Optical probing of the dispersive ‘b’-mode in 1L-MoS_2

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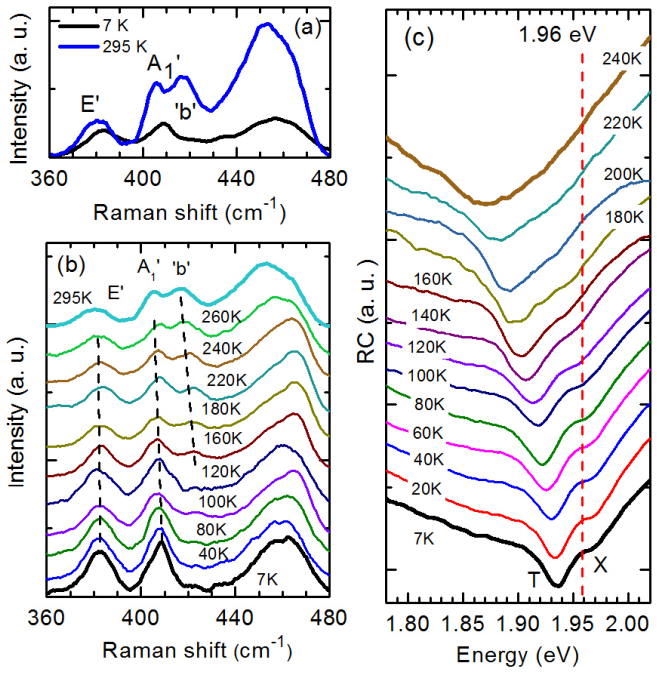

Fig.1 Micro-Raman (μ-Raman) and reflective contrast (RC) spectra of 1L-MoS_2: comparison of the μ-Raman spectra recorded at T =7 and 295 K, in vacuum (a), and the temperature evolution of the μ-Raman (b) and RC (c) spectra.

We report temperature-dependent (7 - 295 K) micro-Raman and reflective contrast (RC) spectroscopy of one layer (1L) MoS_2 exfoliated on the SiO_2/Si substrate. We employ resonant laser excitation (E = 1.96 eV) to probe the so-called dispersive mode ‘b’.

In the resonant Raman spectra of 1L-MoS_2 recorded in vacuum at T = 295 K we observe first-order Raman lines attributed to the in-plane E’ and out-of-plane A’ modes at frequencies 386 cm^{-1} and 404 cm^{-1}, respectively. We can also distinguish a dispersive ‘b’ mode at 420 cm^{-1} and the combined 2 LA(M) process (Fig. 1a). In contrast to the bulk crystal, in 1L-MoS_2 the ‘*b*-band’ is not detected in the Raman spectra at lower temperatures (T = 7 K). Interestingly, as the temperature increases above 100 K, this mode is emerging in the Raman spectra and simultaneously rising in intensity up to 295 K (Fig 1b). In order to elucidate the nature of this mode, we performed comprehensive, temperature-dependent micro-RC measurements. In the RC spectra at the lowest temperatures we observed two distinct resonances, attributed to the neutral exciton (X) and trion (T) transitions. They shift toward lower energies and become broader as temperature increases. Above T = 100 K, when the laser excitation energy crosses the energy of the neutral exciton, the ‘b-band’ is showing up in the Raman spectra. This observation shows that the effective photon - “b” phonon coupling is realized only for the laser excitation resonant with the neutral exciton.