Electronic and Magnetic Properties of Intrinsic Defects in TiS_2

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Transition metal dichalcogenides (TMDCs) are materials with unique electronic properties due to their two-dimensional nature. Recently, there is a large and growing interest in synthesizing ferromagnetic TMDCs for applications in electronic devices and spintronics. Apart from intrinsically magnetic examples, modification via either intrinsic defects or external dopants may induce ferromagnetism in non-magnetic TMDCs [1-2]. Our study focuses on intrinsic defects in TiS_2, which is a system known for potential applications in energy storage. We use scanning tunneling microscopy (STM) and superconducting quantum interference device (SQUID) magnetometry to characterize the crystal structure and magnetic properties of TiS_2 crystals. Atomically resolved STM images suggest the formation of sulfur vacancies and possibly interstitial defects creating brighter triangular shape regions. Preliminary analysis of magnetic data indicates low-spin paramagnetic response, with a saturated magnetization of ~0.16 emu/g and 80% saturation by ~2.5 T. To rule out ferromagnetism, hysteresis loops were analyzed and showed the coercive field to be zero within experimental error. Concurrently, DFT calculations on formation energy and electronic density were also being performed for proper identification of defect formations. Additionally, simulated STM images were generated by calculations that map the electronic density of the surface for the energetically favorable defects. An initial comparison to experimental STM images corroborates with the initial hypothesis of sulfur vacancies and titanium interstitial defects. Further studies include doping of TiS_2 with transition metals and further investigation of the electronic and magnetic properties of these doped TMDC systems.

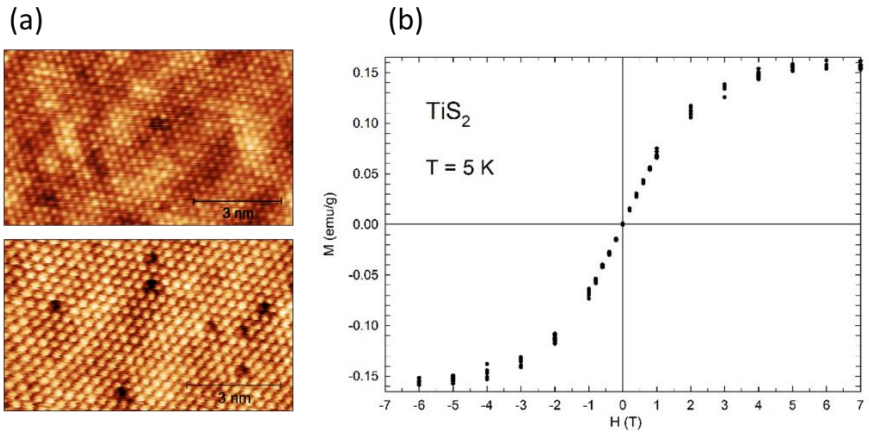

Figure: (a) Atomic resolution STM image on pristine. Empty states image was taken at a positive bias of V_B=200mV and I_T=0.7nA. Top layer sulfur atoms appear brighter in image and some brighter regions with possibly interstitial defects with a brighter contrast (upper panel) and vacancies as dark depression (lower panel). (b) Magnetization versus field measurements at 5 K up to 7 T for pristine TiS_2. Initial analysis indicates paramagnetism. Diamagnetic contribution has been subtracted.

[1] Magnetic doping in transition metal dichalcogenides, PM Coelho, J. Phys.: Condens. Matter 36 203001 (2024).
[2] Room-Temperature Ferromagnetism in $MoTe_2$ by Post-Growth Incorporation of Vanadium Impurities, PM Coelho, HP Komsa, K Lasek, V Kalappattil, J Karthikeyan, MH Phan, AV Krasheninnikov, and M Batzill, Adv. Electron. Mater., 1900044 (2019).