Atomic-Scale Composition Profiles of MOCVD-grown InGaN/GaN quantum wells: Modeling and Characterization

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Recently, a number of approaches has been proposed aimed at improving performance of blue and green LED structures and based on fine tuning of the composition profiles in InGaN quantum wells (QWs) [1-4]. These and other similar approaches do not take, however, into account some limitation on the composition profiles originated from the growth of the structures by MOCVD. It has been shown, in particular, that InGaN composition profile in a QW does not strictly follow the time-variation of the gas phase composition in the MOCVD reactor but becomes broadened asymmetrically along the growth direction [5]. Among various theoretical considerations of this effect, the one involving indium surface segregation during the growth [6] seems to be most relevant. This paper reports on a coupled theoretical and experimental study of the impact of MOCVD conditions on the resulting composition profiles in the grown QWs.

The surface-segregation/kinetic MOCVD model developed in [6] was used to predict theoretically the InGaN composition profiles in the InGaN/GaN QWs. The model exploits the idea that the profile is determined by adsorption/desorption balance under the near-equilibrium conditions between the crystal and adsorbed layer. The original formulation of the model and its parameters were validated by comparison of theoretical predictions with the data of [7,8]. Since that time, much progress has been made in the development of high-resolution characterization techniques capable of providing new data on the QW composition profile in the sub-nanometer scale. This has stimulated us for further refinement and detailed validation of the kinetic MOCVD model.

To understand better what particular physical effects have the major impact on the QW composition profile, we have developed by simulation growth recipes for a number of InGaN/GaN QW structures that were then implemented in a Veeco K300 MOCVD reactor. The recipes differed from each other by variation of the process parameters, i.e. by growth temperature maintained after deposition of QW, duration of the QW growth, and flow rates of TMIn, TEGa, and ammonia precursors. The grown structures were characterized using dark-field electron holography (DFEH) which is as a powerful tool for mapping strain at the nanoscale by measuring the geometric phase of diffracted beams [9]. DFEH experiments were carried out with the Hitachi I2TEM-Toulouse (in situ interferometry TEM), an HF3300 equipped with a cold field-emission gun, imaging aberration corrector (CEOS Aplanator) and multiple biprisms. The multiple biprisms allow more flexibility in choosing holographic fringe spacing and field of view, and Fresnel fringes can be eliminated [10]. Strain maps were obtained with a resolution of 0.3 nm that corresponds to a 0.15 nm distance between hologram fringes. The chemical composition was calculated from Vegards and Hooks laws using the measured strain corrected for a thin foil relaxation effect.

The experimentally obtained InGaN composition profiles exhibit relatively sharp fore fronts of the grown QWs, a rather uniform indium distribution in the QW core, and a broadened rear fronts, the so-called indium “tails”, which evidence penetration of indium atoms from the QWs into the following barriers. The application of the kinetic MOCVD model to the suggested growth recipes demonstrates good agreement between the predicted and measured composition profiles (see Fig.1). The data reveal a rather weak expansion of the indium "tails" in the QW barriers at lower temperatures maintained after the InGaN QW growth. The refined model reproduced quantitatively the observed trends in the composition profile behavior under variations of the QW growth duration and TEGa flow rate. The observed trends will be discussed in the paper in detail.

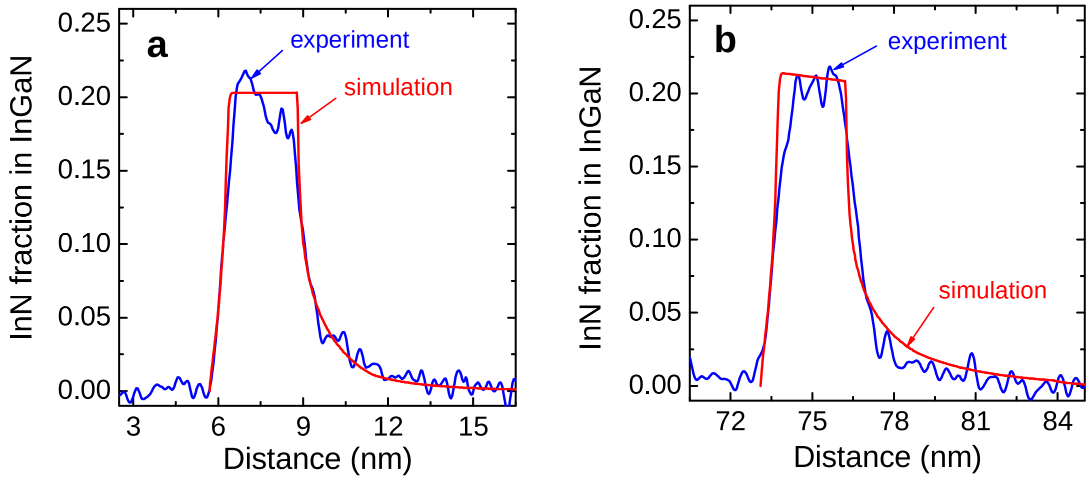

Fig. 1. Experimental and simulated composition profiles of an InGaN/GaN QW at different temperatures maintained after the QW growth: *a* – 810°C, *b* – 750°C (the QW growth temperature is 730°C for *a* and 722-727°C for *b*, the QW growth duration is 90 sec, and the pressure is 200 mbar).

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