Direct Growth of Layered Boron Nitride films on MoS_2 using Atomic Layer Deposition for 2D based Nano-electronics

Jaebeom Lee[1], Lanxia Cheng[1], Hui Zhu[1], Arul Ravichandran[1], Antonio T. Lucero[1], Zifan Che[1], Massimo Catalano[1], Moon Kim[1], Robert M. Wallace[1], Luigi Colombo[2], Jiyoung Kim[1]

[1] *Department of Material Science and Engineering, The University of Texas at Dallas, 800 West Campbell Road, Richardson, TX, 75080, USA*

[2] *Texas Instruments, Analog Technology Development, Dallas, TX 75243*

Hexagonal boron nitride (*h*-BN), a graphene analogue with strong covalent bonding of boron and nitrogen, is an atomically thin two-dimensional (2D) dielectric material having interesting properties, such as atomic flatness, high stiffness, near lattice matching with graphene, and low surface energy. These unique properties have made *h*-BN a widely-studied dielectric as a substrate material and a gate dielectric for graphene based device. However, direct integration of *h*-BN with other 2D semiconductors, such as graphene and MoS_2, remains a major challenge because of their low surface reactivity which leads to poor surface nucleation of *h*-BN, thus preventing the synthesis of large area films with controllable thickness and grain size.

We used atomic layer deposition (ALD) using BCl_3 and NH_3 as precursors in the temperature range of 600~800 ℃ as shown in figure S1 to grow *h*-BN thin films. We evaluated the growth of layered BN on different substrates, such as Co, SiO_2, HOPG and MoS_2 and found that the nucleation mechanism depends on the substrates. The distinct nucleation mechanisms of layered BN are likely attributed to the unique surface reactivities of the various substrates. Both Co and SiO_2 shows uniform nucleation sites, while growth on HOPG and MoS_2 showed growth mostly at the step edges due to the presence of dangling bonds and the inert nature of the basal plane. In order to increase the nucleation density we used an O_3 pretreatment to functionalize the surface of MoS_2. The AFM images revealed enhanced nucleation of the layered BN with an average grain size of ~ 20nm for a growth rate of ~ 0.22 Å/cycle. We also performed XPS measurements of the B 1s and N 1s peaks at 190.66 and 398.07 eV respectively, and the B:N ratio was estimated to be close to 1. The formation of layered BN was also verified further with the identification of satellite features at the higher binding energy shoulders of the XPS peaks, which is in good agreement with the layered BN structure observed in our HR-TEM images that show an interlayer spacing of 0.34nm (Fig S2). The band-gap of the ALD grown BN was also estimated to be around 5.1 eV based on the analysis of N 1s XPS loss feature, and the dielectric constant was estimated to be about 3.8 from capacitor measurements. Our results suggest that polycrystalline *layered* BN can be grown by ALD on Co, SiO_2, HOPG and MoS_2. Further studies will have to be performed to improve the crystalline quality of the films.

We acknowledge partial financial support from the Southwest Academy on Nanoelectronics (SWAN) sponsored by the Nanoelectronic Research Initiative (NRI) and NIST and we thank TMEIC for providing the ozone generator.