Thermoelectric voltage study of $1T$-TaS_2 using temperature dependent scanning tunneling spectroscopy

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Using an ultra high vacuum (UHV) scanning tunneling microscope where the sample is cooled while the tip remains close to room temperature, we measured the thermoelectric voltage induced by the large thermal gradient between the tip and sample. Using tunneling thermometry technique we studied the change of electronic structures of $1T$-TaS_2 from room temperature to 40 K. At the temperature for the nearly commensurate to commensurate transition, we found an abrupt change of the thermoelectric power from a very small value to about 0.15 mV/K.

1. INTRODUCTION

Recently, there have been several attempts to measure the thermoelectric voltage across the tunneling barrier made of the STM tip and sample by the tunneling thermometry technique[1, 2, 3]. It is known that a thermal gradient across the tunneling barrier induces an electric field. The thermoelectric voltage is shown to be related to the logarithmic derivative of electronic states close to the Fermi energy of the tip and sample[4]. Hence it would be possible to study the change of electronic states of the sample near the Fermi level (E_F) by measuring the thermoelectric voltage. Using this method, we have studied the change of electronic states of $1T$-TaS_2 near E_F. $1T$-TaS_2 shows a dramatic change of physical properties at the nearly commensurate (NC) to commensurate (C) transition temperature[5]. We found an abrupt increase of the thermopower from a very small value to about 0.15 mV/K caused by the metal-insulator transition

2. EXPERIMENTAL DETAILS

We used a commercial variable temperature UHV STM (Omicron Vakuumphysik GmbH) equipped with a He flow cryostat[6]. In our STM the sample is cooled separately while the microscopic stage, including the tip remains at room temperature. Since the thermal coupling between the tip and sample is negligible in UHV condition compared with the thermal conductance of tip and sample, the tip can remain at a constant temperature close to room temperature (Fig 1). This enables us to measure the thermoelectric voltage of the sample induced by a large thermal gradient between the tip and cooled sample. The experiments were made below 8×10^{-11}mbar. Electrochemically etched W tips were used. By measuring tunneling spectra and observing the shift of voltage required for zero tunneling current, we got a value of the thermoelectric voltage at each temperature between 40 K and 300 K.

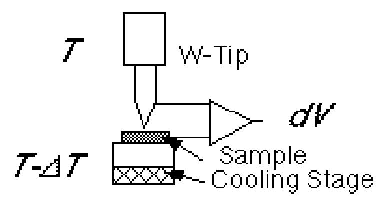

Figure 1: Experimental setup for measuring the thermoelectric voltage.

3. RESULTS AND DISCUSSION

A resistivity measurement of our sample showed that the NC-C phase transition occurs around 187 K during cooling, and that the unbounded increase of resistivity starts below 50 K as shown in inset of Fig 2(a). Fig 2(a) shows the measured thermoelectric voltage developing between the tip and sam-

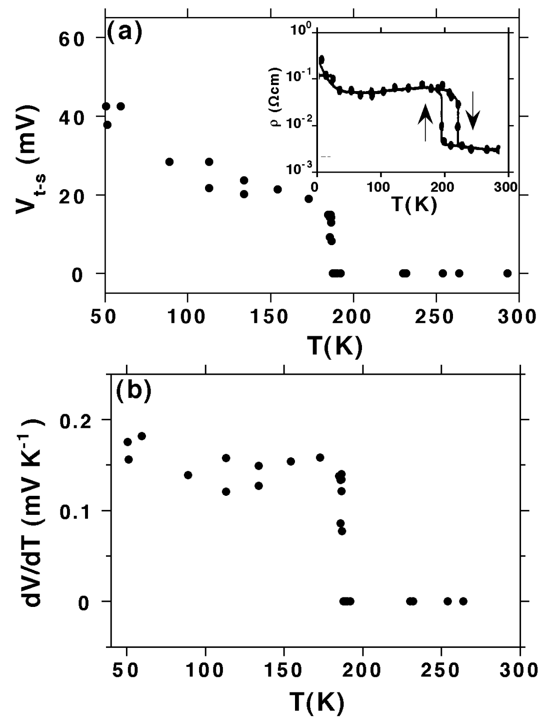

Figure 2: (a) The measured thermoelectric voltage between the STM tip and the sample. Inset: Temperature dependent resistivity of the $1T$-TaS_2 single crystal. (b) The thermoelectric voltage divided by the temperature difference.

ple with decreasing temperatures. At high temperatures, that is above the NC-C transition, the thermoelectric voltage remained at a very small value below 0.1 mV. Around 187 K where the discontinuity of resistivity takes place, the thermoelectric voltage increased abruptly from about 0.1 mV to over 10 mV. At temperatures below the abrupt transition, there was a gradual increase of magnitude of thermoelectric voltage. At the lowest temperature, about 40 K, the thermoelectric voltage developing between the tip and sample became as large as 40 mV. This large thermoelectric voltage, of course, originates from the large thermal gradient between the tip and sample, which is over 200 K. We believe that UHV environment better than 10^{-11} prevent heat exchanges between the tip and sample so that we could observe such a large thermoelectric voltage. Fig 2(b) shows the thermoelectric voltage divided by the temperature difference between the sample and tip. Assuming that the temperature of the tip remains constant during the measurement, the thermoelectric voltage for a certain temperature gradient (dV/dT) should be related to the thermopower for the couple consisting of tip and sample[4]. If the thermopower of the W tip remains constant and small during the transition, a large change of thermopower at the NC-C transition would mainly originate from the sample. The abrupt change of the thermopower from a very small value to about 0.15 mV/K as shown in Fig 2(b) indicates a drastic change of electronic structures near E_F. Our results are also quite consistent with the existing conventional thermoelectric power measurement made by Tani *et al.*[7]. Considering the typical value of the thermopower for metals, 1-10 μV/K, and for semiconductors, 100 μV-1 mV/K, we interpret our large increase of thermopower as a transition from a metallic state to a semiconducting state, that is, carrier excitation from E_F to the mobility edge, E_c, between at least 50 K and 180 K. This is consistent with the recent temperature dependent high resolution photoelectron spectroscopy[5] and scanning tunneling spectroscopy[8] studies, which shows an opening of a deep pseudo gap structure due to a metal-insulator transition at NC-C temperature. A large drop of thermopower below 20 K is also observed[7] suggesting that the conduction is accomplished by the variable-range hopping process in the localized states near E_F at low temperatures.

4. SUMMARY

We used the tunneling thermometry technique to study the change of electronic structures near E_F in $1T$-TaS_2. We have found an abrupt increase of thermoelectric voltage developing between the tip and sample at NC-C transition temperature, which indicates a drastic change of the electronic structure, a metal-insulator transition, near E_F.

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