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Study on the Growth Mechanism of Monolayer and Few-Layer Hexagonal Boron Nitride Films on Copper Foil

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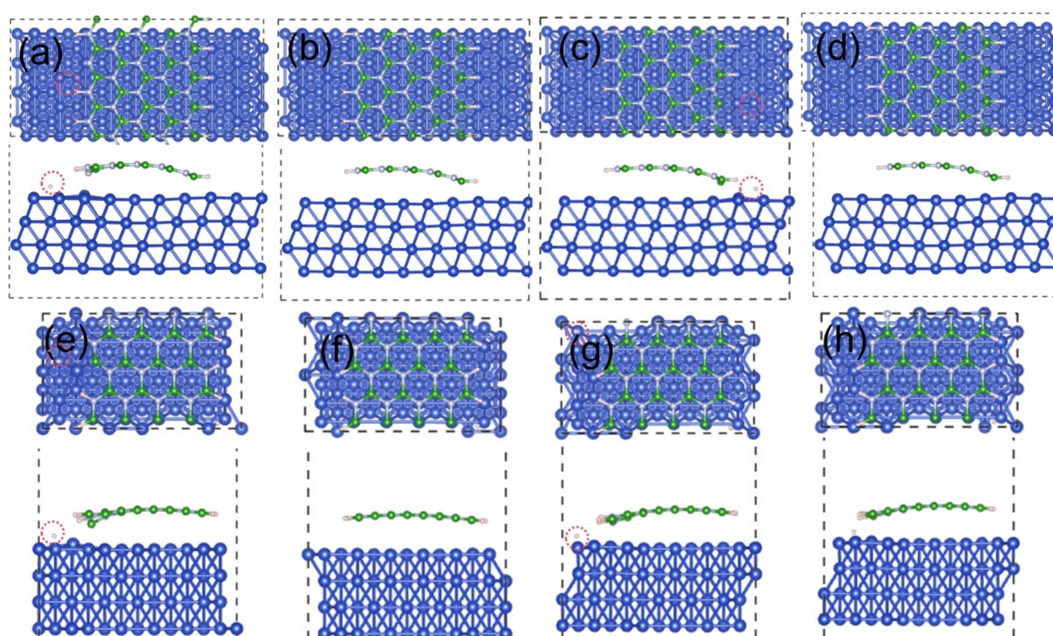

Fig. S1 Initial and final structures of H atom bond to (a, b) N and (c, d) B atoms at the ZZ edge of h-BN on Cu(111). Initial and final structures of H atom bond to (e, f) B and (g, h) N atoms at the AC edge of h-BN on Cu(111). The green, silvery, white and blue balls represent the B, N, H and Cu atoms, respectively. The red dashed circles represent the diffusion process of the marked atoms.

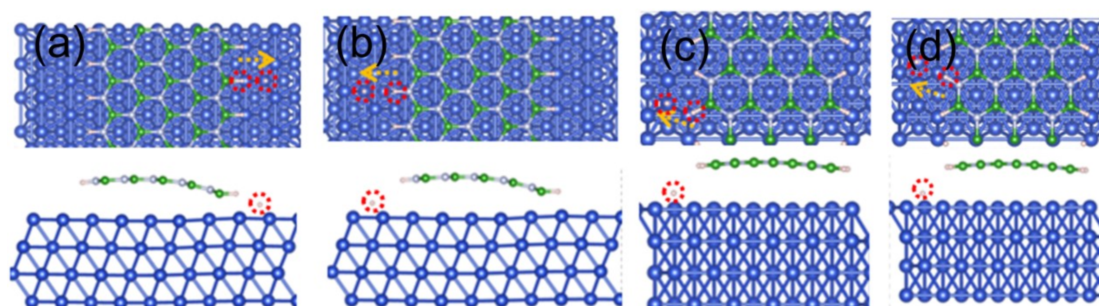

Fig. S2 (a-d) Schematic diagram for H atom desorption from the B and N atoms for BN-ZZ-H and BN-AC-H. The green, silvery, white and blue balls represent the B, N, H and Cu atoms, respectively. The red dashed circles and yellow arrows represent the diffusion process of the marked atoms.

