MgB₂ with \( T_c = 39 \) K. The measurements were done at 5 K using a Pt-Ir tip and the single-crystal grain. The STM images show characteristic hexagonal patterns with the distances of nearest neighbour atoms to be 0.3 – 0.35 nm and 0.15 – 0.2 nm, respectively, which are consistent with the Mg and B lattice sizes. The STS measurements clarify the superconducting gap \( 2D = 20 - 24 \) meV, which leads to the strong-coupling ratio \( 2D/k_B T_c = 5 – 6 \). The tunnelling spectra can be described by the correlated 2-gap model. These features are consistent with our previous break-junction measurements. The gap structure is homogeneous at least within the range of 200 nm x 200 nm.

1. Introduction

The AIB₂-type layered compound MgB₂ has been well investigated since the discovery of the superconductivity with the critical temperature \( T_c = 39 \) K [1]. It is now believed that the superconductivity possesses an \( s \)-wave pairing symmetry, which arises from the strong electron-phonon interaction in the B honeycomb lattice plane. The most intriguing feature is the existence of the multiple gaps consisting of the 2 dimensional \( \sigma \) band and 3 dimensional \( \pi \) band [2]. Such a phenomenon has been introduced theoretically and discussed in terms of raising the \( T_c \) with the help of inter-band scatterings that enhance the effective electron-phonon interaction responsible for the superconductivity [3].

In the previous study, we have observed the multi-gap structures in the break-junction tunnelling spectroscopy (BJTS), and compared them with the correlated 2-gap model of the proximity effect [4], which is mathematically equivalent to that of the 2-band superconductivity [3]. The observed tunnelling spectra were well reproduced in details by this model, thereby indicating that the multiple gaps are intimately correlating with each other. From the agreements between the experimental data and the calculations, we have obtained the representative gap values \( 2\Delta = 4 - 5 \) meV, 8 - 14 meV, and 18 - 24 meV [5,6]. The smallest gap is commonly observed except for the NMR technique, and the existence of the middle-size gap is consistent with the photoemission data suggesting the surface gap...
For the largest gap, the tunnelling conductance can be described by the Gaussian gap distribution model, which suggests the existence of the spatial inhomogeneity and/or the gap anisotropy arising from the layered crystal structure [5, 9].

Although the break-junction technique provides the cleanest junction interface and the reliable tunnelling spectra, it has no spatial resolution [10]. To have further insight into the multiple-gap features for this layered compound, the local gap measurements with atomic resolution are desirable. For this purpose, we have started nano-scale measurements using a low-temperature, ultra high-vacuum scanning tunnelling microscopy and spectroscopy (STM/STS) apparatus. In this paper, we report on the atomic images and the local tunnelling measurements at the temperature of ~ 5 K.

2. Experiments

The crystallographic structure of MgB$_2$ is hexagonal with the space group P6/mmm, which is the AlB$_2$ type. The B honeycomb planes are sandwiched by the Mg hexagonal planes (Fig. 3). The surface of MgB$_2$ was obtained by the submicron-sized crystalline facets in the polycrystalline pellets. The STM/STS apparatus used in the present measurements was an OMICRON LT-UHV-STM system equipped with a low-temperature preparation chamber and other additional functions. The measurements were carried out using a Pt-Ir tip. The STM chamber temperature is kept at 5 K during the measurements. For the STM measurements, the applied bias voltage $V = 15$ mV refers to the sample, and the tunnelling current range is $I = 0.05 - 0.3$ nA. The typical scanning range is 200 nm x 200 nm. For the STS measurements, in which the superconductor - insulator (vacuum) - normal metal (SIN) junction is formed, the bias range is extended up to $V = \pm 30$ meV. The tunnelling conductance $dI/dV$ is calculated numerically from the I-V characteristics with the resolution better than 0.5 mV.

