Exploiting residual mechanical strain in CVD grown two-dimensional MoS_2 crystals

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Molybdenum disulphide (MoS_2) is a layered Van der Waals solid enabling, as in the case of graphene, the isolation of a single MoS_2 layer which is essentially a 2D-crystal. Being an indirect-gap (1.3 eV) semiconductor in its bulk form, MoS_2 attracted significant attention in the past years when it was found that its 2D counterpart is a direct-gap (~1.9 eV) material [1, 2]. Before this material can be properly incorporated into commercial devices, efficient large area growth methods are required.

In this work, a two-step atmospheric pressure CVD method is presented, exhibiting controlled and large area growth of single and few-layered 2D-MoS_2 crystals through the reaction between sulphur vapours and pre-deposited sodium molybdate (Na_2MoO_4) on a Si/SiO_2 substrate. Depending on the precursor concentration the lateral size of the crystals can be controlled. Moreover, a monotonic increase of the substrate coverage with the precursor concentration is established, which enables the preparation of either isolated monolayers homogeneously distributed on the substrate or continuous MoS_2 films with single and few-layer domains. X-ray photoelectron spectroscopy was used to verify the stoichiometry of the produced crystals, while Transmission Electron Microscopy confirmed the high quality of the crystals. Raman and Photoluminescence (PL) spectroscopies are employed to thoroughly study the fabricated crystals before and after transferring them onto a polymer substrate. Significant spectral variations between the as-grown and transferred crystals were found. An optical analysis [3] was conducted, identifying mechanical strain as the main source of the spectral variations. It was found that strain relaxation takes place due to the transferring of the 2D-crystal. The magnitude of the residual strain imparted on the as-grown crystals - which can be as large as 0.5%- is adequate to shift the direct transition of MoS_2 by almost 80 meV. The large residual strain experienced by the as-grown crystals enabled an estimation of the deformation potential of the direct optical transition of MoS_2.

References

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Figures

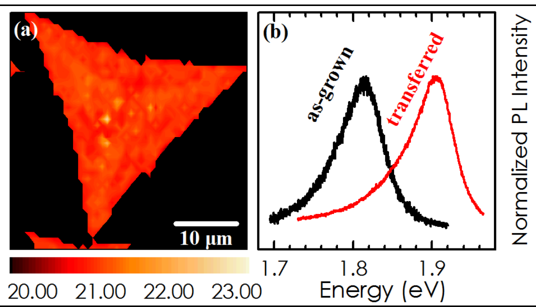

Figure 1 : (a) Raman image of the $\Delta\omega$ *value* of an as grown-CVD MoS_2 monolayer on Si-SiO_2 substrate. The average $\Delta\omega$ value is 20.7 cm^{-1}. (b) PL spectra of as grown and transferred crystal. The PL peak in this case is shifted roughly by 100 meV.

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