

Spectral signatures of phase transformations in the valence energy loss spectra of 1T-TaS₂ intercalated with C₆H₁₂N₂(Triethylenediamine)

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Charge density wave (CDW) materials are characterized by periodic modulations of charge density. Charge density waves are also coupled to a periodic lattice distortion (PLD) which results in periodic modulation of atomic positions. 1T/2H-TaSe₂, 1T/2H-TaS₂, and 1T-TiSe₂ are some of the low dimensional structures that exhibit strong CDW distortions whose transition temperature and commensuration varies with temperature, doping, and dimensionality.¹ Due to their layered nature, these CDW materials can be also be intercalated with metal ions, and organic molecules. The intercalation of the molecules and ions takes place within the van-der-Waals gap.² The intercalation process can result in large changes to the atomic structure, electronic and magnetic structure of the host structure.^{1, 2}

We have investigated the changes in the atomic and electronic structure of 1T-TaS₂ due to intercalation with C₆H₁₂N₂.³ We show that the intercalation process leads to strong modifications in the atomic, electronic, and the CDW structure of 1T-TaS₂. This is mainly characterized by a structural transformation from the octahedrally coordinated 1T-TaS₂ phase to the trigonal-prismatic 4H-TaS₂ phase. The effect of this structural transformation is observed in the electron diffraction pattern of the intercalated phase. Figure 1 (a) shows the electron diffraction pattern from 1T-TaS₂ at 350 K characterized by super-lattice spots due to a nearly-commensurate CDW distortion. The resulting electron diffraction of 1T-TaS₂ intercalated with C₆H₁₂N₂ is shown in Figure 1(b). The electron diffraction pattern of intercalated 1T-TaS₂ is similar to the observed diffraction pattern for 4H-TaS₂ which is due to two orientations of a (13)^{0.5} x (13)^{0.5} superlattice.⁴

Structural phase transformation with the intercalation is also reflected in the valence electron energy loss spectra (VEELS). Figures 2(a), (b) and (c) compares the valence loss electron spectra for pristine 1T-TaS₂, 1T-TaS₂ intercalated with C₆H₁₂N₂, and 2H-TaS₂. The inset shows the peak features in the energy region 0-6 eV in greater details. In this energy region the VEELS spectra of 1T-TaS₂ is characterized by a strong peak between 2-2.5 eV. This peak is shifted to 3.5-4 eV in both 2H-TaS₂ and intercalated 1T-TaS₂. We discuss the nature and origin of changes in the VEELS spectra and the relationship to the structural transformation observed during the intercalation process

References

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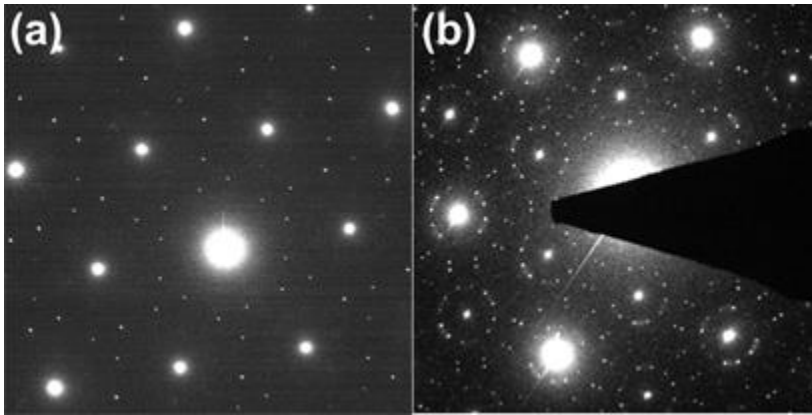


FIG. 1. (a) Electron diffraction pattern for 1T-TaS₂ at 300 K showing the superlattice spots arising from nearly commensurate charge density wave. (b) 1T-TaS intercalated with C₆H₁₂N₂ at 300 K

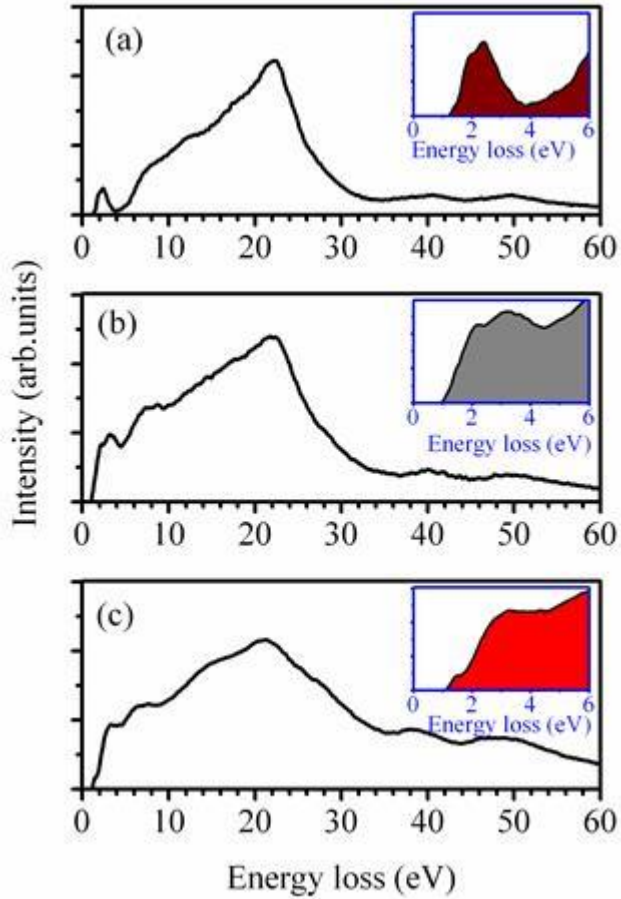


FIG. 2. Valence electron energy loss spectroscopy for (a) 1T-TaS₂ (b) 1T-TaS₂ intercalated with C₆H₁₂N₂ (c) 2H-TaS₂