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High Resolution Photoemission Investigation of Phase Transitions in 1T-TaS_2.

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Abstract. Photoelectron spectroscopy with very high energy resolution reveals both dramatic and subtle changes in the electronic density of states of the quasi-2D material 1T-TaS_2, in coincidence with transitions between different charge density wave phases. Our results are consistent with the occurrence of a zero-gap Mott transition at ~185 K and of a subsequent Anderson localization in the pseudogap between the Hubbard subbands, and provide new insight into the unusual electronic properties of this material.

The layered compound 1T-TaS_2 exhibits unique physical properties which are related to, but are not fully explained by, the presence of a charge density wave (CDW) with a complex phase diagram. Especially the tenfold increase in the resistivity observed at the transition from a *quasi-commensurate* (QC) to a commensurate (C) CDW structure calls for an explanation other than the simple opening of a Peierls gap over portions of the Brillouin zone. Previous photoelectron spectroscopy (PES) studies have provided experimental support to a model predicting the occurrence of a Mott localization in coincidence with the QC-C transition. However, the values of the Mott-Hubbard gap (100-200 meV) estimated from PES data are incompatible with the results of transport measurements, which suggest a gap of the order of 1 meV.
We have addressed this controversial issue by a careful investigation of the temperature dependence of the electronic density of states (DOS) in the various CDW phases. The selected results presented here concern the QC-C transition. Our high resolution (ΔE~15 meV) PES spectra are very sensitive to small variations of the DOS occurring in the critical energy region, within a few k_BT of the Fermi level (E_F), that determines the low-energy properties of the material. The dramatic effect that the QC-C transition produces on the DOS of 1T-TaS_2 is well illustrated by the valence band spectra of Fig.1, which show that the sample evolves from a metallic to an apparently semiconducting state in less than 5 degrees. The prominent structure observed at a binding energy of 180 meV in the 186 K spectrum corresponds to the occupied Hubbard subband on the nonmetallic side of the Mott-Hubbard transition, and its binding energy is a measure of the on-site Coulomb correlation (U) in the Ta 5d band. Our results reveal the details of the growth and shift of this structure throughout the transition. We observe, at the transition temperature, a sharp

increase of the peak intensity, correlated with the resistivity jump, and with the sudden drop of the photoemission intensity at the Fermi level. This drop, reproduced in Fig.2, is a very direct evidence of the abrupt disappearance of most of the Fermi surface in coincidence with the QC-C transition. However, our results make clear that a finite electron density persists at E_F below the transition temperature and down to the experimental limit of 20 K. The separation of the Hubbard subbands is therefore incomplete and the Fermi level lies in a *pseudogap*. 1T-TaS_2 would therefore remain a metal, if localization due to disorder associated with the random distribution of impurities and defects, for which evidence exists from low-temperature resistivity data, did not occur in this pseudogap[2], probably around 180 K. Our results show that the relevant energy scale for the transport properties of this material is not defined by the binding energy of the Hubbard subband (~U) but by the difference between the Fermi energy and the mobility edge (which we estimate at ~5meV). They also demonstrate that PES with state-of-the-art resolution can greatly contribute to our understanding of Fermi surface driven electronic instabilities.

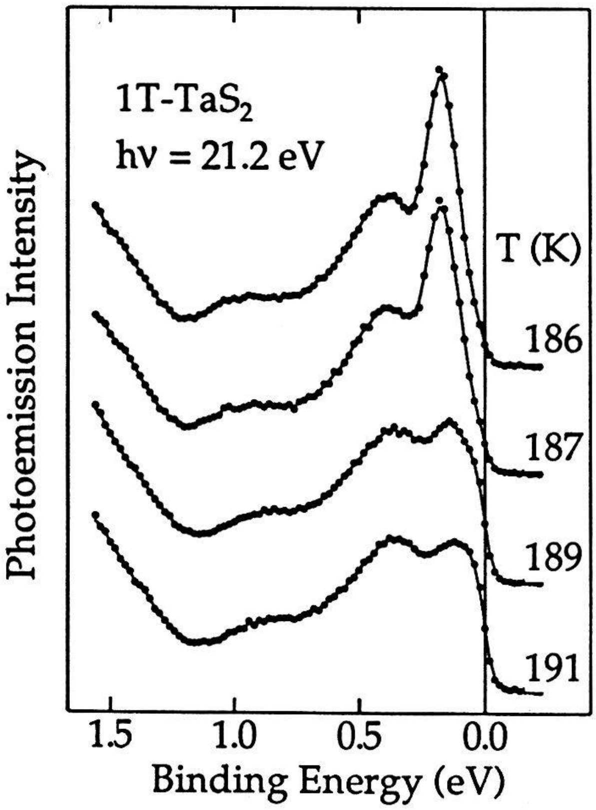

Fig.1. PES spectra of the valence band of 1T-TaS_2 through the QC-C CDW transition.

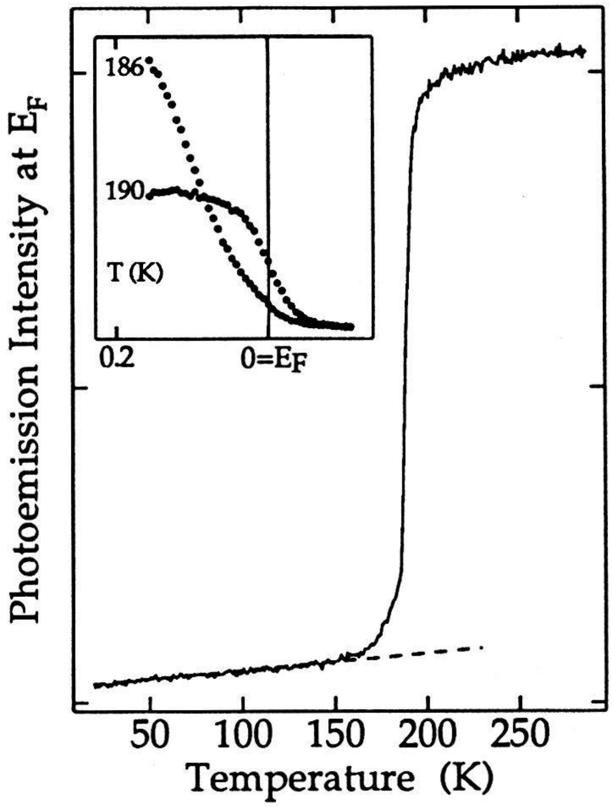

Fig.2. Temperature dependence of the PES intensity at E_F. **Inset**: Close-up of PES spectra near E_F.

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