Figure 1 shows the cracked surface of MgB$_2$ monitored by scanning electron microscope (SEM). The characteristic crystalline facets can be seen with their sizes smaller than 1 $\mu$m x 1 $\mu$m. We have used such a crystalline piece for the STM/STS measurements. For the BJTS measurements, a thin platelet polycrystalline sample is cracked to form a superconductor-insulator-vacuum (SIS) junction at 4 K [9], which thereby possesses the interface structure similar to Fig.1. The actual tunnelling area of the latter, however, could no be identified. In both cases, the sample is in situ cracked just before the measurements.

![Figure 1. SEM image of the cracked surface of a polycrystalline MgB$_2$.](image1)

![Figure 2. STM image of the MgB$_2$ surface at 5 K. The bright spots indicate the Mg atoms. $V = 15$ mV, $I = 0.3$ nA.](image2)

3. Results and discussion

We have scanned several single-crystal facets to find the topmost flat ab plane normal to the c axis, which is expected from the layered hexagonal structure of MgB$_2$. Figure 2 shows the typical STM
image of a clean single-crystal facet of MgB₂ in the superconducting state at 5 K. The characteristic
hexagonal patterns of the spots can be seen with ridges between the spots. The image exhibits slight
corrugation, but no apparent modulations can be seen. The sample bias voltage of 15 mV is well above
the gap-edge voltage of $\Delta/e = 10$ mV. Therefore, the density of states at this energy is similar to that of
the normal state. The bright spots represent the atomic positions, while the dark color corresponds to
the depression region. The configuration and the average separation between the bright spots are
consistent with that of Mg atoms [1], thereby certificating what we observed is the Mg atomic layer on
the ab plane. To our knowledge, this is the first observation of the surface atomic pattern of MgB₂ in
the superconducting state, although there exists the room temperature observations [11].

Figure 3 shows the STM images for two kinds of the atomic arrangements (a) and (c). The Fig. 3
(a) is a magnified part of the scan presented in Fig. 2, while the Fig. 3 (c) is obtained at $V = 15$ mV and
$I = 0.05$ nA. Both the atomic patterns exhibit the hexagonal structures with (a) or without (c) the
centered atom. The appearance of either (a) or (c) depends on the cracked surface condition. The
distances between the nearest neighbor atoms for (a) and (c) are 0.3 - 0.35 nm and 0.15 - 0.2 nm,
respectively, which are consistent with the Mg and B lattice sizes as shown in (b). Therefore, these
STM images are attributed to the Mg and B planes. We have also observed the complex lattice
structures consisting of both Mg and B lattices at 5 K, which is similar to Ref. [11].

![Figure 3. STM images of (a) Mg ($V = 15$ mV, $I = 0.3$ nA, 1 nm x 1 nm) and (c) B ($V = 15$ mV, $I =
0.05$ nA, 0.5 nm x 0.5 nm) planes at 5 K. (b) The structures of Mg and B lattices.](image)

We have next measured the superconducting energy gap by the STS mode. Figure 4 shows the
representative STS conductance. The bias polarity refers to the MgB₂ sample. There exists slight
asymmetry in the conductance with respect to the bias (the more pronounced asymmetric feature is
seen in Fig. 5), which is a general tendency of the present STS measurements. The similar
conductance asymmetry (the higher conductance at negative sample biases) can be seen in the STS
measurements of the high-$T_c$ copper-oxide superconductors [12]. The gap structure is broadened as
compared with the standard BCS model. For the quantitative evaluation of the gap structure, we have
fitted the conductance. As shown in the figure, the conductance is better fitted by the correlated 2-gap
model than by the single-gap broadened BCS model, especially for the depression in the zero-bias
region[3, 4]. This is consistent with the existence of the second gap commonly observed in this
compound [5, 6], although there is no apparent double-gap structure in the fitted curve. In terms of the
correlated 2-gap model, the gap broadening in Fig. 4 can be due to the strong mutual scatterings of
quasiparticles between two phases, which perhaps results in the broadening feature similar to that for
the probability distribution of the gap [5]. The gap value of $2\Delta = 20 - 24$ meV obtained from these
fittings almost corresponds to the conductance peak separation, and this is the largest gap value among
the STS measurements [2]. Figure 5 compares the conductance from the STS and BJTS measurements.
The bias range of the BJTS is adjusted twice wider than that of the STS, because the gap-edge peak separation for the former becomes $4\Delta/e$ for the SIS junction instead of $2\Delta/e$ for the latter SIN junction. It is obvious from Fig. 5 that the gap value of the STS is very consistent with that of the BJTS [5, 6]. The conductance of the STS is almost two orders of magnitude lower than that of the BJTS, and it is broadened in comparison with that for the BJTS. These differences are probably due to the difference in the junction geometry between the STS (SIN) and the BJTS (SIS). Since the observed gap value $2\Delta = 20-24$ meV is the largest reproducible one among our measurements, this is believed to be the predominant gap of MgB$_2$. Therefore, the gap ratio $2\Delta/k_B T_c = 5-6$ is now confirmed from both the STS and BJTS measurements. This is the largest ratio among the non-copper oxide superconductors, and consistent with the NMR measurements [7].

