Lateral Junctions of Twisted and Zero-twisted Transition Metal Dichalcogenide Heterobilayers via Atomic Reconstruction

Hyeongseok Lee
Ji-Hean Baek, Seong Chul Hong, Donghoon Moon, Gwan-Hyoung Lee
Department of Material Science and Engineering, Seoul National University, Gwan-Ak ro 1,08826 , Seoul, Republic of Korea
hsleee54@gmail.com

In vertically stacked bilayers of transition metal dichalcogenides (TMDs), their interfacial van der Waals (vdW) energies vary with twist angles between TMD layers. It has been reported that the stacked TMD layers with a marginally small twist angle induce reconstruction into a relaxed structure to reduce the interfacial vdW energy. In our previous study, we observed thermally induced atomic reconstruction of the stacked bilayers into a fully commensurate (FC) structure regardless of the twist angle via encapsulation annealing.

Here, we report effect of atomically thin spacer between two TMD layers on the atomic reconstruction. We fabricated the twisted $WSe_2/MoSe_2$ heterobilayers, and monolayer graphene was inserted as a spacer between WSe_2 and $MoSe_2$. In this case, we verified that there is no atomic reconstruction in the WSe_2/Gr/$MoSe_2$ heterostructures even after encapsulation annealing at 1000˚C. It implies that the graphene spacer greatly reduces dependence of twist angle on the interfacial vdW energy. Therefore, the TMD bilayer regions with or without the graphene spacer maintained the twisted structure and changed into aligned FC structure, respectively. By using the graphene spacer, we constructed lateral junction of the twisted and aligned TMD bilayer regions by partially placing the graphene spacer between twisted TMD bilayers. At this junction boundary, we observed defect pairs of 5-7 rings, suggesting the possibility for spatial patterning of defect pairs.

Figures