Low frequency Raman modes and coupling constants of $MoS_xSe_{(2-x)}$ layers

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Raman spectroscopy is a versatile tool to characterise graphene and related materials[1]. Here we present a Raman and photoluminescence (PL) investigation of $MoS_xSe_{(2-x)}$ compounds prepared by chemical vapour transport as a function of number of layers and composition ranging from x=0 to 2. We find tuneable PL emission ranging from ~1.55 to 1.85eV corresponding to ~650-800nm. Thus, these compounds are of interest for electronics and optoelectronics applications as they allow one to tune and engineer the band gap. We find that the Raman spectra change significantly with number of layers and are sensitive to the composition. We monitor the shear (C peak) and layer breathing modes (LBMs), due to the relative motion of the layers either parallel or perpendicular to each other [2,3]. Representative Raman spectra for x=0.9 as function of number of layers are shown in Fig. 1, while Fig. 2 shows the C peak position, Pos(C), for a fixed number of layers as a function of x. A linear chain model to fit Pos(C) and Pos(LBM) position is used to describe the data: $Pos_{C,LBM}(N)=\sqrt{[\alpha^{\parallel,\perp}/(m_{Mo}+2m_{S,Se})]}\sqrt{[1\pm\cos(N_0\pi/N)]}/\sqrt{2}\pi c$, where N is the number of layers, $\alpha^{\parallel,\perp}$ are the force constants related to shear and LBMs, respectively, $m_{Mo,S,Se}$ are masses per unit area and c is the velocity of light. $\alpha^{\parallel,\perp}$ are then used to derive the layer coupling constants related to the in-plane and out-of plane Young's moduli. We find a non-linear dependence of the coupling constants with composition. Our results give insights into fundamental material properties such as van-der-Waals coupling in compounds and prove that the linear chain model can be applied to any layered material.

References

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[3] X.Zhang et al., Phys.Rev.B **87**, 11541 (2013)

Figures

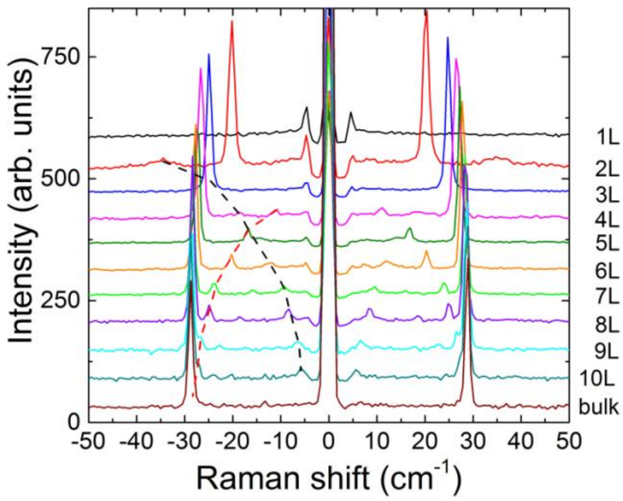

Figure 1: ULF Raman spectra for $MoS_xSe_{(2-x)}$ compound for x=0.9 recorded at 514.5 nm.

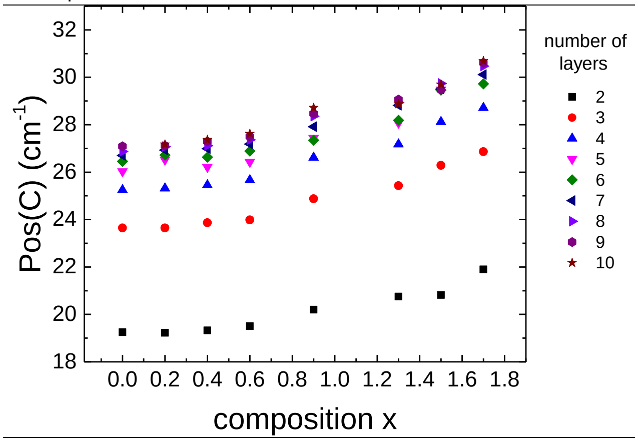

Figure 2: C peak position as function of composition for fixed number of layers.