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High-Mobility Two-Dimensional Electron Gases at AlGaN/GaN Heterostructures Grown on GaN Bulk Wafers and GaN Template Substrates

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ABSTRACT

We report a comparative study of the mobility of two-dimensional electron gases (2DEG) formed at AlGaN/GaN heterostructures by simultaneously growing on substrates with very different dislocation densities. The mobility is seen to depend on the 2DEG charge density directly, but surprisingly, dislocations do not cause a discernible impact on the mobility of the samples within the measured region < 25,000 cm^2/Vs. This experimental observation questions the generally accepted belief that dislocations are the dominant low-temperature scattering mechanism for low-density 2DEG at AlGaN/GaN structures.

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The two-dimensional electron gas (2DEG) at AlGaN/GaN interfaces has been actively studied due to its use in GaN-based high electron mobility transistors (HEMTs). There is no need for intentional modulation doping to induce such 2DEGs, which are enabled by the difference of spontaneous and piezoelectric polarization across heterojunctions in nitrides.[1] This is an advantage for AlGaN/GaN 2DEGs because it potentially eliminates scattering from intentional dopants. Owing to its unique origin, the density of the 2DEG in such AlGaN/GaN structures can be manipulated by either the thickness or Al concentration of the AlGaN barrier layers.

In the early 2000s, there were efforts to improve the mobility of 2DEGs in the AlGaN/GaN system. Two research groups independently reported ~4 K mobilities exceeding 100,000 cm^2/Vs for a 2DEG density of 1×10^{12} cm^{-2}.[2,3] Interest in obtaining very high mobility 2DEGs in nitride semiconductors has been rekindled as a potential path to topologically interesting heterostructures by the epitaxial combination of AlGaN and the nitride superconductor NbN.[4] It is generally believed that a key factor to higher mobility is the ever-improving quality of GaN substrates, and that in the density range $<10^{12}$ cm^{-2} the electron mobility is limited by scattering from threading dislocations of densities $>10^8$ cm^{-2}.[5,6,7] The recent availability of high quality single-crystal GaN substrates with very low dislocation densities have enabled the observation of quantum interference effects in III-nitride heterostructures resonant tunneling transport[8,9] and the demonstration of pn diodes with nearly-ideal characteristics[10,11,12].

Electron scattering by dislocations are believed to be Coulombic or long-range in nature, originating from charged cores and deformation potential scattering from strain fields surrounding them.[13,14] In order to improve the 2DEG mobility, researchers have used GaN bulk crystals as substrates with dislocation densities considerably below 10^8 cm^{-2}.[3] There have been a

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few studies on the impact of dislocations on the mobility of 2DEG at AlGaN/GaN system with different Al compositions.[15,16] Within the range of dislocation densities studied (> ~1×10^8 cm^{-2}), it was found that the dislocation scattering seems to detrimentally affect the mobility.[15,16] Thorough, comparative studies are still missing since the 2DEG formation depends not only on the Al composition, but also the AlGaN thickness. In addition, the role of dislocations on the 2DEG mobility for very low dislocation densities well below 10^8 cm^{-2} has not been reported yet. In this work, we have performed a systematic study aimed at investigating the effect of dislocation scattering on the low-temperature mobility of low-density AlGaN/GaN 2DEGs. We have grown two different series of AlGaN/GaN heterostructures simultaneously on single-crystal GaN bulk wafers with very low dislocation densities, and a GaN template with high dislocation density and compared the mobilities.

Two types of substrates with a sharp contrast in dislocation density were chosen to examine the role of dislocation scattering on mobility: (1) semi-insulating (Mn-doped) single-crystal GaN (0001) bulk wafers[17] from Ammono with a dislocation density of ~5×10^4 cm^{-2} and (2) semi-insulating (Fe-doped) GaN on sapphire template substrates from PAM-Xiamen with a dislocation density of ~1×10^8 cm^{-2}. For each epitaxial growth run, diced substrates of each type of size 7×7 mm^2 were co-loaded side-by-side using indium on a Si carrier holder to guarantee the same growth conditions. All the samples in this study were grown in a Veeco Gen10 MBE reactor equipped with standard effusion cells for elemental Ga and Al, and a radio-frequency plasma source for active N species. The base pressure of the growth chamber was in the range of 10^{-10} Torr under idle conditions, and 2×10^{-5} Torr during the growth runs primarily due to N_2 gas. As a measure of the purity of the growth chamber, secondary ion mass spectrometry (SIMS) measurement on a

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separate unintentionally doped GaN layer grown in this chamber condition showed an unintentional background oxygen level of ~1×10^{16} cm^{-3}.

