Scanning Tunneling Spectroscopy of $1T$-TaS$_2$ between 300 K and 40 K

Inger Ekvall[a], Ju-Jin Kim[a,b], and Håkan Olin[a]

[a] Department of Physics, Chalmers University of Technology and Göteborg University,
S-412 96 Göteborg, Sweden

[b] Department of Physics, Chonbuk National University,
Chonju 560-756, Korea

We have used scanning tunneling spectroscopy to measure temperature dependent tunneling spectra of $1T$-TaS$_2$ from room temperature to $\sim$ 40 K. An abrupt transition from the charge-density-wave induced broad depletion to an opening of a deep pseudo gap was observed within $\sim$ 1 K of the nearly commensurate to commensurate transition temperature. This pseudo gap was deep enough to form localized states at the Fermi level. Our tunneling results therefore suggest, in contrast to inverse photoelectron spectroscopy, that the band splitting of the Ta 5d band is due to the electron correlation effect.

1. INTRODUCTION

$1T$-TaS$_2$ has a complex charge-density-wave (CDW) phase diagram. An abrupt change of physical properties at the nearly commensurate (NC) to commensurate (C) CDW transition occurs at $\sim$190 K [1], and is interpreted as a Mott transition [2]. Photoelectron Spectroscopy (PES)[3] and Inverse Photoelectron Spectroscopy (IPES)[4] have been used to study the Density of States (DOS) near the Fermi level (E_{F}) at this transition. The PES study shows an opening of a deep pseudo gap atE_{F}. The IPES study do not reveal any change, suggesting that the gap opens only below E_{F} and that E_{F} is pinned at the lowest unoccupied band. Spectroscopy of $1T$-TaS$_2$ by macroscopic tunneling shows a gradually increasing CDW gap with no change at the NC-C transition[5]. We present a temperature dependent Scanning Tunneling Spectroscopy (STS) study, which showed an abrupt transition from the CDW induced depletion to an opening of a deep pseudo gap near E_{F} at the NC-C transition. This pseudo gap was deep enough to form localized states at E_{F}.

2. EXPERIMENTAL DETAILS

The sample was cleaved in air and set into a commercial variable temperature ultrahigh vacuum STM (Omicron Vakuumphysik GmbH) equipped with a He flow cryostat. Pressure was below 8×10^{-11}mbar. Electrochemically etched W tips were used. We measured tunneling spectra in a 11×11 array over a 200 Å×200 Å area and averaged these spectra for each temperature to improve the signal to noise ratio.

3. RESULTS AND DISCUSSION

A resistivity measurement of our sample showed that the NC-C transition occurs around 187 K during cooling, and that an unbounded increase of resistivity starts below 50 K. Above 187.7 K, our tunneling spectra showed a broad opening of the CDW gap, see Fig 1. The CDW driven band splitting of the Ta 5d band, which is found in high resolution PES was not clear in our spectra[3]. This might reflect that STS represent Fermi surface averaged spectra and is more related to angle integrated PES than angle resolved PES. Between 187.7 K and 186.6 K, the DOS at E$_F$ dropped drastically, but remained finite, indicating a pseudo gap. Simultaneously a peak structure appeared at -0.25 V in the occupied band. By further decreasing the temperature, a small but clear gap structure in the unoccupied band appeared at 0.20 V, and the gap structure at -0.25 V increased and widened slightly.

Comparing our tunneling results with earlier PES spectra, the sharp peak in the occupied band can be interpreted as representing the lower Hubbard band[3]. We can then explain the peak structure in the unoccupied band as the upper Hubbard band. This gap structure is observed in an earlier tunneling experiment at 77 K[6]. Using our spectra we

