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Mean inner potential variation with strain in III-nitrides studied by off-axis electron holography

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Background incl. aims

Wurtzite III-nitride semiconductors are well known for their intense spontaneous and piezoelectric polarization fields. A deeper understanding of these properties is relevant for applications in various fields such as optoelectronic or power electronic devices. Off-axis electron holography is a powerful tool to measure directly and with a nanometer resolution the total electrostatic potential in these materials. However, to be able to study the polarization fields in III-nitrides, we need to remove the contribution from mean inner potential (MIP), which corresponds to the volume average of the Coulomb potential in the specimen. In the literature, MIP is traditionally derived for bulk materials within density functional theory (DFT).^{1,2} Evaluating the MIP using electron holography, we noticed disparities with values from the literature. One explanation that we propose is that the calculation for bulk material does not reflect the reality of heterostructures that are used in devices, with for instance the importance of strain. We propose here a deep analysis of the MIP evaluation for III-nitrides, comparing electron holography results with DFT calculation of the MIP that include the variation of strain.

Methods

MIP was computed through ab-initio simulations performed using GPAW code with plane wave basis-set of 300 eV cutoff energy, PBE functional, and 8x8x1 k-point sampling. The calculations were performed in a slab containing 11 atomic layers terminated in nonpolar m-{10-10} facets, centered in a 6.2-nm-long vacuum region with periodic boundary conditions. The MIP was obtained by averaging the Coulomb potential in the center 7 atomic layers, to prevent surface effects. The effect of strain has been modelled considering a biaxial strain configuration for layers grown along the <0001> direction.

From the experimental point of view, we study here 4 different samples. The first structure consists in a 6-period non-polar AlN/GaN (13nm/16nm) on 60 nm of AlN deposited on a (1-100) SiC substrate. The second sample is a 10-period polar AlN/GaN (20nm/20nm) superlattice grown by plasma-assisted molecular beam epitaxy (PAMBE) on 100 nm of GaN deposited on 1- μ m-thick AlN-on-sapphire templates.³ The third and fourth samples consist in 5-period GaN/InGaN multi-quantum wells (MQWs) grown on a 2 μ m-thick GaN layer that is itself grown on a 220-nm thick AlN buffer layer on patterned Si(111) templates using low-pressure metal organic vapor phase epitaxy (MOVPE). In

one of the samples, the MQW consists in 5 periods of In_{0.13}Ga_{0.87}N (2 nm)/GaN (12 nm). In the other one, the indium content in the barriers is higher, between 14 and 16%.⁴ These samples have been studied using off axis electron holography performed in a double corrected FEI Titan Ultimate TEM operating at 200kV. Electron holograms were recorded on a Gatan One View 4k camera. TEM specimen were prepared by in-situ lift-out focus ion beam (FIB) using a FEI Strata 400.

Results

III-nitride heterostructures are usually grown along a polar axis, resulting in strong polarisation-induced internal electric fields that contribute to the total potential measured in electron holography. Additional contributions come from dopants, which can partially screen the internal electric fields, and from the MIP. Our first experiment consist in an attempt to measure MIP in an AlN/GaN heterostructure. To avoid the presence of internal electric fields, the heterostructure was grown along a non polar axis, and we verified that the lattice was fully relaxed. We obtained a difference of MIP between GaN and AlN of 1.53 V which is very different from the generally accepted 1.01 V, calculated by Schowalter et al. [1], and the 2.77 V that we obtain from our DFT calculations for relaxed materials. This opens a question about the real value of MIP for these compounds.

We used then a polar superlattice of AlN/GaN (second sample) to repeat the same measurement. In this case, the MIP difference between GaN and AlN, extracted from the electron holography result, was 1.3 V, i.e. slightly lower than in the non polar sample. We assumed that the difference could be attributed to a different strain in the structure. However, keeping in mind that AlN is under tensile strain and GaN is under compressive strain, the expected result is rather an increase of the MIP difference, which might reach up to 3 V. In summary, we conclude that current uncertainties in the AlN MIP value make it extremely difficult to extract precise information about the potential profile field in GaN/AlN heterostructures.

We have extended this work to InGaN/GaN, now obtaining more reliable results. The TEM specimen from the third sample was prepared with a gradient of thickness, so that there is a different degree of surface-induced relaxation in the 5 quantum wells. In this sample, we can show experimentally the variation of MIP with respect to strain, with the MIP of GaN and InGaN being almost equal for a completely relaxed sample. The experimental results match closely our DFT computation, including the strain dependence.

In the last sample, also InGaN/GaN but with different indium concentration, we could further confirm the effect of strain on the MIP, including a clear evaluation of the MIP difference between GaN and In_{0.16}Ga_{0.84}N.

Conclusion

The understanding and computation of MIP is highly important for a correct interpretation of the potential profiles measured in electron holography. In this work, we provide a theoretical and experimental evaluation of the MIP in III-nitrides. We outline the important disagreement between theory and experiments in the case of AlN/GaN heterostructures, even taking the strain into account. In contrast, we were able to provide reliable values of MIP for InGaN/GaN, showing excellent agreement between experimental and theoretical estimations, and confirming the effect of strain predicted by the calculations.

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Graphic:

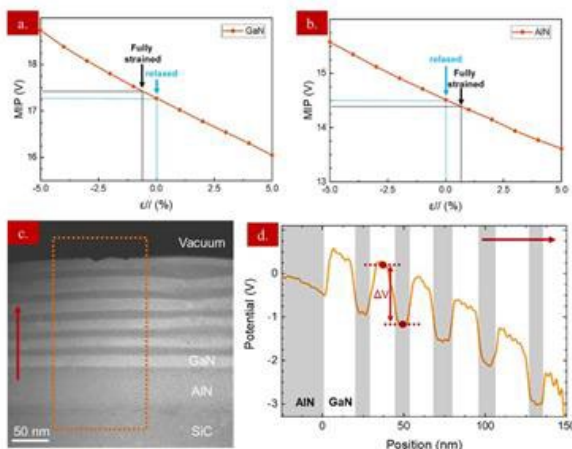


Fig.1: The red arrow represents the [0001] growth direction. [a] MIP computation of GaN and [b] AlN as a function of the biaxial strain. [c] Phase image of the non-polar AlN/GaN multilayer sample and [d] resulting potential profile. The difference of MIP between AlN and GaN is estimated as represented in [d], taking the difference of potential between the middle of AlN and GaN layers.

Keywords:

Holography, III-nitride, Mean inner potential

Reference:

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