Atomic structure determination of the (2×2) reconstructions of the polar AlN(0001) surface and atomic metallic deposition

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Group-III nitride semiconductors are ideal candidates for high-power electronic applications. Among these materials, aluminium nitride (AlN) has the largest band gap. It also has unique properties such as small density, large stiffness, large piezoelectric constant, large fracture resistivity and chemical inertness. Unfortunately, defects and interface states seriously compromise devices based on these materials and there is an urgent need for high-quality interfaces and surfaces. For these reasons, its surface reconstructions have received a lot of attention theoretically. Furthermore, due to its high ionicity, AlN crystallizes in the wurtzite structure and its (0001) growth surface is polar, like other zinc blende (001) semiconductor surfaces. The consequence of this polarity is that the crystal should be stabilized by the apparition of surface charges that can be generated by different mechanisms like surface reconstructions. Experimentally, due to the large gap of AlN (6.2 eV) it is not possible to observe its surface by scanning tunneling microscopy (STM) except for the Al rich phase. One effective way to get information at the atomic scale is to use atomic-force microscopy in the non-contact mode (NC-AFM) under UHV.

The growth of AlN samples was carried out in a MBE chamber equipped with a RHEED gun working at 15 keV. The AlN layer is grown on a 4H-SiC(0001) substrate following a recipe described elsewhere [1]. With the help of density functional studies, we determine new protocols for growing the technologically interesting N-rich AlN surfaces. This is achieved by dosing the precursor gases at unusually low rates. The measured surface reconstructions are in good agreement with our calculated structures [2]. Our protocols permit us to access the surface based on one additional N atom in a (2×2) cell. These N-rich AlN surfaces could open new routes to dope AlN layers with important implications in high- power and temperature technological applications.

Additionally, we have studied the adsorption of metallic components with the perspective of fabrication of planar atomic nanopads on AlN. Examples with Mg, Ag, and Au metallic deposition will be shown both experimentally and theoretically.

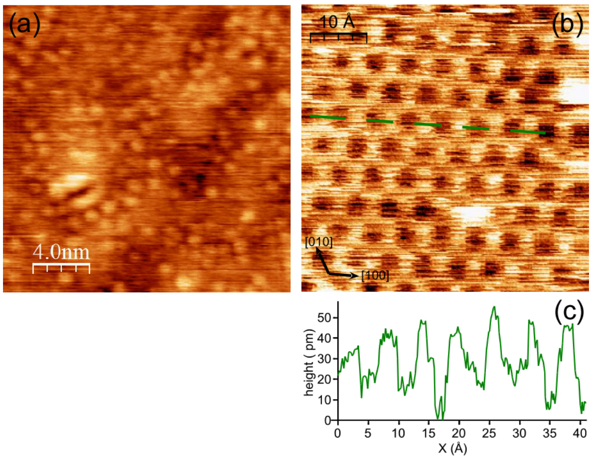

Figure 1 : NC-AFM topography image of AlN(0001) surface after growth of 200 nm thick sample at $T_{substrate}$ = 950°C, $BEP_{NH3} = 10^{-5}$ Torr and a growth rate of 100 nm/h (a) and 5 nm thick at 10 nm/h (b). (c) Cross section along the dashed line in (b).

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References

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