Electronic supplementary information

Interface microstructure and band alignment of hexagonal boron nitride/diamond heterojunction

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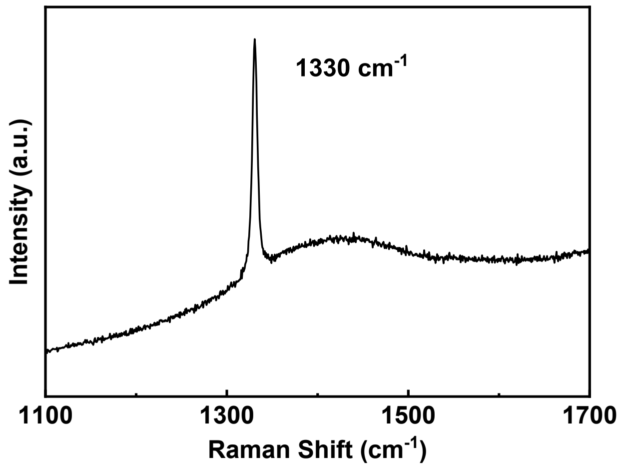

Fig. S1 Raman spectrum of the CVD-grown polycrystalline diamond substrate.

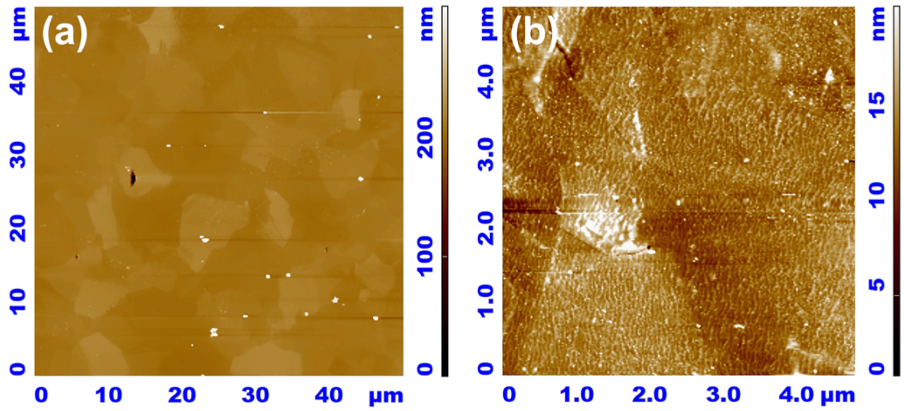

Fig. S2 AFM images of diamond substrate with a scanning area of (a) 50 μm × 50 μm and (b) 5 μm × 5 μm. The RMS roughness is determined to be about 0.90 nm within a 5 μm × 5 μm region.

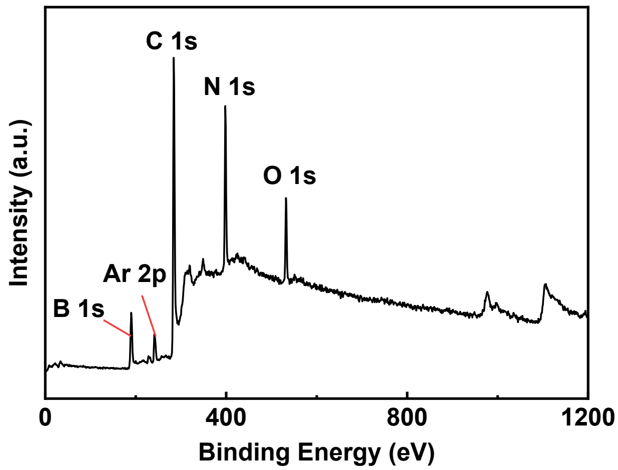

Fig. S3 Full XPS spectrum of the h-BN layer grown on diamond. Besides the B and N constituents from the h-BN layer, Ar, C, and O signals can also be detected. The presence of Ar is attributed to the incorporation from the growth atmosphere, while C and O originates from the surface contaminants and adsorption as well as the diamond substrate.

