Interplay of anomalous strain relaxation and minimization of polarization changes at nitride semiconductor heterointerfaces

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We present a methodology to quantify polarization and electron affinity changes at interfaces by combining scanning tunneling spectroscopy, off-axis electron holography in transmission electron microscopy (TEM), and self-consistent calculations of the electrostatic potential and electron phase change. We use a precisely known grown-in doping structure to calibrate the surface potential of the TEM lamella and thereby achieve a quantitative analysis of electron phase changes measured by off-axis electron holography. Using this calibration, we deduce quantitatively polarization and electron affinity changes for $Al_{0.06}Ga_{0.94}N/GaN$ and $In_{0.05}Ga_{0.95}N/Al_{0.06}Ga_{0.94}N$ interfaces. The latter interface reveals, as expected, biaxial relaxation as well as polarization and electron affinity changes. However, at the $Al_{0.06}Ga_{0.94}N/GaN$ interface anomalous lattice relaxations and vanishing polarization and electron affinity changes occur, whose underlying physical origin is anticipated to be total energy minimization by the minimization of Coulomb interactions between the polarization-induced interface charges.

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I. INTRODUCTION

Group III nitride semiconductors became the material system of choice for solid-state lighting and high-power semiconductor devices. Functioning of such devices is highly dependent on the presence and characteristics of doping and/or heterointerfaces. However, such interfaces may introduce new localized features: Besides lattice mismatch-induced strain, interdiffusion, and segregation, interfaces typically lead to a variety of localized electronic properties, such as atomically localized electronic states, band offsets, and polarization changes. These localized electronic features and, particularly, polarization changes, giving rise to two-dimensional sheets of bound charges [1,2], are partly desired (e.g., in high electron mobility transistors), but partly, they have the potential to affect, e.g., quantum wells and hence device performance adversely [3].

Thus far, polarization fields in group III nitride semiconductors grown along the *c* direction have been considered to be the most critical problem for spatial carrier separation in quantum wells. In order to avoid such polarization fields, growth on nonpolar or semipolar planes flourished [4]. However, polarization fields in the *c* direction and their detrimental effects on quantum wells can be avoided, too, by so-called polarization matching, i.e., by adjusting ternary or quaternary compositions to tune the polarization of the barrier materials relative to that of the quantum well [3,5]. This strategy, allowing the removal of polarization changes at interfaces, implicitly assumes that composition in conjunction with linear elastic biaxial strain at the interfaces fully determine the polarization. However, this approach ignores a possible interplay between the polarization, charge sheets, and the lattice relaxation at interfaces, potentially creating unexpected interface polarization and relaxation structures.

Here we quantitatively probe polarization and electron affinity changes at group III nitride heterointerfaces by combining off-axis electron holography, scanning tunneling spectroscopy, and self-consistent simulations. Although some interfaces exhibit the expected polarization change and biaxial lattice strain, we unravel, against expectations, for another interface anomalous lattice relaxations combined with a disappearance of polarization change. We argue that the driving force for the anomalous relaxation is the minimization of the total energy by reduction of the Coulomb interaction energy between bound charges arising from polarization changes at the heterointerfaces. Such effects have the potential to critically change the efficiencies of devices based on interfaces with anomalous relaxation and polarization changes.

II. METHODS

For this work we needed to probe quantitatively the polarization change and lattice relaxation at interfaces. It is,

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