Anisotropic Transition-Metal Nitride van der Waals Epitaxy on Two-Dimensional Materials: A First-Principles Study

Shao-Chen Hwu(胡紹晨)[1], Kuan-Bo Lin (林冠伯)[2]*, Shu-Jui Chang (張書睿)[3], Chao-Hsin Chien(簡昭欣)[1] ,and Chenming Hu (胡正明)[2, 4]*

[1]*Department of Electronics Engineering, National Yang Ming Chiao Tung University, Hsinchu 30010, Taiwan*
[2]*International College of Semiconductor Technology, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*
[2]*Corporate Research, Taiwan Semiconductor Manufacturing Company (TSMC), Hsinchu 30078, Taiwan*
[4]*Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, California 94720, United States*
g00869@nycu.edu.tw

Abstract

Transition-metal nitrides (TMNs) such as TiN, ZrN, and HfN exhibit distinctive physical properties for their anisotropic crystalline. For instance, the (111) orientation of TMNs is known for its higher workfunction (> 4.5 eV) [1], making it a promising candidate for p-type transistor contacts. In our first-principles study, we further demonstrate that the TMN (111) orientation can form a short-range van der Waals epitaxial superlattice on a transition-metal dichalcogenide (TMD) substrate such as WS_2, MoS_2 (a lattice mismatch is lesser than 2 % observed for a 5 x 6 supercell periodicity). Notably, based on the calculated interfacial binding energy and density of states, the N-terminal TMN (111) configuration shows the strongest p-type contact properties on the TMD substrate.

Keywords - first-principles, short-range van der Waals epitaxy, anisotropy, transition-metal nitride, transition-metal dichalcogenide.

[1] Arrigo Calzolari and Alessandra Catellani Controlling the TiN electrode work function at the atomistic level: a first principles investigation (2016)