## Experimental and DFT Study of Boron Nitride Films Grown on SiO<sub>2</sub>/Si Substrates via Chemical Vapor Deposition

Mingyuan Wang,<sup>a,b,\*</sup> Ruo-wang Chen,<sup>a</sup> Hui Shi,<sup>a</sup> Guiwu Liu,<sup>c</sup> Shuangying Lei,<sup>a</sup> Neng

## Wan<sup>a,\*</sup>

<sup>a</sup>Key Laboratory of MEMS of Ministry of Education, School of Integrated Circuits, Southeast University, 210096, Nanjing, China;

<sup>b</sup>School of Mechanical Engineering, Jiangsu University, Zhenjiang, 212013, China

°School of Materials Science and Engineering, Jiangsu University, Zhenjiang, 212013,

## China;



**Fig. S1** (a, b) AFM topography images and corresponding (c, d) phase images of BN thin films grown on a  $SiO_2/Si$  substrate after the surface of the Ni film was etched with  $FeCI_3$  solution.



Fig. S2 (a) The X-ray photoelectron spectroscopy, and (b) Si 2p and (c) O 1s spectrum of





**Fig. S3** EDS mapping of the direct growth of BN on SiO<sub>2</sub>/Si substrate after the partial removal of polycrystalline Ni films.



**Fig. S4** (a) The X-ray photoelectron spectroscopy, and (b) Ni 2p spectrum for the surface of Ni. (c) The X-ray photoelectron spectroscopy, and (d) Ni 2p spectrum for the reverse side of Ni.



**Fig. S5** The structures of the initial state (IS), transition state (TS), and final state (FS) structures for N and B atoms from the first layer to the third layer for Ni(111), Ni(110) and Ni(111)&(110). The purple, green and silver balls represent the Ni, B and N atoms, respectivelly.