The Band Structure of The Quasi-One-Dimensional Layered Semiconductor TiS₃(001)

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Two dimensional (2D) materials are attractive choices for field effect transistor channels because of the reduced source-drain “cross-talk” at very small spatial dimensions, that occurs because such materials are so thin. ¹ To date, experimental studies have mostly focused on graphene and the transition metal dichalcogenide (TMDC) materials with MX₂ composition (M = Mo, W; X is a chalcogen), such as MoS₂, MoSe₂, WS₂, and WSe₂. The disadvantage with such materials is that in scaling down to 10 nm widths or less, edge scattering will become significant. Concern about edge scattering has attracted the attention of theorists²–⁷ and is now seen to be a major influence in experiment.⁸–¹¹ To overcome this complication, the transition metal trichalcogenide (TMTC) family are attractive materials. In this talk, we will present the first experimental mapping of the electronic band structure of TiS₃, which expected to have a band gap of about 1 eV and a mobility higher than 10,000 cm²/(V·sec).

The experimental mapping of the band structure of TiS₃(001), by momentum resolution nano-spot angle resolved photoemission (nano-ARPES), is presented in Figure 1. The experimental band structure, derived from angle-resolved photoemission, confirms that the top of the valence band is at the center of the Brillouin zone. This trichalcogenide has a rectangular surface Brillouin zone where the effective hole mass along the chain direction is -0.95 ± 0.09 mₑ while perpendicular to the chain direction the magnitude of the effective hole mass is much lower at -0.44 ± 0.1 mₑ. The placement of the valence band well below the Fermi level suggests that this is an n-type semiconductor.

Figure 1. Comparison of the experimental band structure for TiS₃(001), obtained from angle resolved photoemission spectroscopy, along the chain direction, i.e. Γ to Y (right), and perpendicular to the chain direction, i.e. along Γ to B (left), where the critical points, at the surface Brillouin zone edge, are at 0.95 Å⁻¹ and 0.65 Å⁻¹ respectively. The red dashed lines indicate the parabolic fits to the data.

Crystallographic picture

Brillouin Zone

References:
⁷ O. V. Yazyev, Reports Prog. Phys. 73, 056501 (2010).