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**Surface Structure and Analysis  
With Scanning Tunneling Microscopy  
and Electron Tunneling Spectroscopy**

**PROGRESS REPORT**

May 1, 1989 - April 30, 1990

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**MASTER**

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During the current grant period we have continued to develop the spectroscopic applications of the STM and have carried out a large number of measurements on the gap structure due to charge-density waves and superconductivity. The measured energy gaps in 2H-TaSe<sub>2</sub>, 2H-TaS<sub>2</sub> and 2H-NbSe<sub>2</sub> are  $\Delta = 80, 50$ , and  $34$  mV giving values of  $2\Delta/k_B T_c$  of 15.2, 15.4 and 21.9. Measured energy gaps in 1T-TaSe<sub>2</sub> and 1T-TaS<sub>2</sub> are  $\Delta \simeq 150$  mV with  $2\Delta/k_B T_c \simeq 5.8$ . In the linear chain compounds, initial measurements have determined  $\Delta = 30$  mV in NbSe<sub>3</sub> and  $\Delta = 120$  mV in orthorhombic TaS<sub>3</sub>.

The spectroscopic mode of the STM is extremely sensitive to the precise local surface structure and the tip structure. Particular tip-sample combinations can exhibit large zero bias anomalies which modify the characteristic tunnel curves. We are currently exploring such factors by inducing surface and tip modifications and by adsorbing impurities on the surface. We are also designing chambers that will allow vacuum cleaning of the surface and tip for more careful control of surface contamination. The results of the spectroscopic studies on the layer structure dichalcogenides have been submitted to the Physical Review B (See present DOE-ER45072-38).

We have continued work on the high temperature superconducting oxides and metallic oxides. These are very difficult materials on which to obtain atomic resolution at low temperature, but success on several runs has been obtained at 4.2 K. More elaborate cleaving and surface preparation techniques need to be developed. The spectroscopic mode works fairly well and good measurements of the gap have been obtained on Bi<sub>2</sub>Sr<sub>2</sub>CaCuO<sub>8</sub> at 4.2 K. The best gap value is  $\Delta = 30$ -35 mV giving a value of  $2\Delta/k_B T_c \simeq 8$  as reported in preprint DOE-ER45072-38.

We continue to develop techniques for studying the linear chain compounds NbSe<sub>3</sub>, TaS<sub>3</sub> and TaSe<sub>3</sub>. During the current grant period we have succeeded in obtaining atomic resolution images of orthorhombic TaS<sub>3</sub>. We have shown that the single charge-density wave forming below 215 K consists of charge modulations on two of the three chains and are 180° out of phase. This work has been published as a rapid communication in Physical Review B (See DOE-ER45072-36). It supports the proposal by Wang et al. that the two charge modulations are coupled to form a CDW with a single  $\vec{q}$ -vector.

We continue to work on the 1T-phase of  $\text{TaSe}_2$ ,  $\text{TaS}_2$  and  $\text{VSe}_2$  with STMs that operate at different temperatures and over variable temperature ranges. In 1T- $\text{TaS}_2$  we have been studying the incommensurate CDW phases that exist at temperatures above 150 K. At room temperature we have shown the existence of a long range amplitude modulation of the CDW with a wavelength of  $\sim 6$  CDW wavelengths as shown in the grey-scale scan and profile in Fig. 1. This two dimensional modulated structure demonstrates the sensitivity of the STM to the detailed electronic structure of the material. The result also indicates that the CDW is continuously incommensurate rather than forming commensurate domains. More detail of these experiments can be found in preprint (DOE-ER45072-29).

**I. Preprints and Reprints of Publications Prepared During Current Grant Period**

1. "Scanning Tunneling Microscopy of Orthorhombic  $\text{TaS}_3$ ," C.G. Slough and R.V. Coleman, Phys. Rev. B 40, 8042 (1989) (DOE-ER45072-36).
2. "Scanning Tunneling Microscopy of the Linear Chain Compounds  $\text{NbSe}_3$ ,  $\text{TaS}_3$  and  $\text{TaSe}_3$ ," Journ. Vacuum Science and Technology, to be published (DOE-ER45072-37).
3. "Energy Gaps Measured by Scanning Tunneling Microscopy," Chen Wang, B. Giambattista, C.G. Slough and R.V. Coleman, submitted to Phys. Rev. B (DOE-ER45072-38).