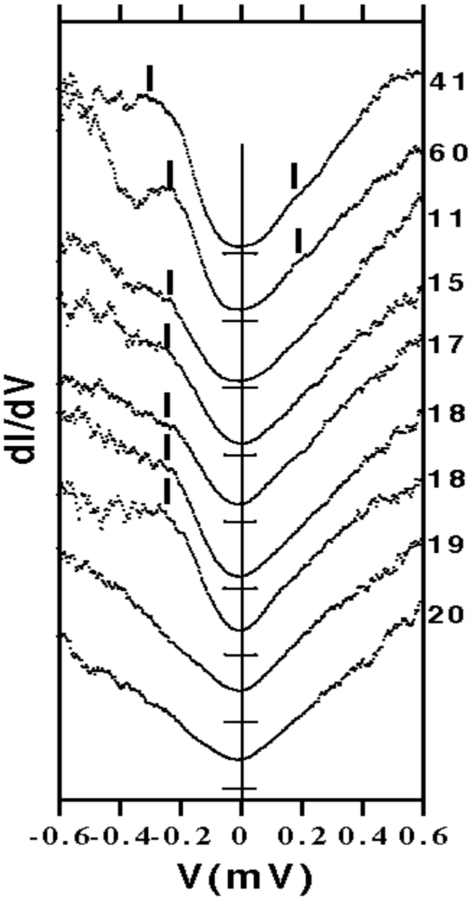

Figure 1: Tunneling spectra at different temperatures. $V_{\rm bias} = 0.3$ V and $I_{\rm tunnel} = 0.75$ nA. Small horizontal bars represent zeros for each dI/dV curve.

estimate the pseudo gap to 0.45 eV-0.5 eV, which is consistent with an optical measurement at 80 K[7]. The normalized zero-bias conductance, Fig 2, is a rough measure of the thermally smeared DOS at the Fermi level, N($E_{\rm F}$). This shows that the ten fold increase of resistivity at the NC-C transition is caused by the drop of N($E_{\rm F}$), and not by the decrease of mobility. If the pseudo gap is deep enough the DOS in the gap should be localized. Mott's criterion for Anderson localiztion reads g=N($E_{\rm F}$)/N($E_{\rm F}$)$_{\rm free}$ $\approx$ 0.3, where N($E_{\rm F}$)$_{\rm free}$ is the free electron value of N($E_{\rm F}$). If we assume that N($E_{\rm F}$)$_{\rm free}$ is equivalent to N($E_{\rm F}$) before the transition, although it might be underestimated because of CDW depletion, we can from the data in Fig 2 roughly estimate $g\sim$ 0.23 below the transition. Hence N(E$_F$) should then be localized. The weak metallic character between 180 K and 60 K can be explained by excitation of carriers

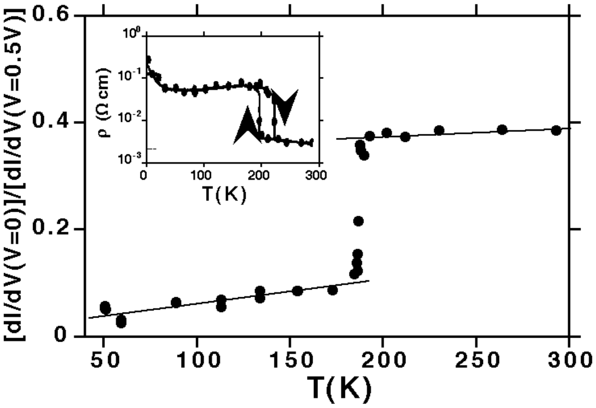

Figure 2: Temperature dependence of the normalized zero-bias conductance, which is a rough measure of DOS at $E_{\rm F}$. Inset: Temperature dependent resistivity of our 1T-TaS$_2$ crystal.

to the mobility edge, in line with Mott's idea[8], and the unbounded increase of resistivity below 50 K is explained as thermally activated hopping processes.

4. CONCLUSIONS

Our STS study showed an abrupt appearance of a pseudo gap at $E_{\rm F}$ below the NC-C transition temperature. The measured pseudo gap turned out to be deep enough to form localized states at $E_{\rm F}$. This indicates a splitting of the Ta 5d band due to the electron correlation effect rather than the pinning of $E_{\rm F}$ as suggested by the IPES study.

REFERENCES

[1] J. A. Wilson, F. J. DiSalvo, and S. Mahasan, Adv. Phys. 24 (1975) 117.
[2] P. Fazekas and E. Tosatti, Phil. Mag. 39 (1979) 229.
[3] B. Dardel, M. Grioni, D. Malterre, P. Weibel, Y. Baer, and F. Levy, Phys. Rev. B 45 (1992) 1462.
[4] R. Claessen, B. Burandt, H. Carstensen, and M. Skibowski, Phys. Rev. B 41 8270 (1990) 8270.
[5] S. Noutomi, T. Futatsugi, M. Naito, and S. Tanaka, Solid State Commun. 50 (1984) 181.
[6] J. -J. Kim, W. Yamaguchi, T. Hasegawa, and K. Kitazawa, Phys. Rev. Lett. 73 (1994) 2103.
[7] A. S. Barker, Jr., J. A. Ditzenberger, and F. J. DiSalvo, Phys. Rev. B 12 (1976) 2049.
[8] N. F. Mott and E. A. Davis, Electronic Processes in Non Crystalline Materials, (Clarendon Press, Oxford, 1979).