Correlation between optical properties and thickness of the exfoliated transition metal dichalcogenides – MoS_2, $MoSe_2$, $MoTe_2$, WSe_2

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Transition–metal dichalcogenide crystals (TMDCs) have emerged as a new class of materials that display exceptional physical and optical properties [1]. Thickness is one of the fundamental parameters that define their surprising and unique electronic properties. A monolayer of these materials have the direct bandgap which gives an advantage over the indirect bandgap in bulk TMDCs, thus makes them promising candidates for several interesting applications as light emitters, detectors, and photovoltaic devices [2].

The typical representative compounds of the TMDCs family are molybdenum disulfide (MoS_2), molybdenum diselenide ($MoSe_2$), molybdenum ditelluride ($MoTe_2$) and tungsten diselenide (WSe_2) - natural and synthetic crystals, whose structures are characterized by strong intralayer covalent bonds within planes of hexagonally arranged transition metal (*M*) and chalcogen atoms *(X*) and by weak out-of-plane van der Waals interactions *X*-*M*-*X* layers.

It's important for applications and research purposes to have easy, quick and nondestructive methods of determining of layer thickness. Optical microscopy can give inconclusive results, so we propose using two different wavelengths in order to effectively determine number of layers of TMDCs and visualize defects. We use characteristic difference of relative reflections to determine the exact number of TMDC layers. TMDs crystals were mechanically exfoliated using PDMS-based exfoliation technic and were deposited onto a clean silica oxide substrate of 75 nm thickness. A confocal microscope was used for scanning the surface of these samples and for studying different defects formed during the exfoliation process. The measurements were carried out at room temperature using red (650 nm) and green (532 nm) laser light illumination. We use characteristic difference of relative reflections to determine the exact number of TMDC layers. This method also provides a quick method of visualization of the presence of defects in 2D materials.

We demonstrate that the correlation between the number of layers in a flake and the intensity of light reflected from the flake can be used for preliminary determination of the flake's thickness. The experimental results have been verified by Raman spectroscopy. The energy difference between E_{2g}^{1} (active out-of plane vibrational mode), A_{1g} (active in-plane vibrational mode) and B_{2g}^{1} (inactive in-plane vibrational mode) allowed for the independent measurement of the thickness of our samples. The new method was checked by theoretical model. We used transfer matrix method to obtain dependence between the number of TMDC layers and the intensity of reflected light. Main parameters of the model was thicknesses of materials and their indices of refraction at the given wavelength of light. Consistency of experiment and theoretical model was confirmed.

[1] Y. Li, A. Chernikov, T. F. Heinz et al., *Measurement of the optical dielectric function of monolayer transition-metal dichalcogenides: MoS_2, $MoSe_2$, WS_2, and WSe_2*, Physical Review B **90**, 205422 (2014).

[2] W. Zhao, Z. Ghorannevis, G. Eda et al., *Lattice dynamics in mono- and few-layer sheets of WS_2 and WSe_2,* Nanoscale **5**, 9677–9683 (2013).