MOCVD and Transistor Performance of MoS_2/WSe_2 Heterostructures

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Abstract

Two-dimensional (2D) transition metal dichalcogenides (TMDCs) are widely studied as potential channel materials for ultra-scaled field-effect transistors (FETs) beyond conventional CMOS technology. Two representatives are MoS_2 (inherently n-type) and WSe_2 (p-type). In addition to TMDC monolayers (MLs), vertically-stacked heterostructures consisting of two distinct TMDC-MLs have demonstrated many intriguing properties for (opto)electronic applications. However, most of these heterostructures are fabricated via mechanical transfer and stacking, which limits interface purity and scalability. A bottom-up approach to directly synthesize such vertical heterostructures is highly demanded to support technical advancements in this field.
In this work, employing a state-of-the-art AIXTRON close-coupled showerhead reactor, metal-organic chemical vapor deposition (MOCVD) processes for wafer-scale vertical MoS_2/WSe_2 heterostructures are designed. Tungsten/molybdenum hexacarbonyl (WCO/MCO), di-tert-butyl sulfide (DTBS) and di-iso-propyl selenide (DiPSe) are used as precursors with either H_2 or N_2 as carrier gas. 2" c-plane sapphire with a nominal 0.2° off-cut to m-plane is chosen as substrate, and a standard sapphire desorption procedure (150 hPa H_2, 1050 °C, 30 min) is carried out before deposition.
Firstly, the growth mechanism of MoS_2 on top of a WSe_2 ML surface is discussed. It is found that on the WSe_2 ML, the edges of prematurely formed WSe_2 bilayer (BL) domains serve as favorable growth sites for MoS_2. Compared to the desorbed sapphire surface, the growth rate of MoS_2 is accelerated on WSe_2, which can be explained by the promoted adsorption and migration of Mo adatoms on the WSe_2 ML surface. A change of MoS_2 domain shapes from triangular (on sapphire surface) to hexagonal (on WSe_2 ML surface) is also observed.
Multi-step MOCVD processes can be employed to reduce premature BL nucleation and achieve a planar interface between MoS_2 and WSe_2. By finetuning the growth conditions of MoS_2, a series of MoS_2-on-WSe_2 heterostructures were deposited with different coverages of the MoS_2 layer. Inverted WSe_2-on-MoS_2 heterostructures were also deposited.
The stoichiometry of MoS_2-on-WSe_2 heterostructures is examined by X-ray photoelectron spectroscopy, indicating a partial substitution of Se by S atoms. In the case of the inverted WSe_2-on-MoS_2 heterostructure, unchanged triangular domain growth and no chalcogen substitution are observed.
Optical characterizations indicate strong interlayer coupling between MoS_2 and WSe_2 in the as-grown heterostructures. MoS_2-on-WSe_2 vertical heterostructures with varied coverages of MoS_2 were processed into globally back-gated FETs. An increase in the electron current is observed with increasing MoS_2 coverage, while the hole current remains mostly unchanged.
The exact conduction mechanism of heterostructure FETs is still under investigation. The possible explanations include interlayer charge transfer doping and hybridization of band structures.