Topological phase transitions and isostructural phase transition in 1T-$TiTe_2$ single crystal under pressure

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Trigonal $TiTe_2$ (1T-$TiTe_2$) has been studied for a few decades, showing some novel properties such as the enhanced superconductivity under uniaxial strain[1] and the charge density wave (CDW) transition in monolayer form[2]. However, there has been no experimental exploration for its high pressure behavior. In this work, the pressure-induced phase transitions were investigated by Raman scattering and electric resistivity for 1T-$TiTe_2$ single crystal under high pressure up to 17 GPa at room temperature. The result indicated that 1T-$TiTe_2$ single crystal undergoes three phase transitions at 1.7 GPa, 3 GPa and 8 GPa, respectively. The first-principles calculations manifest that the first two transitions at 1.7 and 3 GPa are accompanied with the band inversion near Fermi level, the further parity analysis shows that both two belong to the topological transition. Meanwhile, the structural distortion marked by the calculated c/a minimum was observed and proposed to induce the isostructural phase transition at 8 GPa. The observation of the two topological phase transitions and one isostructural phase transition for 1T-$TiTe_2$ single crystal under high pressure immensely enriches the physical understandings for this material family.

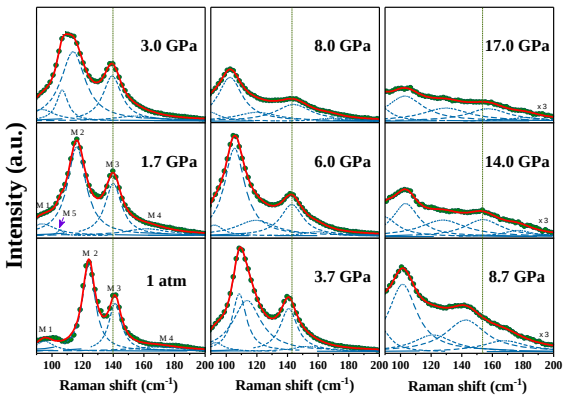

Figure 1 Raman spctra under high pressure

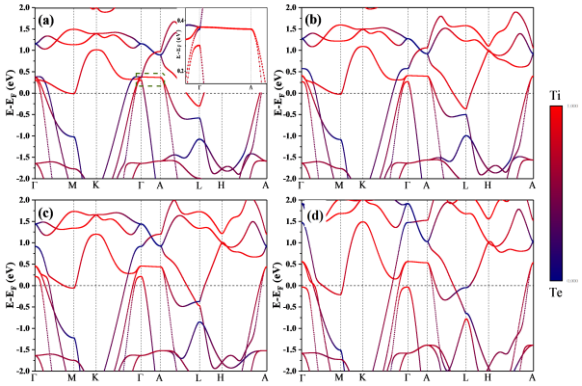

Figure 2 band structure at various pressure

[1] R. C. Xiao, Journal of Materials Chemistry C 5, 4167 (2017).
[2] P. Chen, Nature communications 8, 516(2017).