Infrared spectroscopic measurements of structural transition and charge dynamics in 1*T*-TiTe2 under pressure

S. Karmakar[1,2,*], U. Dutta,[1,2] S. Sahoo,[1] P. Malavi,[1] F. Piccirilli,[3] P. Di Pietro,[4] A. Perucchi,[4] and S. Lupi,[5]

[1]*HP&SRPD, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India*
[2]*Department of Physical Sciences, Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
[3]*CNR-IOM, Laboratorio TASC, S.S. 14 Km 163.5, 34149 Basovizza, Trieste, Italy*
[4]*Elettra Sincrotrone Trieste, S.S. 14 Km 163.5 in Area Science Park, 34149 Basovizza, Trieste, Italy*
[5]*CNR-IOM and Dipartimento di Fisica, Università di Roma Sapienza, P. le Aldo Moro 2, I-00185 Roma, Italy*

Keywords: high pressure, infrared spectroscopy, transition metal dichalcogenide

*e-mail: sdak@barc.gov.in

Quasi-2D layered transition metal dichalcogenides, a nonmagnetic family of compounds, provide an important playground to reveal exotic ground-state electronic order exhibiting the verities of charge density wave (CDW) transitions and superconductivity [1]. 1*T*-structured $TiTe_2$ is isostructural to 1*T* -$TiSe_2$, the latter being a model system of layered dichalcogenides that illustrates competing electronic orders (charge density wave order and superconductivity) upon intercalation or by external pressure [2,3].

Our recent investigations on isostructural semi-metal 1T-$TiTe_2$ have revealed pressure-induced superconductivity (with $Tc \sim 6$ K) and its persistence upon decompression [4] where CDW ordering was found to coexist with the superconducting state. Our results indicated that phase separated undeformed semi-metallic domains are responsible for the emergence of superconductivity.

We now have performed high pressure infrared measurements (at SISSI beamline, ELETTRA) on this system to understand the effect of pressure on its charge dynamics and electronic structure [5]. Our far-IR measurements help identifying a subtle and irreversible structural transition into a non-centrosymmetric structure (space group *P*3*m*1) at ~2.5 GPa. This structural modification results in dramatic change in low-energy electronic structure with enhanced Drude spectral weight (increased free carrier / metallicity), favoring superconductivity to emerge with a high transition temperature. This spectral weight transfer is found to be irreversible, as supported from irreversible structural modification under nonhydrostatic compression. This helps understand the persistence of a superconducting state upon decompression. The low-energy characteristic band (near 2000 cm^{-1}) of 2D correlated metal also gains in intensity irreversibly, indicating increased electronic correlation at higher pressure and its persistence nature. The broken inversion symmetry in the high-pressure structure in the presence of strong spin-orbit interaction may turn this gapped semimetallic compound into a possible topological semimetal, warranting more detailed high-pressure optical measurements and also theoretical investigations.

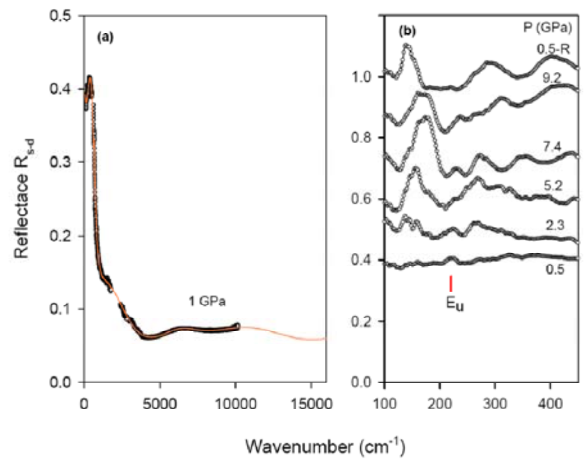

Fig. 1(a) Room-temperature IR reflectance spectra at the diamond-sample interface $R_{s-d}(\omega)$ for 1T -$TiTe_2$ at 1 GPa. Open circles are the experimental data, and the orange solid line is the calculated reflectance spectra using Drude-Lorentz oscillators (shown up to 16000 cm^{-1}). (b) Room-temperature far-IR $R_{s-d}(\omega)$ spectra at various high pressures. Spectra at higher pressures are arbitrarily shifted. R represents the released pressure.

Acknowledgments: Financial support by the Department of Science and Technology (Government of India) and ICTP (Italy) is gratefully acknowledged.

[1] R. Klemm, *Layered Superconductors* (Oxford University Press, Oxford, UK) 2012, Vol. 1.
[2] E. Morosan, et. al., Nat. Phys. 2006 **2**, 544.
[3] A.F.Kusmartseva, et. al. Phys. Rev. Lett. 2009, **103**, 236401
[4] U. Dutta et. al. Phys. Rev. B 2018, **97**, 060503(R)
[5] U. Dutta et. al. Phys. Rev. B 2019, **99**, 125105