AlN/NbN epitaxial heterostructures on Si: polytypes, strain and polarity

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The combination of metal/superconductor NbN with III-N semiconductors opens the way to a wide range of innovative applications. Notably, it is possible to epitaxially integrate NbN and III-N. NbN can exist in different crystalline structures, commonly referred as polytypes. We found that by a fine-tunning of the growth conditions, a precise control of the NbN polytype formed on AlN can be obtained. This work focuses on a detailed analysis through advanced scanning transmission electron microscopy (STEM) of AlN/NbN/AlN heterostructures epitaxially-grown on Si (111) substrates by NH_3-molecular beam epitaxy (MBE).

Figure 1 (a) show a high angle annular dark field (HAADF) image of a δ-NbN layer viewed along the $AlN_{[11\text{-}20]}$ zone axis where the ABC cubic stacking is clearly observed. The epitaxial relationship is $AlN_{<11\text{-}20>} || \delta\text{-}NbN_{<1\text{-}10>}$ and $AlN_{<0001>} || \delta\text{-}NbN_{<111>}$. Conversely, it is also possible to achieve a predominantly ε-NbN layer. Figure 2(a) show a HAADF image of such a layer observed along the $AlN_{[11\text{-}20]}$ zone axis. While the first monolayers adopt the δ-polytype, the majority of the NbN layer exhibit the AA-BB stacking corresponding to the ε-polytype. The observed epitaxial relationship is $AlN_{<11\text{-}20>} || \varepsilon\text{-}NbN_{<11\text{-}20>}$ and $AlN_{<0001>} || \varepsilon\text{-}NbN_{<0001>}$.

The lattice mismatches between AlN and NbN depends on the NbN polytype. Specifically, the in-plane lattice mismatches are -0.7% and -4.7% for δ- and ε-NbN respectively. Figure 1(b) and 2(b) show strain maps obtained using the geometrical phase analysis (GPA) method for both heterostructures, with the AlN lattice distance used as reference. These maps reveal that, due to the low mismatch, δ-NbN is fully strained on AlN without introduction of misfit dislocations. For the NbN layer consisting of δ-polytype at the bottom and ε-polytype at the top, the δ-region is strained on AlN whereas the ε-region is fully relaxed.

A key distinction between wurtzite III-N and NbN is that III-N are polar materials whereas NbN is non-polar. Our observations using integrated differential phase contrast (iDPC) (figure (3)) confirm previous results: adding a thin epitaxial NbN layer reverses the polarity of AlN from Al-Polar to N-Polar.

Our STEM study demonstrates that is possible to control the NbN polytype by adjusting the growth conditions. Whatever the polytype, the introduction of a thin NbN layer consistently reverses the polarity of the AlN top layer. Another interesting finding obtained from our analyses is that the AlN/δ-NbN/AlN heterostructures are pseudomorphic with no misfit dislocations paving the way for the realization of high crystalline quality hybrid semiconductor/superconductor heterostructures and also hybrid Al-Polar/N Polar AlN layers.

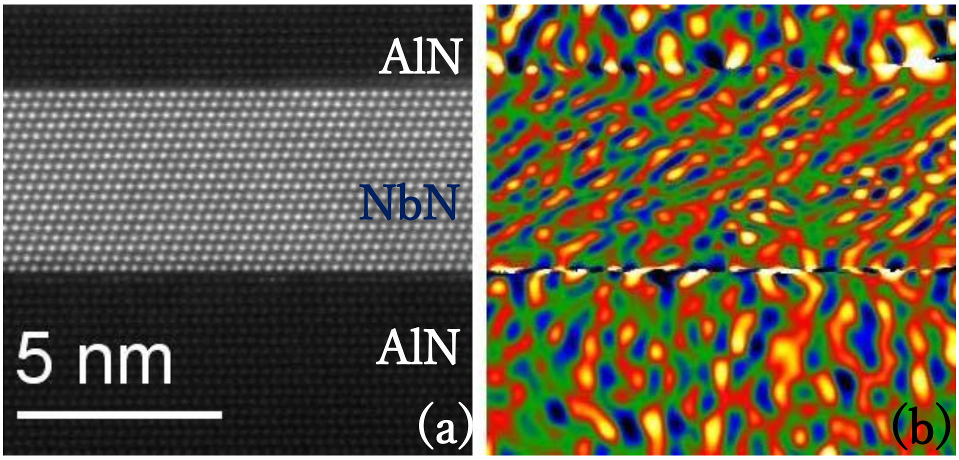

Figure 1: HAADF image of a δ-NbN layer (a) and corresponding GPA strain map for in plane distances (b).

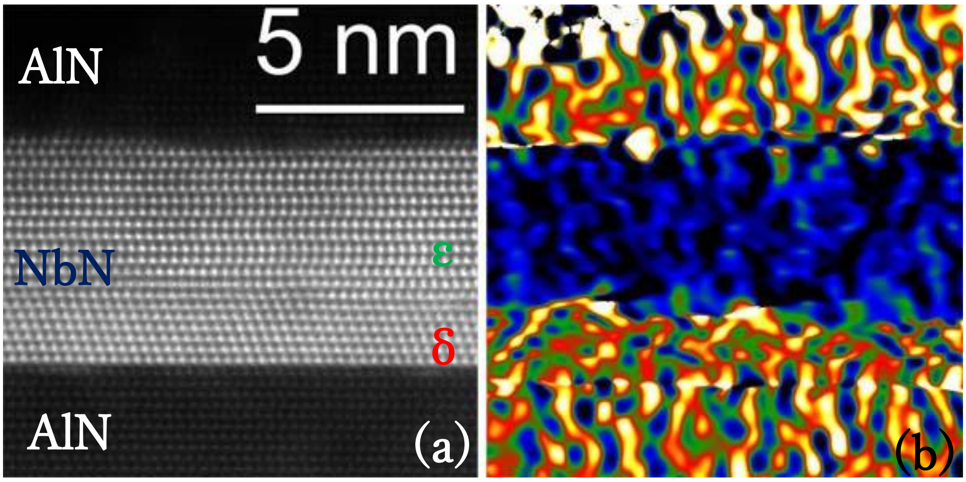

Figure 2: STEM-HAADF image of a mixed δ-NbN/ε-NbN layer (a) and corresponding GPA strain map for in plane distances (b).

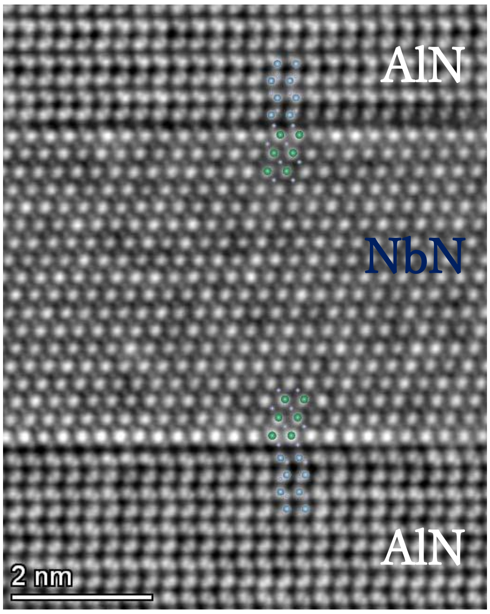

Figure 3: STEM-iDPC image of a δ-NbN layer. Both heavy (Nb, Al) and light (N) elements, are observed revealing the polarity reversal between the bottom and top AlN layers. Ball-and-stick model is superimposed on the experimental image with Nb in green, Al in blue and N in grey.