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Unraveling the Atomic Structure of GaN(0001) Pseudo-1×1: Surface-Electron-Gas Mediated Dimer Ordering[1]

TIANJIAO CHEN, Ohio University Nanoscale and Quantum Phenomena Institute, NOBORU TAKEUCHI, Centro de Nanociencias y Nanotecnologia, Universidad Nacional Autonoma de Mexico, KANGKANG WANG, DANDA ARCHAYA, YINGHAO LIU, SAW-WAI HLA, ARTHUR SMITH, Ohio University Nanoscale and Quantum Phenomena Institute — Gallium nitride based light emitting devices have seen a steep rise of attention in recent years because of their potential in revolutionizing the current lighting industry. Of great importance in advancing the material technology is the understanding of the GaN(0001) surface, onto which most of the commercial devices are grown. We report a novel dimer-based model for Ga-rich GaN(0001), which exhibits an intriguing reconstruction known as the pseudo-1×1. To unravel its atomic structure, we have cooled the surface to cryogenic temperatures while monitoring the reconstruction by reflection high-energy electron diffraction and scanning tunneling microscopy. Upon cooling, the pseudo-1×1 phase transforms into a new phase consisting of buckled Ga-dimers on the surface. This observation then strongly suggests the existence of Ga dimers also at the room-temperature surface, although only partially ordered compared to the low temperature case. Combined with first-principles calculations, we propose a new model for the pseudo-1×1 consisting of dimers that are spaced ∼1.9 nm (6a) apart along <11$\bar{2}$0> azimuths, while being randomly distributed along other directions. The mechanism of this partial ordering is identified to be through the surface electron gas residing within the bulk band-gap.

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