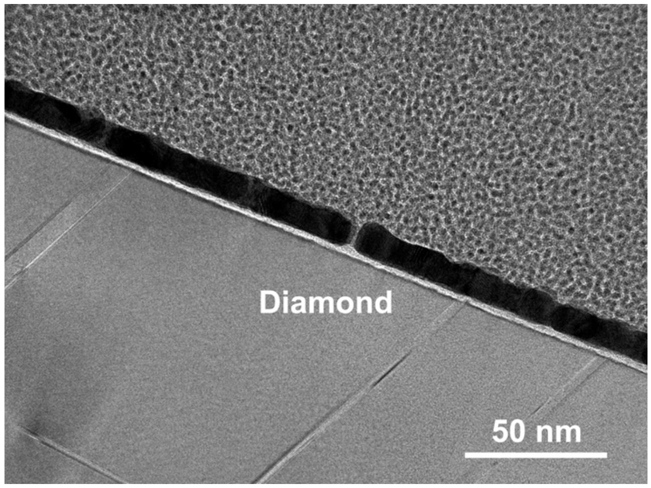

Fig. S4 A typical low-magnification TEM image of h-BN/diamond heterojunction, showing a very uniform thickness of the h-BN layer (the brightest thin layer).

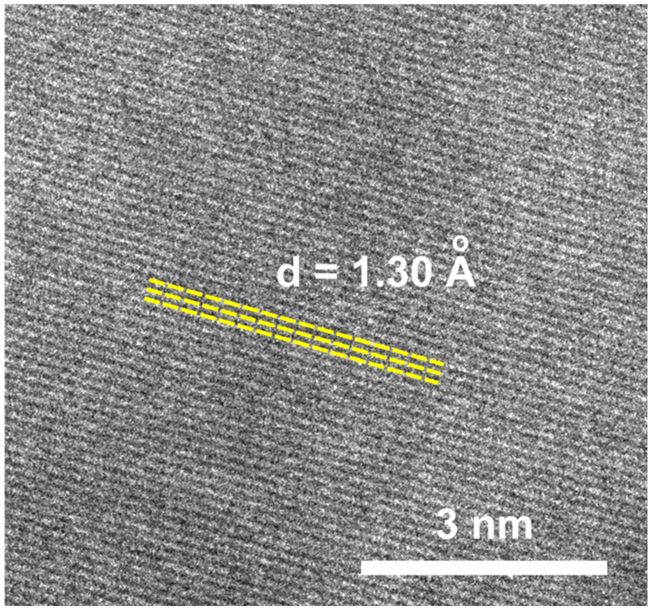

Fig. S5 HRTEM image of diamond substrate, showing a lattice fringe of diamond (220) planes with a lattice spacing of 1.30 Å.

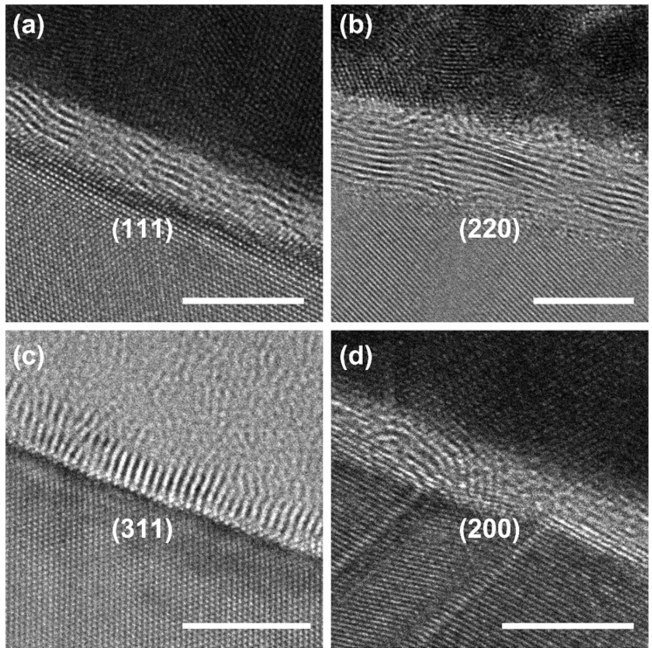

Fig. S6 HRTEM images of h-BN/diamond heterointerface focused on different crystal facets of diamond substrate. The scale bars denote 5 nm in these images.

Calculation of surface energy

We deduced the surface energy using the following equation:

$$E^{S}_{(hkl)} = \frac{\sigma}{2} \times N \times d_{(hkl)} \times \rho$$

where $E^{S}_{(hkl)}$ is the surface energy of the sample terminated by specific facet, σ is the bond energy of specific atom, N is the quantity of dangling bonds for each atom at the specific crystal plane, $d_{(hkl)}$ is the d-spacing of the crystal plane and the ρ is the volume density of atom of the sample.

