Understanding Gallium Nitride Nucleation Layer Evolution

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Motivation—The use of GaN nucleation layers (NLs) promotes 2D growth on sapphire and reduces dislocation density in the final GaN film. However, dislocations in GaN grown on sapphire have been observed to originate in the NL, making the study of how they evolve imperative for further dislocation reduction. While low temperature (T) GaN NLs are commonly used to improve GaN growth on sapphire, there is little understanding how the NLs evolve during the ramp to high T and how they influence the high T GaN growth.

Accomplishment—For this study, GaN NLs were grown at 550 ^{o}C to a thickness of 30 nm using metalorganic chemical vapor deposition (MOCVD). Once grown, the NLs were heated under hydrogen and ammonia up to 1050 ^{o}C and held at 1050 ^{o}C before high T GaN growth proceeds. In Fig. 1, atomic force microscope (AFM) images of the GaN NL morphology during the annealing procedure are shown. As shown in Fig. 1, the GaN NL changes from a smooth (1 nm roughness) film to a rough film with nuclei approaching 1 µm in width and 200 nm in height. The nuclei that form on the NL are the initial GaN grains that continue to grow when the Ga source is turned back on. With further annealing of the NL at constant T, the GaN nuclei become smaller in size.

To quantify the GaN NL evolution the AFM images from Fig. 1 and the optical reflectance waveform shown in Fig. 2 were analyzed. Detailed analysis of the reflectance waveform showed that the reflectance signal could be used to extract the GaN NL thickness during the ramp to high T. Since the NL was losing thickness during this ramp and not substantially roughening until T > 1000 ^{o}C, the NL decomposition rates were obtained using the reflectance signal. From this work it was determined that the GaN NL decomposed with an activation energy of 2.7 eV, consistent with a rate limiting step of Ga desorption. Analytic fits were developed to fit the initial curvature in reflectance waveform, i.e. points (a-e) in Fig. 2. During decomposition, the desorbed Ga atoms were reincorporated into the growing GaN nuclei as shown in Fig. 1(e-i), reaching a maximum height in Fig. 1(i). Further annealing led to full decomposition of all of the original NL. At this point the GaN nuclei began to decompose and decreased in size as shown in Fig. 1(j-l).

Calculation of the height-height correlation function from the AFM images yielded information on the smoothing process during the NL annealing. It was found that the GaN nuclei shown in Fig. 1(e-j) had a smoothing exponent ($n = 2.3 \pm 0.3$) consistent with an evaporation and recondensation mechanism, while the films in Fig. (a-d, k, l) had a smoothing exponent ($n = 3.7 \pm 0.1$) consistent with a surface diffusion mechanism. The observation of an evaporation and recondensation smoothing mechanism for the growth of the GaN nuclei is entirely consistent with the NL decomposition kinetics mentioned above.

Significance—Heteroepitaxial growth of new materials will become increasingly important because single crystal substrates for these new materials rarely exist. Developing a more complete understanding of hetero-nucleation will aid in quick testing and evaluation of these new material systems. Using GaN as a test case, a clearer physical understanding of the GaN nuclei formation from the NL has been achieved.

