

The Symmetry Of The CDW Related Raman Modes In 2H-TaSe₂

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Two-dimensional layered materials, such as transition metal dichalcogenides display many interesting properties, among them the charge density wave (CDW) is one of the great interests for researchers. One of such materials is 2H-TaSe₂ characterised by two or three CDW phases, the transitions of which depend on whether the material is heated or cooled down. As the crystal's unit cell grows during the phase transition in the CDW phase, a series of new phonon modes emerge, rendering Raman scattering (RS) spectroscopy an attractive way of investigating the phase transitions. Although some simple polarisation measurements of Raman modes have already been done [1], there is no comprehensive study devoted to the modes' symmetries. Moreover, recent studies [2] show interesting chiral properties of phonon modes.

In this work, we investigate the symmetry of the CDW-related RS modes in 2H-TaSe₂ at a low temperature of 5 K as well as their temperature evolutions during crystal heating and cooling. Moreover, we assign the influence of the excitation energy on the RS spectra.

Figure 1 presents a comparison of the RS spectra measured at low ($T=5$ K) and room ($T=300$ K) temperatures. Although the low-temperature spectrum is composed of twelve phonon modes, its room-temperature counterpart displays only three narrow Raman peaks and a single broader one. The disappearance of nine phonon modes above approximately 120 K indicates the phase transition from CDW to normal. However, no clear sign of hysteresis was observed in the RS spectra between the cooling and heating procedures. Using polarisation-resolved RS experiments, we undeniably assigned the phonon modes to two families of symmetries, *i.e.* A_{1g} and E_{2g} , see the insets in Figure 1. We also found that some of the observed RS modes highly depend on the incident light energy, visibly varying for used 405 nm, 515 nm, 632 nm and 785 nm lasers. This indicates that the resonant conditions may play an important role in the measured Raman spectra.

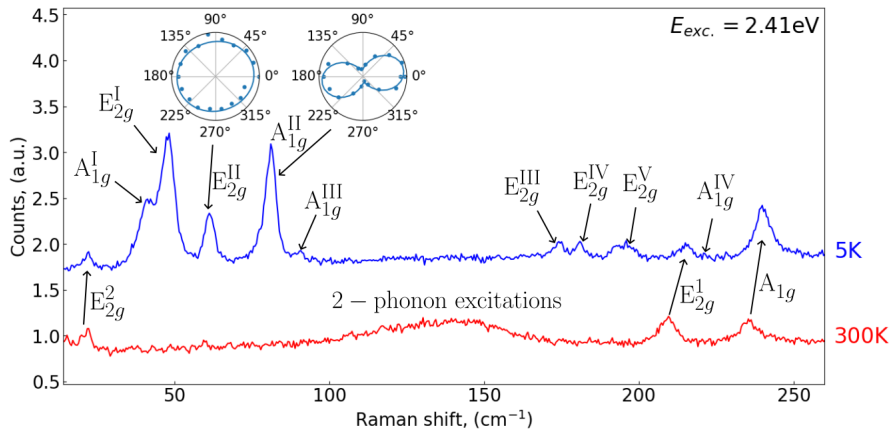


Figure 1: Raman spectra in 5K (Commensurate CDW) and 300K (normal phase). The insets show angular plots of linear polarisation of E_{2g}^{II} and A_{1g}^{II} modes.

[1] S. Sugai and K. Murase, *Phys. Rev. B* **25** 2418 (1982)

[2] Lacinska EM, et al., *Nano Lett.* **22**(7) 2835 (2022)