PHYSICAL REVIEW B 70, 121201(R) (2004)

Identification of Ga-interstitial defects in GaN_yP_{1-y} and $Al_xGa_{1-x}N_yP_{1-y}$

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(Received 29 June 2004; revised manuscript received 4 August 2004; published 13 September 2004)

Two Ga-interstitial (Ga_i) defects are identified by optically detected magnetic resonance as common grown-in defects in molecular beam epitaxial GaN_yP_{1-y} and $Al_xGa_{1-x}N_yP_{1-y}$. Characteristic hyperfine structure arising from spin interaction between an unpaired electron and a Ga nucleus is clearly resolved. The observed strong and nearly isotropic hyperfine interaction reveals an electron wave function of A_1 symmetry that is highly localized at the Ga_i and thus a deep-level defect. Our analysis based on first-principles calculations suggests that these defects are complexes containing one Ga_i^{2+}.

DOI: 10.1103/PhysRevB.70.121201 PACS number(s): 61.72.Ji, 61.72.Bb, 71.55.Eq, 76.70.Hb

Self-interstitials, together with vacancies and antisites, belong to an important class of defects, i.e., intrinsic defects, in compound semiconductors. They are commonly found in semiconductors grown under nonequilibrium conditions or subjected to high-energy particle bombardment, and could play a crucial role in the electronic and optical properties of semiconductors. Among a few successful experimental techniques, magnetic resonance techniques have been shown to be a powerful probe for investigating the chemical identity and microscopic structure of defects.[1–5]

Since the middle 1980s, optically detected magnetic resonance (ODMR) studies revealed that Ga self-interstitials (Ga_i) are common residual defects in bulk GaP (Refs. 6–8) and in epitaxially grown $Al_xGa_{1-x}As$ (Refs. 9 and 10), AlAs/GaAs superlattices,[11] and $GaAs/Al_xGa_{1-x}As$ heterostructures.[12] Recently, Ga_i has been shown to be among the dominant defects in epitaxial GaN films when they are exposed to high-energy electron irradiation after growth.[13,14] In one case, a complex involving a Ga_i was observed in as-grown Zn-doped GaN.[15] Though many models were proposed, the microscopic structures of Ga_i are still largely unknown.

In this work, we were able to identify two types of Ga_i defects (denoted below as Ga_i-*A* and Ga_i-*B*) by ODMR in the GaN_yP_{1-y} and $Al_xGa_{1-x}N_yP_{1-y}$ alloys. Both defects are shown to possess an electron wave function of A_1 symmetry that is rather highly localized at the Ga_i site. By taking advantage of the degree of freedom provided by this alloy system, the defects were investigated under varied compositions of both group-III and group-V atoms in the two sublattices.

The GaN_yP_{1-y} and $Al_xGa_{1-x}N_yP_{1-y}$ epilayers (with a thickness of 0.75–0.9 μm) studied in this work were grown on GaP substrates, by gas-source molecular beam epitaxy (MBE). Two sets of samples were used to investigate the effect of Al and N compositions on the defects. One set is $Al_xGa_{1-x}N_yP_{1-y}$ with a fixed N composition of $y=0.012$ but different Al compositions of $x=0$, 0.02, and 0.3. The other set is GaN_yP_{1-y} with varied N compositions ($y=0.012$, 0.023, 0.031). To examine if the defects under study are common in this class of alloy system, a 0.15-μm-thick $GaN_{0.018}P_{0.982}$ epilayer grown on a Si(100) substrate by solid-source MBE was also studied.

The ODMR measurements were performed at two microwave frequencies (~9.3 GHz and ~95 GHz). Photoluminescence (PL) was excited by the 532 nm line from a solid state laser and was detected by a cooled Ge detector and a GaAs photodiode for the near infrared and visible spectral range, respectively. ODMR signals were detected as spin-resonance-induced changes in PL intensity. The success of the ODMR technique in identifying the chemical nature of the Ga_i interstitials relies on its ability to measure the hyperfine (HF) interaction between an unpaired electron spin and the nuclear spin of the Ga_i, described by the spin Hamiltonian

$$H=\mu_B \mathbf{B}\cdot\mathbf{g}\cdot\mathbf{S}+\mathbf{S}\cdot\mathbf{A}\cdot\mathbf{I}. \quad (1)$$

Here the first and second terms describe electron Zeeman and HF interaction terms, respectively; μ_B is the Bohr magneton, **B** is the magnetic field; **g** is the Zeeman splitting tensor, and **A** is the HF interaction tensor for each of the two naturally abundant Ga isotopes (^{69}Ga and ^{71}Ga). The effective electron spin is $S=1/2$ and both Ga isotopes have the same nuclear spin of $I=3/2$. Both **g** and **A** tensors are de-