**II. Reprints of Articles Previously Published**

1. "Scanning Tunneling Microscopy of Charge-Density Waves in Transition Metal Chalcogenides," R.V. Coleman, B. Giambattista, P.K. Hansma, A. Johnson, W.W. McNairy and C.G. Slough, Advances in Physics 37, 559-644 (1988). (DOE-ER45072-30).
2. "Scanning Tunneling Microscopy of Charge-Density Waves in  $\text{NbSe}_3$ ," C.G. Slough, B. Giambattista, A. Johnson, W.W. McNairy, and R.V. Coleman, Phys. Rev. B 39, 5496 (1989). (DOE-ER45072-32).

**III. Ph.D. Degrees Awarded**

Brian Giambattista, "Scanning Tunneling Microscopy of Atoms and Charge-Density Waves in Transition Metal Chalcogenides at 4.2 K."

Ph.D. Awarded June 1989

**IV. Papers Presented at Conferences**

1. Gordon Conference on the Phenomenology of High Temperature Superconductors, Invited June 1989  
"Tunneling Measurements of Energy Gaps in High Temperature Superconductors"
2. STM '89 Oarai, Japan July 1989  
"Scanning Tunneling Microscopy of the Linear Chain Compounds  $\text{NbSe}_3$ ,  $\text{TaS}_3$  and  $\text{TaSe}_3$ ."
3. American Physical Society  
Anaheim, CA March 1990  
"STM Measurements of Energy Gaps in CDW Compounds and Superconductors" (See Abstract Attached).
4. American Physical Society  
Anaheim, CA. March 1990  
"STM Observations of Commensurate and Incommensurate CDWs in 1T Phase Layer Structure Dichalcogenides" (See Abstract Attached).

5. American Association Adv. of Science  
New Orleans February 1990

"Scanning Tunneling and Atomic Force Microscopes," Invited

6. 14th Congress of Scientific Research  
Puerto Rico, February 1990

"Scanning Tunneling Microscopy - A Technique At the Cutting Edge," Invited

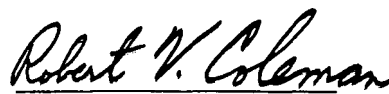
Abstract Submitted  
for the March 1990 Meeting of the  
American Physical Society

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STM Measurements of Energy Gaps in CDW Compounds and Superconductors.\* Chen Wang, B. Giambattista, C.G. Slough and R. V. Coleman, U. of Virginia. -- The scanning tunneling microscope (STM) has been used to measure the energy gap due to charge-density-wave (CDW) formation in the layer structure dichalcogenides. Structure in the  $I$  versus  $V$  and in the  $dI/dV$  versus  $V$  curves measured at 4.2 K has been clearly identified with the CDW gap. The presence of variable strength zero bias anomalies (ZBAs) can complicate the measurement, but a systematic analysis can separate the effects. Enhanced STM deflections and low barrier heights can also be correlated with the strength of the ZBA. Measured energy gaps in  $2H-TaSe_2$ ,  $2H-TaS_2$  and  $2H-NbSe_2$  are  $\Delta = 80, 50$  and  $34$  meV giving values of  $2\Delta/k_B T_c$  of 15.2, 15.4 and 21.9. Measured energy gaps in  $1T-TaSe_2$  and  $1T-TaS_2$  are  $\Delta \approx 150$  meV with  $2\Delta/k_B T_c \approx 5.8$ . Measured energy gaps in  $NbSe_3$  and  $TaS_3$  are  $\Delta = 30$  and  $120$  meV. The best measurements on the superconductor  $Bi_2Sr_2CaCuO_8$  give  $2\Delta/k_B T_c \approx 8$ .

\*Research supported by the Department of Energy.

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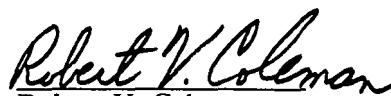
Abstract Submitted  
for the 1990 March Meeting of the  
American Physical Society

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STM Observations of Commensurate and Incommensurate CDWs in 1T Phase Layer Structure Dichalcogenides.\* C.G. Slough, W.W. McNairy and R.V. Coleman, U. of Virginia. -- The 1T phase layer compounds 1T-TaSe<sub>2</sub>, 1T-TaS<sub>2</sub> and 1T-VSe<sub>2</sub> have been studied by scanning-tunneling microscopy (STM) in the temperature range 4.2 to 300 K. At low temperatures the CDWs are commensurate with the lattice and the CDW amplitude is uniform in regions where the crystal lattice is perfect. The absolute amplitudes depend on the strength of the CDW, but are also a sensitive function of the effective barrier heights which also show a strong dependence on barrier thickness. The presence of zero bias anomalies (ZBAs) can also affect the amplitude. At higher temperatures incommensurate CDW phases are present in 1T-TaS<sub>2</sub> and 1T-VSe<sub>2</sub> and long range amplitude modulations of the CDW are observed. In 1T-TaS<sub>2</sub> at 300 K a continuous modulation of the CDW amplitude with a period of ~6 CDW wavelengths is observed. In 1T-VSe<sub>2</sub> various competing CDW structures are observed with a more complex amplitude distribution.