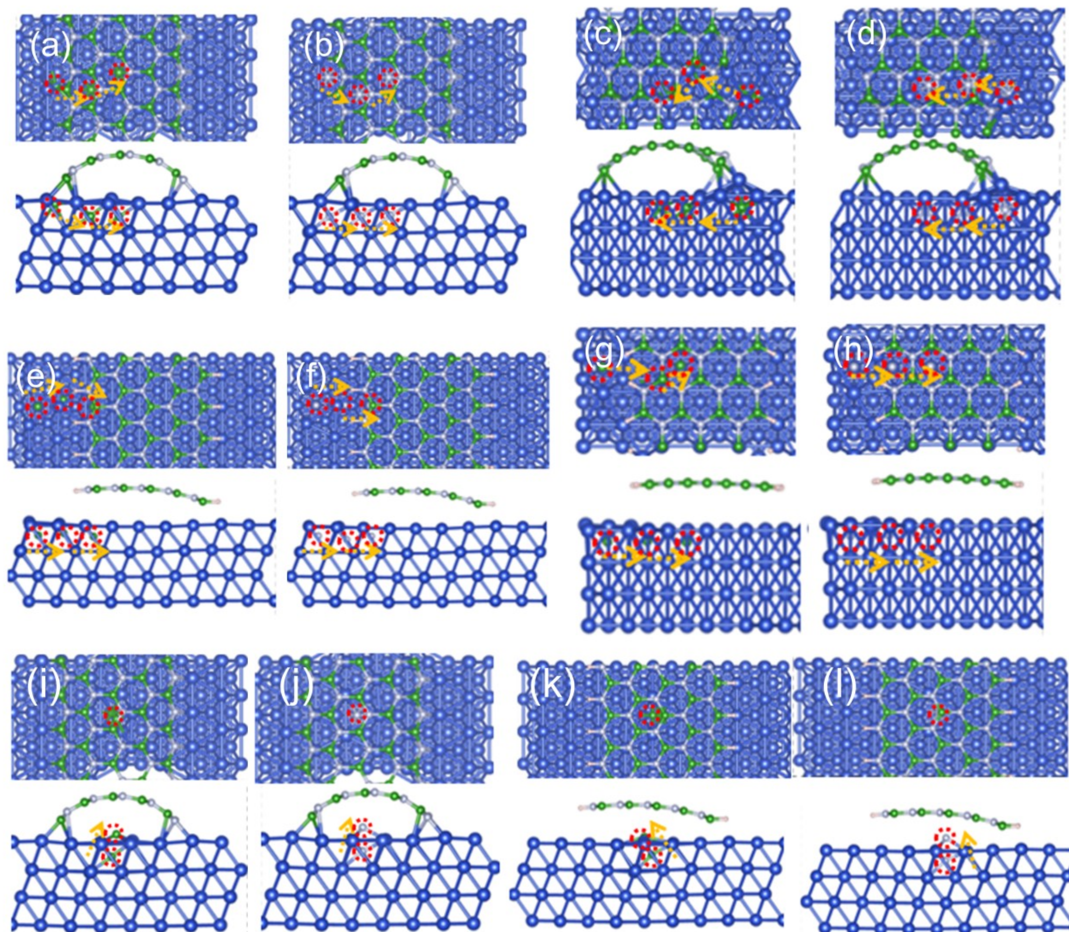

Fig.S3 (a-h) Diagram for the diffusion of B and N atoms along subsurface for BN-ZZ, BN-AC, BN-ZZ-H and BN-AC-H. (i-l) Diagram for the diffusion of B and N atoms from subsurface to surface for BN-ZZ and BN-ZZ-H. The green, silvery, white and blue balls represent the B, N, H and Cu atoms, respectively. The red dashed circles and yellow arrows represent the diffusion process of the marked atoms.

