Strain distribution in ultra-thin In(Ga)N/GaN quantum wells

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Abstract: In the field of III-Nitride compound semiconductors, a lot of emphasis is being placed on the effort for growth of ultra-thin pure InN or high In-content InGaN quantum wells (QWs). It has been shown that, through tailoring of the internal polarization, it is possible that such layers exhibit topological insulator properties, making them suitable for applications in spintronics and quantum computing [1]. Two-dimensional electron gas properties and a temperature-independent behavior in the diagonal resistance, indicating the topological nature of the 2DES, were demonstrated in monolayer-thick, nominally InN QWs [2]. At the same time, the internal quantum efficiency of optoelectronic devices can be benefited by the band gap engineering that is feasible by short period In(Ga)N/GaN superlattices (SPSs). However, the stress-strain state of such heterostructures has not been clarified so far, as it may deviate from the conventional biaxial one, i.e. the plane stress state also referred to as 'tetragonal distortion'. In the present contribution we have considered the interfacial accommodation at SPS samples comprising nominally 1, 2, and 4 monolayer (ML) thick QWs that were grown by molecular beam epitaxy (MBE) on (0001) GaN templates. We have employed high resolution transmission electron microscopy (HRTEM), and high resolution Z-contrast scanning TEM (HRSTEM) in order to correlate the chemical composition with the strain, focusing on the influence of pseudomorphic accommodation on the out-of-plane strain component. Phenomena of interfacial sharpness and indium clustering have also been considered. Experimental observations were analyzed using geometrical phase analysis, peak finding, and Z-contrast quantification. Experimental results were compared to theoretical simulations, in particular, energetic calculations using *ab initio* density functional theory and molecular dynamics with a modified Tersoff interatomic potential. In both cases, deviation from the biaxial stress state of InN was identified for these QWs in agreement with the experimental observations.

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