Unlocking of Schottky Barrier near the Junction of MoS2 Heterostructure under Electrochemical Potential

Kubra Aydin[1], Mansu Kim[2], Hyunho Seok[1], Chulwoo Bae[1], Muyoung Kim[3], Jonghwan Park[1], Joseph T. Hupp[2], Dongmok Whang[1], Hyeong-U Kim[3], and Taesung Kim[1]

[1]Sungkyunkwan University - Natural Sciences Campus
[2]Northwestern University
[3]Korea Institute of Machinery & Materials

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Abstract

The exploration of heterostructures composed of two-dimensional (2D) transition metal dichalcogenide (TMDc) materials has garnered significant research attention due to the distinctive properties of each individual component and their phase-dependent unique properties. Using the plasma-enhanced chemical vapor deposition (PECVD) method, we analyze the fabrication of heterostructures consisting of two phases of molybdenum disulfide (MoS2) in four different cases. The initial hydrogen evolution reaction (HER) polarization curve indicates that the activity of the heterostructure MoS2 is consistent with that of the underlying MoS2, rather than the surface activity of the upper MoS2. This behavior can be attributed to an energy barrier arising from the physical contact resistance between the two different phases of MoS2 layers, which is mediated by van der Waals bonds. Remarkably, the energy barrier at the junction dissipates upon reaching a certain electrochemical potential, indicating surface activation from the top phase of MoS2 in the heterostructure. Notably, the 1T/2H MoS2 heterostructure demonstrates enhanced electrochemical stability compared to its metastable 1T-MoS2. This fundamental understanding paves the way for the creation of phase-controllable heterostructures through an experimentally viable PECVD, offering significant promise for a wide range of applications.

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