The value of N can be determined from the structure models as shown in Figure S6. Such as for the (111) plane of diamond, half carbon atoms bond with the upper-layer atoms and the other part bond with the down-layer atoms. As a result, only half carbon atoms have one dangling bond represented as 1×1/2+0×1/2.

The other computational details and the results are shown in Table S1.

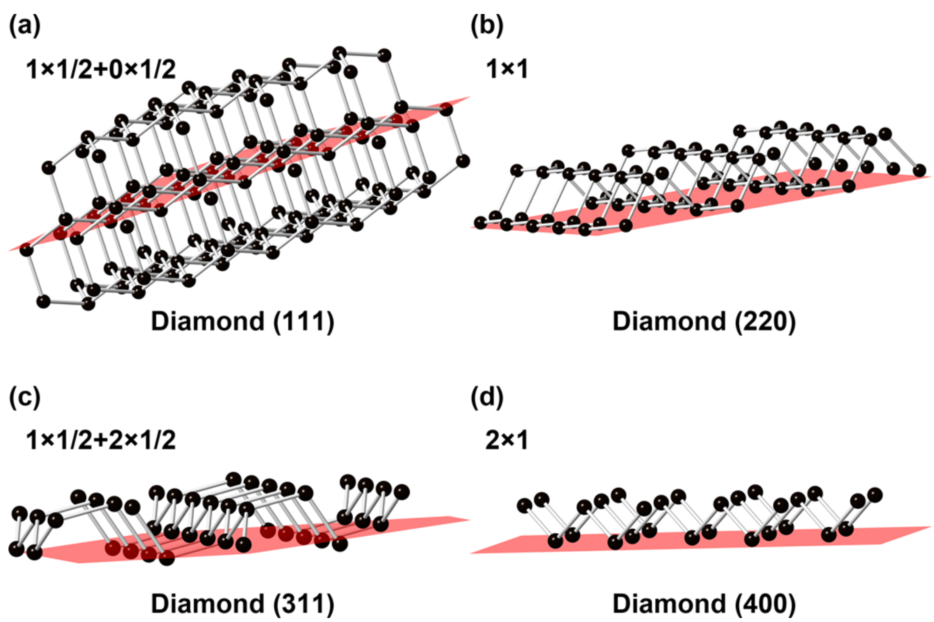

Fig. S7 Structure models of diamond terminated by specific facet (red plane).

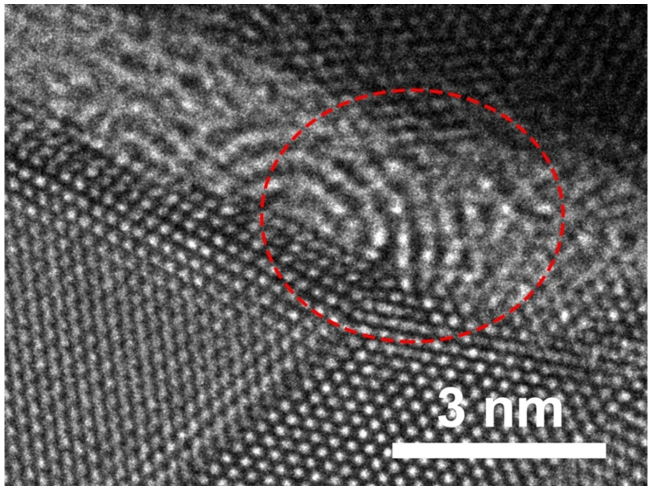

Fig. S8 HRTEM images of h-BN/diamond heterostructure focused on the grain boundary region of diamond substrate.

Table S1. Computational details of the surface energy.

Surface	σ [eV]	N	$d_{(hkl)}$ [Å]	ρ [$Å^{-3}$]	$E^{S}_{(hkl)}$ [eV $Å^{-2}$]
Diamond (111)	3.78	1×1/2+0×1/2	2.06	0.18	0.35
Diamond (220)	3.78	1×1	1.26	0.18	0.43
Diamond (311)	3.78	2×1/2+1×1/2	1.07	0.18	0.55
Diamond (400)	3.78	2×1	0.89	0.18	0.61
h-BN ($1\bar{1}00$)	3.98	1×1/2+0×1/2	2.16	0.11	0.24