Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A Comparative Study of Graphene and h-BN Growth on Cu(100) based on DFT Calculations[1] WEI CHEN, University of Tennessee; University of Science and Technology of China; Harvard University, LEI LIU, GONG GU, University of Tennessee, ZHENYU ZHANG, University of Science and Technology of China — Using density functional theory (DFT) calculations, we carry out a comparative study of the epitaxial growth of graphene and hexagonal boron nitride (h-BN) on Cu(100) foils. We first show that van der Waals interactions play an important role in stabilizing the h-BN islands as they are nucleated on the metal substrate, similar to the physical picture from our previous study of graphene nucleation on Cu(111). By exploring the atomic structures of characteristic graphene and h-BN islands, we reveal the contrasting behavior between the orientations of graphene and h-BN clusters on the Cu(100) substrate, and correlate the differences with the differences in bond strength. We further advance the understanding on the spatial orientation at the nucleation stage to grain boundary (GB) formation, and provide insights in explaining the characteristic angle distribution of the GBs in graphene growth on Cu foils. The present theoretical study clearly explains our experimental observations, and may prove to be instrumental in modifying growth methods for large-scale fabrication of high-quality graphene and h-BN without GBs.

[1]Supported by USNSF, USDOE, and NNSF of China.

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Date submitted: 13 Nov 2013 Electronic form version 1.4