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Transition between the 1×1 and $(\sqrt{3} \times 2\sqrt{3})R30°$ surface structures of GaN in the vapor-phase environment

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Out-of-plane structures of the GaN(0001) surface in the metal-organic chemical vapor deposition (MOCVD) environment have been determined using *in situ* grazing-incidence x-ray scattering. We measured $11\bar{2}l$ crystal truncation rod intensities at a variety of temperatures and ammonia partial pressures on both sides of the 1×1 to $(\sqrt{3} \times 2\sqrt{3})R30°$ surface phase transition. The out-of-plane structure of the $(\sqrt{3} \times 2\sqrt{3})R30°$ phase appears to be nearly independent of temperature below the transition, while the structure of the 1×1 phase changes increasingly rapidly as the phase transition is approached from above. A model for the structure of the 1×1 phase with a partially-occupied top Ga layer agrees well with the data. The observed temperature dependence is consistent with a simple model of the equilibrium between the vapor phase and the surface coverage of Ga and N. In addition, we present results on the kinetics of reconstruction domain coarsening following a "quench" into the $(\sqrt{3} \times 2\sqrt{3})R30°$ phase field.

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A. Introduction

The use of GaN-based materials has allowed dramatic improvements to be made in optoelectronic devices such as blue lasers [1]. The production of these devices typically relies on epitaxial crystal growth using metal-organic chemical vapor deposition (MOCVD) [2]. Although the understanding of atomic-scale surface structure during MOCVD growth would greatly facilitate optimization of GaN-based devices, there are few probes of surface structure compatible with the near-atmospheric-pressure, high-temperature, reactive vapor-phase environment of this process. Our approach to this challenge has been to use x-ray scattering to conduct *in situ* measurements of GaN surface structure in the MOCVD environment [3].

In previous work [4], we presented grazing-incidence x-ray scattering results that characterize the in-plane surface structure of GaN(0001) in the MOCVD environment. We found that the surface equilibrium phase diagram as a function of temperature and ammonia partial pressure shows a transition between two phases with structures having 1×1 and $(\sqrt{3} \times 2\sqrt{3})R30°$ symmetries. We determined the in-plane structure of the $(\sqrt{3} \times 2\sqrt{3})R30°$ phase to be a novel "missing row" structure with 1/3 of the surface Ga atoms absent, as shown in Fig. 1. In this paper, we present further x-ray scattering results that characterize the out-of-plane surface structure of these surface phases. A model for the structure of the 1×1 phase with a partially-occupied top Ga layer agrees well with the data. The observed temperature dependence is consistent with a simple model of the interaction between the chemistry of the vapor phase and the surface structure. In addition, we present results on the kinetics of reconstruction domain coarsening following a "quench" into the $(\sqrt{3} \times 2\sqrt{3})R30°$ phase field. Related *in situ* x-ray scattering studies of growth on these surfaces have been published elsewhere [5].

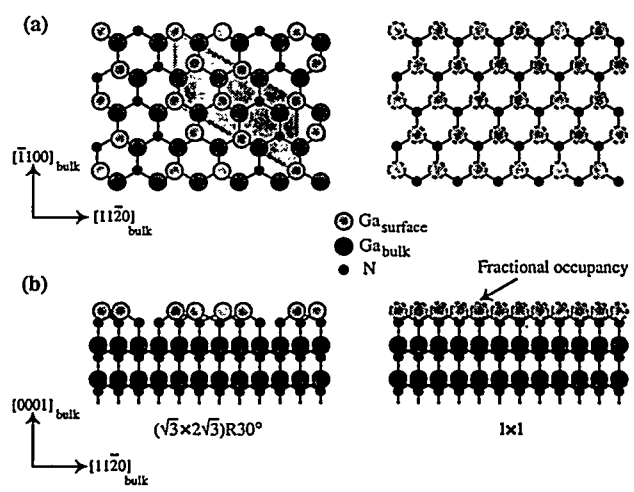

FIG. 1. (a) In-plane structure of the GaN(0001) $(\sqrt{3} \times 2\sqrt{3})$R30° and 1×1 phases, obtained previously [4]. In the 1×1 structure the top Ga-layer has fractional occupancy. (b) Schematic of the GaN(0001) structures normal to the surface.