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Transport properties of in-plane MoS_2 heterostructures from lateral and vertical directions

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Abstract. Two-dimensional (2D) molybdenum disulfide (MoS_2) promised a wide range of potential applications. Here, we report the transport investigations on the MoS_2 from Armchair (AC) and Zigzag (ZZ) directions with different kinds of leads. The conductance of 2H phase MoS_2 depended on the transport directions and lead types (2H phase or 1T phase). System with 1T phase MoS_2 as lead can impressively improve the transport properties compared with the 2H phase lead. Moreover, for the system with metal lead, enhanced conductance can be observed, which contrast to the experiment measurements. Further investigate indicated that the conductance is sensitively rely on the distance between metal lead and 2D material. The present theoretical results suggested the lead material and interface details are both important for MoS_2 transport exploration, which can provide vital insights into the other 2D hybrid materials.

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Key words: lateral heterostructures, phase hybrid materials, MoS_2, transport.

1 Introduction

Recently, two dimensional (2D) materials like molybdenum disulphide (MoS_2) have attracted many interests because of them excellent physical and chemical properties and then promised many potential applications [1–8]. Monolayer MoS_2 appears in many distinct phases depending on the arrangement of its S atoms, two of them are more popular and exhibits substantially different electronic structures: 2H (trigonal prismatic, D_3h) MoS_2 is a semiconductor with a finite band gap between the filled d_{z^2} and empty d_{x^2}-$d_{y^2,xy}$ bands, and 1T (octahedral geometry, O_h) phase is metallic with Fermi level lying in the middle of degenerate $d_{xy,yz,xz}$ single band [9]. The reversible transition between

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2H and 1T phase have been proved by annealing [10], electric doping [11, 12], applying strain [13] or electron-beam irradiating [14]. Moreover, a mixed phase (2H and 1T) structure with the abrupt phase interface and matched lattice has been demonstrated experimentally [15]. This kind of bi-phase material paved a new way to design 2D photoelectric devices based on the in-plane metal/semiconductor heterostructures [16, 17].

Compared with the comprehensive studies on the fabrications [18–21] and applications [22, 23] of graphene/h-BN heterostructures, fewer reports focused on the in-plane 1T/2H MoS_2 hybrid systems. [14–16] By using lithium based chemical exfoliation method, Eda *et al.* [15] firstly synthetized a single layer of exfoliated MoS_2 consisting of both 2H and 1T phases then form chemically homogeneous atomic and electronic heterostructures with potential for novel molecular functionalities. The atomic phase transition mechanism for 2H to 1T in mono-layer MoS_2 have been explored with transmission electron microscopy, in which the controllable area of 1T phase was achieved with essential intermediate phases as the precursor phase [14].

Former studies suggested that the grain boundaries of the 2H monolayer MoS_2 have important effects on the transport properties [24]. They found that only tilt GBs have a significant effect on the mobility and transport characteristics of MoS_2, and these kinds of effects rely mostly on the defect type and density. In another experimental measurement, by using the 1T phase MoS_2 electrodes and well controlled phase interface, the contact resistance of 2H MoS_2 can be significant reduced without the performance loss [16, 17]. They attribute the superior performance of the devices to absence of structural and electrical mismatch between 1T and 2H MoS_2.

In this paper, we performed a first-principle combine with non-equivalent transport investigations on the 2H monolayer MoS_2 hybrid system with 1T and 2H electrodes. We focused on the relationship between the thermodynamics stability of the 1T/2H interface, and transport properties with different kinds of the electrodes. We found that the intermediate phase is unavoidable, and system's conductance is affected by electrodes choices.

2 Threoretical methods

The atomic and electronic structures of the 1T/2H monolayer MoS_2 phase interfaces were investigated using the DFT and the projector-augmented wave method (PAW) [25], as implemented in the Vienna ab-initio simulation package (VASP) [26]. The exchange-correction interaction was described by the Perdew-Burke-Ernzerhof (PBE) [27] functional. The plane-wave basis was expanded up to 550 eV. The 2D Brillouin zones of different interfaces were sampled by a series of k-point grids with constant separations of 0.02 $Å^{-1}$ during geometry optimization and 0.01 $Å^{-1}$ in the DOS calculation. 2D periodic boundary condition was applied in the directions along (y) and perpendicular (x) to the 1-dimensional (1D) interface. A single layer of molybdenum disulfide consists of a 6.7 Åthick slab of a S-Mo-S sandwich layer, [28] here a thickness of 20 angstrom was selected