Kyungnam Kang

Kyungnam Kang[1], Kamalika Ghatak[2], Shichen Fu[1], Xiaotian Wang[1], Siwei Chen[1], Dibakar Datta[2] and Eui-Hyeok Yang[1]

[1] Department of Mechanical Engineering, Stevens Institute of Technology, Hoboken, New Jersey 07030.

[2] Department of Mechanical and Industrial Engineering, New Jersey Institute of Technology, Newark, New Jersey 07102.

eyang@stevens.edu

A study on the growth of WS_2 homobilayers with controlled 0 and 60 degree stacking using two-step van der Waals epitaxy

The crystallographic alignment (0 or 60 degree stacking) of homobilayer shows strong interlayer coupling and leads to magnetoelectric effects for quantum manipulations [1-3]. However, 0 or 60 degree stacked homobilayers are typically fabricated by manually stacking the TMD layers through transfer, which is a low yield process with a high possibility of contaminant trapping between the layers.
In this report, we introduce two-step epitaxial growth technique to synthesize WS_2 homobilayer with a controlled 0 or 60 degree stacking. Since edges of the first monolayer have dangling bonds which work as nucleation sites for second growth, the second WS_2 monolayer grows from the edges and subsequently covers the first WS_2 monolayer. This growth process allows the two- step WS_2 homobilayer growth always gives perfectly aligned 0 or 60 degree stacking, attributed to the edge structures of first grown WS_2 monolayer. In order to elucidate the growth mechanism, we model the growth by *ab initio* first-principles scheme based on density functional theory (DFT), which identifies the most stable inter-layer stacking interactions (0 or 60 degree stacking) as a function of their binding energy. Furthermore, presence of dangling atoms/bonds in between the layers is corroborated from the formation energy calculations.

References

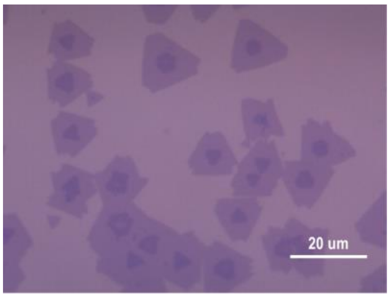
[1] S. Wu, J. S. Ross, G. B. Liu, G. Aivazian, A. Jones, Z. Fei, W. Zhu, D. Xiao, W. Yao, D. Cobden and X. Xu, "Electrical tuning of valley magnetic moment through symmetry control in bilayer MoS_2" Nat. Phys., **9**, 149-153 (2013)

[2] T. Jiang, H. Liu, D. Huang, S. Zhang, Y. Li, X. Gong, Y. R. Shen, W. T. Liu and S. Wu, "Valley and band structure engineering of fold MoS_2 bilayers" Nat. Nanotechnol., **9**, 825-829 (2014)

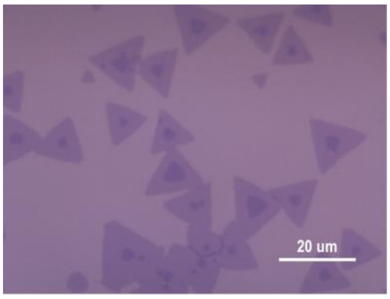
[3] A. M. Jones, H. Yu, J. S. Ross, P. Klement, N. J. Ghimire, J. Yang, D. G. Mandrus, W. Yao and X. Xu, "Spin-layer locking effects in optical orientation of exciton spin in bilayer WSe_2" Nat. Phys., **10**, 130-134 (2014)

Figures

Figure 1: Insert caption to place caption below figure (Arial Narrow 11)



60° of WS2 homobilayer



0° of WS2 homobilayer