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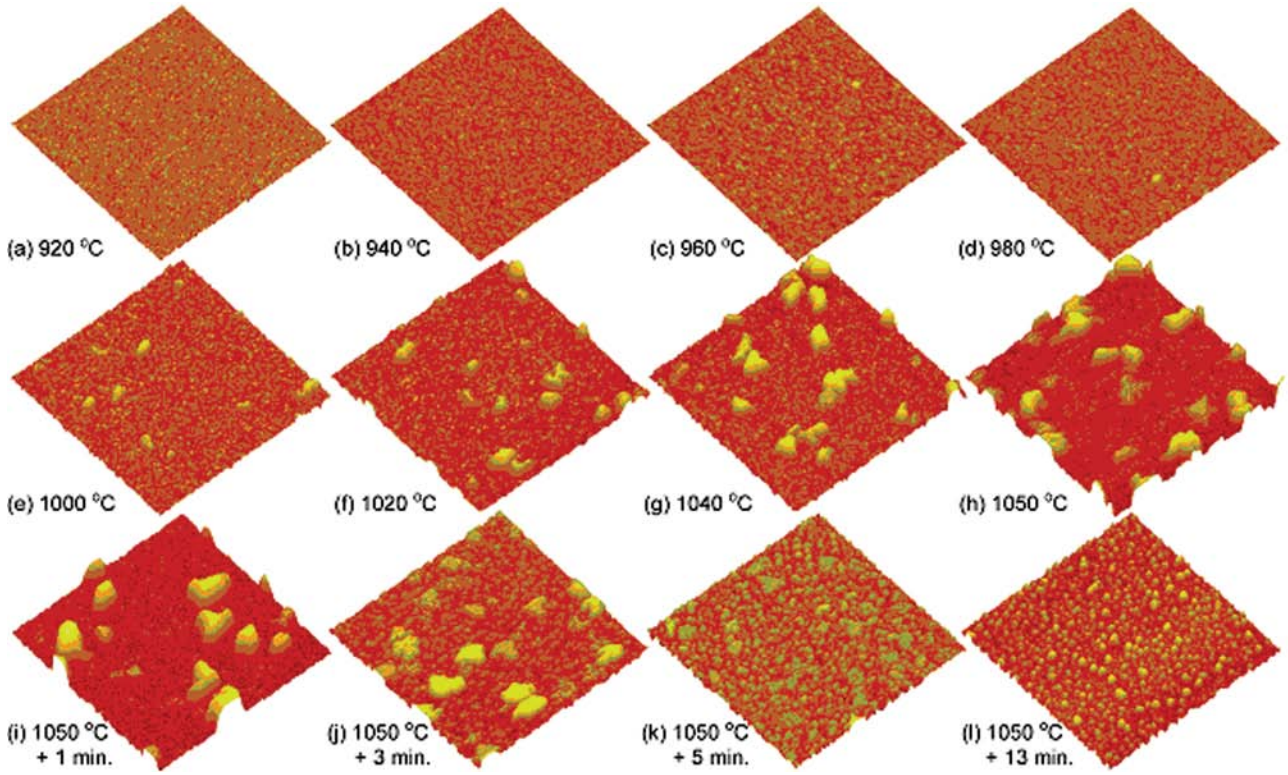

Figure 1. Atomic force microscopy (AFM) images of the GaN nucleation layer morphology for different annealing temperatures and times. The height scale is 200 nm and the scan size is 3 x 3 µm. GaN nuclei reach their maximum size at (i) after ramping to 1050 °C and holding for 1 minute.

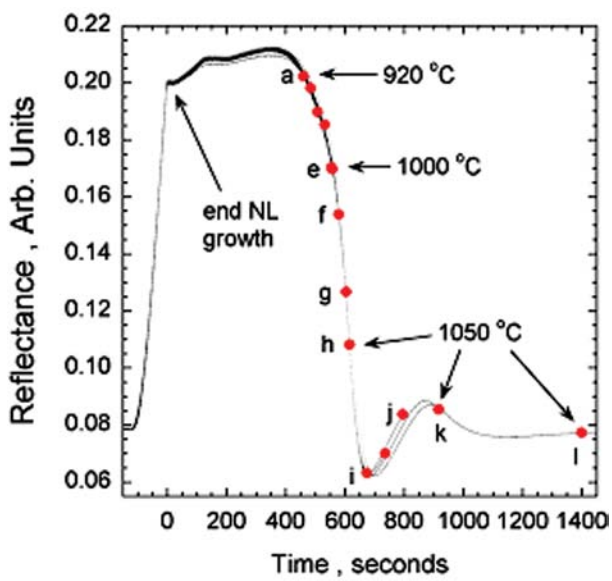

Figure 2. Optical reflectance waveform measured during the anneal to high temper-ature. The letters (a) - (l) denote the stopping point during the anneal and correspond to the AFM images shown in Fig. 1.

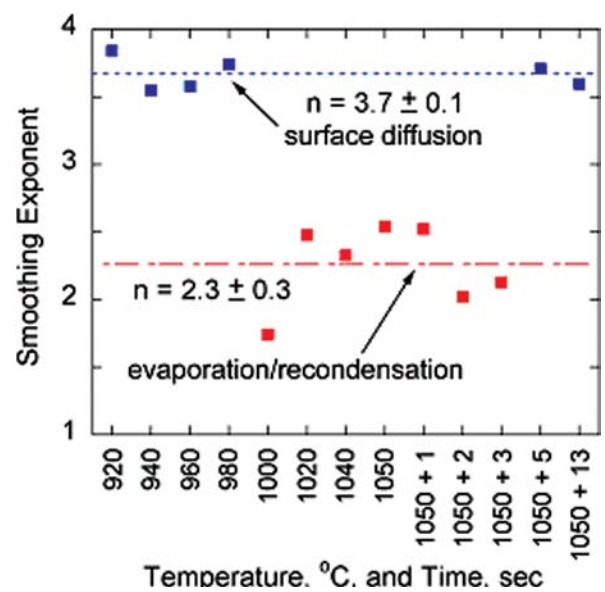

Figure 3. Measured exponents used to determine the smoothing mechanism from the AFM images in Fig. 1. An evaporation and recondensation mechanism accounts for the growth of the GaN nuclei shown in Fig. 1.