CHARACTERIZATION OF STRUCTURED 2D MATERIAL LIKE "TRIANGLES" OF MOS₂ BY RAMAN SPECTROSCOPY

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One of the intensely investigated areas of the material research is the study of low dimensional structures with their unique optical and electronic band structure properties. It should be noted that the performances in applications of 2D crystals are largely influenced by their morphology and microstructure. In our study we used monolayer MoS₂ triangle flakes prepared by the chemical vapor deposition (CVD) method on SiO₂/Si substrate. Raman spectroscopy has been proven to be a fast, convenient, nondestructive technique and play a key role to characterize the fundamental properties of 2DMs. Therefore, we implemented this sensitive vibrational spectroscopy to probe the effect of interaction between the MoS₂ flakes and the Si substrate.



Figure 1. (a) Raman spectra of monolayer MoS_2 under 633 nm laser excitation, inset of the brightfield optical micrograph on MoS_2 deposited on silicon surface, (b) AFM image of a monolayer MoS_2 . Inset: the height profile along the dashed line and the dash-dot line to denote the measured Raman positions, (c) the vibrational modes A_{1g} , E^{1}_{2g} , shifts in dependence of the position from corner to edge of the triangle MoS_2 .

The resonant Raman spectrum of MoS_2 at the 633 nm excitation is composed of two basic vibrational modes; $E_{2g}^1(384 \text{ cm}^{-1})$, A_{1g} (405 cm⁻¹), and a broad asymmetric band at around 454 cm⁻¹ (Fig.1a). The peak frequency difference between those A_{1g} , E_{2g}^1 modes is about 19 cm⁻¹, which is characteristic for monolayer MoS_2 . This was further confirmed by the AFM mapping (Fig.1b). For the E_{2g}^1 vibrational mode we observed small frequency deviations (shifts) in the spectra taken from the corner-center-edge positions (Fig.1c).

It can be postulated that one of the contributing factors to this discrepancy may be the strain resulting from a mismatch in the lattice constants between the substrate and the twodimensional flake. Another factor that can be considered is the binding between the flake and the substrate characterized by a weakening from the center to the edges and corners. The obtained Raman spectra exhibited a good correlation with the results of the density functional theory (DFT) simulations. Also, in this study, transport properties of the MoS_2 flakes were observed with increasing the energy of the laser excitation which modulates the resonance with the electronic bands of MoS_2 occurring in the scattering processes.