Figure 6 shows the STS conductance at 5 K taken at intervals separated by 6 nm along a line of 200 nm on a single-crystal facet. The conductance peak position showing the gap of $2\Delta = 20$ meV is kept almost constant along the mapping line, although the overall conductance magnitude gradually varies. We have also obtained the similar mapping result along the line perpendicular to the first mapping line. These features indicate that the gap-edge peak of MgB$_2$ is homogeneous at least within the domain of $10^4 - 10^5$ nm$^2$. The similar broadening of the gap structure all over the domain shown in Fig. 6 suggests the characteristic minute probability distribution of the gap, which could not be resolved even by the STS measurements. In fact, such a gap feature has been fitted by the Gaussian-gap distribution model, and it is also reflected in the thermodynamic quantities as we have examined specific heat data [9]. The spatially homogeneous gap structure in Fig. 6 is in contrast to the case of the copper-oxide superconductors, in which a large distribution ($\sim \pm 50\%$) of the gap-edge peak energy is observed within a short range of $\sim 2-5$ nm [12].

Figure 7 shows the apparent smallest gap structure observed in the present STS measurements. The $I$-$V$ curve is also shown. The gap-edge peaks occur at $\pm 3$ mV with the severely modulated background conductance. The weak and broadened humps in the conductance centered at around $\pm 9-10$ mV are probably the traces of the main-gap edges as shown in Figs. 4 - 6. We have seldom observed such an apparent small gap of $2\Delta = 5 - 6$ meV, although this is one of the main conductance features of the other STS and point-contact measurements as the $\pi$-band gap of the 2-band superconductivity [2]. The dips at $\pm 4$ mV and the shoulders at $\pm 1.5$ mV in Fig. 7 can be associated with the proximity effect of the superconducting gap. Especially, such intensive dips located just outside the gap-edge peaks are most probably concomitant with the proximity-induced phase. The measurements of the temperature evolution of the gap will be desirable to distinguish its origin.
In summary, we have carried out low-temperature STM/STS experiments on the layered high-$T_c$ superconductor MgB$_2$. The STM measurements at 5 K exhibit characteristic hexagonal patterns of Mg and B atoms. The distances of the nearest-neighbor atoms for the Mg and B layers are 0.3 – 0.35 nm and 0.15 – 0.2 nm, respectively, which are consistent with the Mg and B lattice sizes. The STS measurements clarify the representative gap value $2\Delta = 20 – 24$ meV, which agrees well with our previous BJTS measurements. Thereby, the present STS results reconfirm the extreme strong-coupling superconductivity with the gap ratio $2\Delta/k_BT_c = 5 - 6$. The gap structure is implicitly expressed by the correlated 2-gap model of the proximity effect, although the apparent small gap of $2\Delta = 5 - 6$ meV is seldom observed. We have examined the spatial dependence of the gap, and found almost no variations of the gap in a domain of 200 nm x 200 nm.

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