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Combining Atomic-Scale EDX with Inelastic Multislice Simulations for Quantitative Chemical Analysis of AlGaN/GaN 1 nm-thick Quantum Wells

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Due to their emission properties, III-nitride materials based on GaN/AlGaN alloys have aroused great interest for the development of UV lasers [1]. The control of the quantum wells (QWs) morphology used in these structures, e.g. interface roughness and chemical sharpness, is critical to ensure the good performances of such devices. The objective of this study is to detect and quantify Al content possibly incorporated into the GaN QWs (Figure 1a). Atomic-scale energy-dispersive X-ray (EDX) spectroscopy in the transmission electron microscope (TEM) is a technique of choice for such analysis, in particular with the recent development of detection systems combined with the improved control of the geometrical aberrations of the beam [2].

For a reliable interpretation of atomic-scale mappings, it is essential to understand the interaction mechanisms between the beam and the sample. When travelling through a crystalline material, an electron beam focused on one particular atomic column has a significant probability to interact with the surrounding ones. This phenomenon, named "cross-talk" in the literature, originates from the broadening of the beam, the geometric aberrations, and the channeling effects during scattering. In a non-homogeneous material as QWs, these physical effects can have severe consequences on the relative chemical intensities measured at the interfaces, and may introduce serious biases in the interpretation of the results. Although these problematics have been widely documented and studied by electron beam scattering simulations [3,4], there is still to our knowledge a lack of experimental works proving the relevance of incorporating inelastic simulations to address materials issues. This also leads to a lack of information about how to incorporate such simulations into atomic-scale spectroscopy mappings. In the present work, we show how to correlate EDX mappings with inelastic simulations to determine the Al content in a 1-nm thick GaN QW prepared using a standard focused ion beam (FIB) milling.

High-resolution EDX acquisitions were performed on a TFS Titan Themis probe-corrected microscope operating at 200 kV, with a convergence semi-angle of 20 mrad and a probe current of 50 pA, preventing the degradation of the material. The area covered by the EDX mapping is shown in Figure 1b. In order to optimize the signal/noise ratio while reducing the significant effect of spatial drift, the area is scanned several hundred times using the Velox software. The data cubes obtained are then realigned and summed with a homemade python script. In addition, the contributions of the different crystal lattices in the growth plane (i.e. perpendicular to the c-axis) are projected (Figure 1c). A homemade Fourier filter is performed to more easily identify the location of the Al, Ga and N signals. The experimental Al profile through the QW is presented in Figure 2. The results show that a significant Al signal is detected inside the QW, and that the transition between the two materials is not sharp.

To determine how much this detected signal originates from the electron beam cross-talk when probing the QW or the interface, simulations are carried out using the μSTEM library [5]. The algorithm, based

on a multislice approach, incorporates both the interaction with the phonons as well as the inelastic transitions. As a first step, the input structure is made of a pure (i.e. without Al incorporated) GaN QW, and the electron probe is supposed to be coherent and free of geometrical aberrations. Interestingly, simulations does not provide a sharp AlGaN:GaN interface and exhibit a noticeable Al signal within the QW. This signal, though lower than the one experimentally observed, has to be clearly accounted for an accurate Al content quantification.

In this presentation, we will discuss in more details the impact of the beam configuration (considering aberrations and coherency) on the origin of the signal, and we will propose an approach based on the coupling of atomic-scale EDX and inelastic simulations to accurately describe the atomic distribution of chemical elements through the QWs [6].

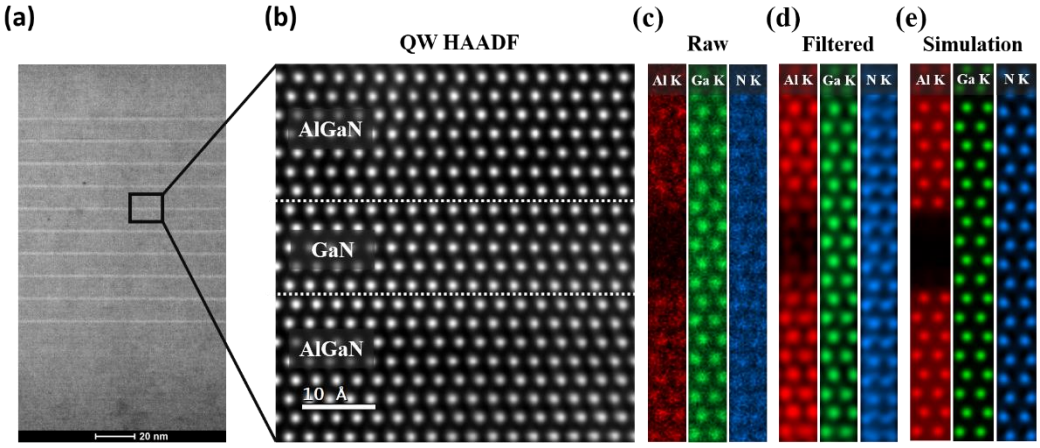

Figure 1. (a) HAADF image of the AlGaN/GaN multiple QWs heterostructure. (b) High resolution HAADF image of a GaN QW surrounded by AlGaN barriers. One can note the poor Z contrast, due to the low concentration of Al in the barriers. (c-d) Experimental atomic-scale EDX maps of the same area before and after filtering, respectively. (e) Inelastic multislice simulation of the heterostructure, convolved with a Gaussian filter (FWHM = 0.8 Å) to include spatial incoherence of the electron beam.

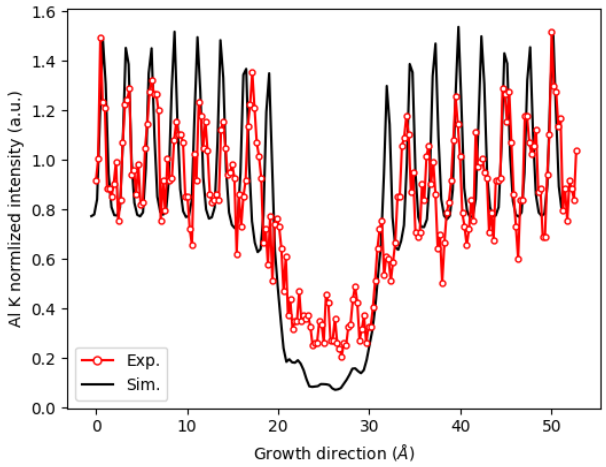

Figure 2. Comparison between experimental (red) and simulated (black) evolution of Al K signal through a GaN QW. Intensities are normalized in the AlGaN barriers to compare the two profiles.

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