IMPRINTS OF NANOSTRUCTURED AND MOTT PHASE IN OPTICAL PHONONS AND CONTINUA OF 1T-TAS₂

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1T-TaS₂ shows two unusual phases whose properties are still intensively investigated: CCDW (Commensurate Charge Density Wave) phase is a Mott phase whose appearance is followed by a reorganization of atoms in David-star(DS)-shaped super-cells throughout the TaS₂ plane; NCCDW (Nearly Commensurate Charge Density Wave) phase is a mixed phase of the CDW and metallic phase where these areas mix on a nanometer scale and in a geometrically ordered fashion. It is known that the mixed NCCDW phase can be stabilized by applying pressure [1] or very small doping (e.g. copper atoms) [2], and that this phase becomes superconducting at low temperatures (T < 5K). In this work, we present optical conductivity measurements of high precision, as well as the analysis of the optical features that emerge upon 13-fold reconstruction of the unit cell in both phases, and nano-structuring in the NCCDW phase. Almost all of observed optical phonons are the consequence of the David-star reconstruction, and their relative strengths in optical spectra reflect the charge redistribution within the stars. The mixed NCCDW phase is analyzed within the Effective Medium Approximation (EMA): The wide maximum in the real part of the optical conductivity, $\sigma_1(\omega)$, is identified as the effect of "surface plasmons" localized on the metallic islands. The mix of DS-modulated and metallic phases also account for "Fano-like" shape of phonon peaks. Finally, the Mott gap appears in the optical response of the CCDW phase as the additional feature at the low-frequency side of the "inter-band" portion of the optical spectra.

Sipos et al., Nature Mater. 7, 960 (2008)
Xu et al., PRB 81, 172503 (2010)