

ABSTRACT

The successful isolation of graphene in the year 2004 attracted substantial interest in exploring potential applications of this unique material and other members of the two-dimensional (2D) materials family in electronics, optoelectronics and emerging interdisciplinary research fields spanning from biomedical applications to information technology. The semiconducting transition metal dichalcogenides (TMDCs), among the two-dimensional materials, possessing atomic scale thickness, high surface area to volume ratio of atoms, varying band alignment and desirable bandgap are promising materials for next-generation electronics. A strong in-plane covalent bonding and a weak out-of-plane van der Waals bonding between atomic layers renders the TMDCs a characteristic layered property which makes them different from the three-dimensional (3D) counterparts. As the layers in these 2D TMDCs reach the atomic scale thickness, in the pursuit of miniaturization beyond Moore's law, 2D semiconducting TMDCs become a natural choice for device fabrication. However, practical implementation of these materials and their heterostructures needs to be preceded by a thorough understanding of their electronic and optoelectronic properties, as a function of number of layers, an issue addressed in the present work. In the present study, chemical vapor deposition technique was used to synthesize single-crystalline, large area films of 2D MoS₂, WS₂ and MoS₂-WS₂ heterostructure. The synthesis is based on reaction between metal-oxide (MoO₃ and WO₃) and sulphur (S₂) powder precursors, following a suitable temperature-time profile. In case of the growth of WS₂ and MoS₂-WS₂ heterostructure, the reaction is catalyzed using NaCl as seed promoter, due to the high sublimation temperature of WO₃. The obtained flakes with varying number of layers are triangular in shape, have large lateral dimension (~ 30– 40 μm) and cover the SiO₂/Si substrate uniformly. Lateral and vertical geometries of MoS₂-WS₂ heterostructure were obtained. Raman spectroscopy, optical microscopy and Atomic force microscopy techniques were used as fingerprint of the number of layers of the formed 2D material. The wavenumber separation between Raman peaks corresponding to 'A' and 'E' (2LA for WS₂) modes is used to determine the number of layers formed. Photoluminescence and UV-visible spectra with their distinct 'A' and 'B' bands confirm the exceptional optical properties of the 2D layers. Kelvin probe force microscopy (KPFM) technique was used to map the nanoscale variations in surface potential and to probe the effect of surface adsorbates on the work function of 2D MoS₂, WS₂ and MoS₂-WS₂ heterostructure, as a function of their number of layers. Surface potential distribution exhibits maximum spread in the monolayer MoS₂ and WS₂ samples which decreases with increase in the number of layers. A similar phenomenon of broad spread in Pt-MoS₂ and Pt-WS₂ junction current observed through point I-V measurements using conductive atomic force microscopy (CAFM) sheds light into the monolayer and few layer character of 2D layers resulting from charge trapping at the crystal defects. The study emphasizes the presence of exceptional electronic and optical attributes of the 2D layers even in presence of surface adsorbates and defects. The nature of metal-2D (MoS₂, WS₂ and MoS₂-WS₂ heterostructure) contact was further investigated as a function of number of layers and applied loading force using conductive atomic force microscopy. The junction formed between MoS₂ (single layer and bulk) and AFM metal tip (Co and Pt coated) was investigated as function of applied loading force (53 – 252 nN). A decreasing junction current with increasing loading

forces for monolayer sample was observed in contrast to negligible change in multilayer sample. A similar behaviour was also observed in metal-WS₂ and metal-heterostructure junction. The above has been attributed to the stress induced charge polarization in odd-layered MoS₂, WS₂ and MoS₂-WS₂ heterostructure materials.

The optoelectronic capability of 2D semiconductors was exploited by fabricating MoS₂ based optical sensors and studying their photocurrent generation mechanisms for light wavelengths in UV (300-450 nm), visible (500-670 nm) and near-infrared (700-1100 nm) range. It was observed that based on the number of layers of 2D MoS₂ a tunable response ranging from broadband in single layer to near infrared (upto 1000 nm) wavelength selective in multilayer is possible. Back-gated field effect transistor devices were fabricated utilizing 3-4L MoS₂, WS₂ and MoS₂-WS₂ heterostructure as the channel material. Successful operation of unipolar n-type and ambipolar conduction paved way towards demonstration of a logic CMOS inverter switch having enormous potential in future electronic devices. These results open opportunities to explore the uninvestigated applications of 2D FETs with precise conductivity modulation for future electronic devices.