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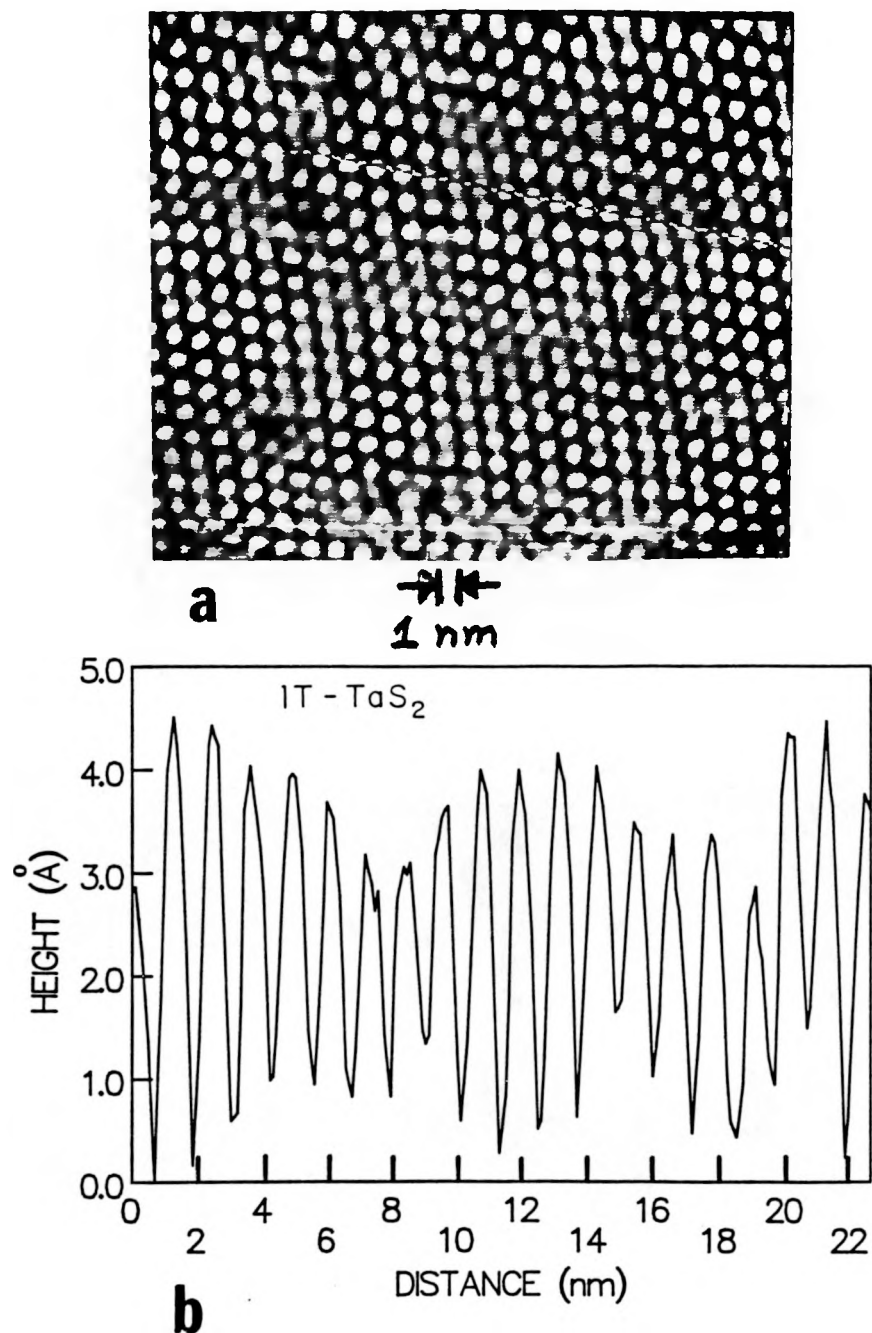


Fig. 1. (a) STM scan of 1T-TaS<sub>2</sub> at room temperature showing a two dimensional modulated structure due to the incommensurate CDW. The pattern shows only the CDW maxima. The surface atoms of S are not resolved. (b). Profile of STM deflection along the track shown in Fig. 2(a). The CDW amplitude is continuously modulated with a period of ~6 CDW wavelengths.

Fig. 1.