Table S1 Growth of h-BN on copper substrate under different conditions

Ref	Substrate	Pressure regime	Growth temperature	Precursor	Atmosphere	Results	Torr
1	Polycrystalline Cu foil	Atmospheric pressure	1000℃	Ammonia-borane 120–130℃	Ar: H_2 =170：30 sccm	2–5 layer film	760
2	Cu foil	Atmospheric pressure	1000℃	Borazine	H_2 =2000sccm	2 to ~20 nm thick film	760
3	Polycrystalline Cu foil	Atmospheric pressure	1000℃	Ammonia-borane, 110–130℃	Ar: H_2 = 80：20 sccm	6–8 layer film	760
4	Cu foil	~500 Torr	950℃	Ammonia-borane, 130℃	Ar: H_2 = 300：50 sccm	5-layer	500
5	Cu foil	Atmospheric pressure	1050℃	Ammonia-borane, 5 mg, 60℃	Ar: H_2 =170：30 sccm	1–2.2 nm thick film	760
6	Cu (solid and molten Cu on W)	Atmospheric pressure	1000℃ 1100℃	Ammonia-borane, 110℃	Ar: H_2 =90：10 sccm	1–10 layers	760
7	Polycrystalline Cu foil	Atmospheric pressure	1030℃	Ammonia-borane, 60–90℃	N_2: H_2 = 180：20 sccm	Monolayer film	760
8	Cu foil	Atmospheric pressure	1020℃	Ammonia-borane, 8.5mg, 80–100 ℃	Ar: H_2 = 95：5 sccm	~3 nm thick film	760
9	Cu foil	Atmospheric pressure	1030℃	Ammonia-borane, 80℃	20-mTorr air and 10-sccm H_2	~3 nm thick film	760
10	Cu foil	Low pressure	1000℃	Ammonia-borane, 55–120℃	Ar: H_2 = 50：50 sccm	Monolayer film	0.5
11	Cu foil	~10^{-6} mbar	≈950–1000℃	Borazine, 1×10^{-4} to 5×10^{-3} mbar	H_2 (~0.2 mbar)	Monolayer films	$7.5*10^{-7}$
12	Cu foil	350 mTorr	1000℃	Ammonia-borane, 60–90℃	H_2, 10 sccm (350 mTorr)	Monolayer film and islands	0.35
13	Polycrystalline Cu foil	30–40 Pa	1000℃	Ammonia-borane, 90–100℃	Ar, 40 sccm	Monolayer film	0.3
14	Cu foil	400 mTorr	1050℃	Ammonia-	H_2,100	Monolayer	0.4

				borane, 130℃	sccm	film	
15	Cu foil	30–40 Pa	1000℃	Ammonia-borane, 50, 70, 90, and 110℃	Different ratio of Ar and H_2	Monolayer film and islands	0.3
16	Polycrystalline Cu foil	UHV, base pressure < 10^{-7} mbar	1000℃	Ammonia-borane, 15 mg	H_2, 10 sccm	Monolayer islands	$7.5*10^{-8}$
17	Cu foil	Low pressure	1050 ℃	Ammonia-borane, 100℃	H_2, 15 sccm	Monolayer film	0.5
18	Polycrystalline Cu foil	Low-pressure	1050℃	Ammonia-borane, 2–3mg, 75–85℃	H_2, 40 sccm	Monolayer islands	0.5
19	Cu foi	Low-pressure	1050℃	Borazine	Ar: H_2 = 70：100 sccm	Monolayer film	0.5
20	single-crystal Cu (110) foil	low pressure (about 200 Pa)	1,035 ℃	Ammonia borane 65 ℃	Ar: H_2 = 5：45 sccm	single-crystal monolayer	1.5
21	Cu (111) films deposited on sapphire	low-pressure 5.0 torr	1,050 ℃	Ammonia borane, roughly 60 mg, 85 ℃	H_2, 30 sccm	single-crystal monolayer	5

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