Two series of samples were grown [Fig. 1 (a)]. For series 1, the structures were grown using the following sequence, starting from the substrate: [300 nm GaN] / [21 nm $Al_xGa_{1-x}N$] / [3 nm GaN cap]. Series 2 was grown as follows, (starting from the substrate): [300 nm GaN] / [*t* nm $Al_{0.03}Ga_{0.97}N$] / [3 nm GaN cap]. The 2DEG density formed at the AlGaN/GaN interface was varied by changing the Al composition x ($0.07 < x < 0.23$) in the 21 nm-thick $Al_xGa_{1-x}N$ (series 1) or by varying the thickness t (t = 42, 63 and 84 nm) of the $Al_{0.03}Ga_{0.97}N$ layer (series 2). For example, Fig. 1 (b) shows the calculated conduction band diagram and electron wavefunction squared at the ground state of the structures of series 1 with x=0.07 and 0.23. It is clearly seen that a 2DEG is formed at the AlGaN/GaN interface farther from the surface because of the metal-polarity of the crystal. The low density 2DEG is also more spatially extended. This implies one must be careful applying theoretical models that assume a perfect 2D electron confinement: the effect of dislocation scattering on more 3D-lke electron concentrations of low density is expected to lead to lower mobilities than for a high-density 2DEG strongly confined in 2D. All the GaN ($\Phi_{Ga} > \Phi_N$) and the (Al,Ga)N layers ($\Phi_{Al} + \Phi_{Ga} > \Phi_N$; $\Phi_{Al} < \Phi_N$) were grown under metal-rich conditions at 730 ^{0}C, where Φ_{Ga}, Φ_{Al} and Φ_N are Ga, Al and active N fluxes, respectively. The growth rate, which is limited by Φ_N, was 7 nm/min. The excess Ga droplets after the growth were first removed in HCl before characterization. Surface morphology of the samples were characterized by atomic force microscopy (AFM). Electrical transport measurements were performed on van der Pauw Hall-effect patterns using indium contacts.

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The samples grown on the bulk GaN wafers are expected to have much less dislocations compared to ones grown on the template substrates. This can be judged to an extent from the populations of spiral hillocks on the GaN surface: a high dislocation density grown by MBE typically reveals a high density of spiral hillocks. The expected difference in dislocation densities is indeed observed in the sample structures grown on the two different substrates. As a representative, AFM micrographs of two identical structures (300 nm GaN / 84 nm $Al_{0.03}Ga_{0.97}N$ / 3 nm GaN) are shown in Fig. 2. Both samples show clear atomic steps enabled by the metal-rich growth condition.[18] However, spiral hillocks are seen only on the sample grown on the template substrate, whereas the sample grown on the GaN bulk wafer does not show any spiral hillocks over an area of 20×20 μm^2, indicating a sharp contrast in dislocation density between the two samples. The same characteristics hold for all the other pairs of samples grown in this study.

Figures 3(a) and (b) show the measured room-temperature (RT) and 77 K electron mobilities versus the measured 2DEG charge densities of all the samples in series 1 and 2 together with the best prior reported data in the literature[3,19,20,21,22,23,24,25]. The measured mobilities lie roughly in the 500–2000 cm^2/Vs window at RT and 10,000–25,000 cm^2/Vs at 77 K over the range of 2DEG densities, with no discernable difference between bulk substrates and GaN templates. First, in the relatively strong confinement regime where for electron sheet densities > 5×10^{12} cm^{-2} at RT and > 2×10^{12} cm^{-2} at 77 K, the mobility decreases with increasing 2DEG density. This is explained by increased alloy scattering due to enhanced penetration of the electron wavefunction into the AlGaN barrier at high 2DEG densities, and enhanced interface roughness scattering due to the movement of the centroid of the 2DEG distribution closer to the interface with increasing density.[6,26,27,28,29] [e.g., see Fig.1(b)] In the low 2DEG density regime, optical phonon scattering and

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dislocation scattering is believed to be the dominant scattering mechanism at RT and low temperature, respectively. Therefore, a sharp contrast in mobilities between the samples grown on the two different substrates is expected especially at low temperature for low 2DEG density (<~2×10^{12} cm^{-2}), due to the reduced screening of dislocation scattering potentials. However, the measured 2DEG mobilities in this study apparently do not depend on the dislocation density. It increases with increasing charge density with a peak mobility at 1–2×10^{12} cm^{-2} at 77 K, no clear difference is observed between the bulk and template substrates. The measured 2DEG mobility vs charge density relation together with the corresponding data [Figs. 3(a) and (b)] from the literature is qualitatively similar to results reported by several other research groups.[7,26,27,30] The decrease of the mobility with decreasing 2DEG density for samples grown on bulk GaN substrates with very low dislocation density is therefore surprising.

It is unlikely that the electron mobility does not depend on the dislocation density, implying that the dislocations are not the limiting scattering channel for the 77 K-mobility in Fig. 3(b). To elucidate this, we compare the spacing between dislocations with the electron mean free path. At a dislocation density of 10^{8} cm^{-2}, which is the density for the template substrates in this study, the average distance between dislocations is ~1 μm. On the other hand, for a carrier density of 1×10^{12} cm^{-2} and a mobility of 20,000 cm^{2}/Vs, the electron mean free path l is approximately 0.3 μm. Here $l \sim v_F \tau$, where v_F is the Fermi velocity and τ is the transport relaxation time. The mean free path is therefore smaller than the dislocation spacing for the template substrates. However, charged dislocation scattering is Coulombic; its long-range nature indicates that the effective electronic scattering distance between such scatterers must be smaller than their physical spacing. Nonetheless, this comparison and the experimental results seem to indicate that dislocation

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scattering is not a major factor affecting the transport in the samples investigated in this study. This might imply that other scattering mechanisms such as acoustic phonons and background impurities - both charged or neutral, are playing a role in limiting the mobility of the samples in the low charge density regime at 77 K. A rough calculation shows that acoustic phonon scattering limits the mobility at 77 K to ~50,000 cm^2/Vs at a charge density of $\sim1\times10^{12}$ cm^{-2}. On the other hand, if one models each dislocation as a charged wire with a linear charge density of $2e/c$, where e is the fundamental charge and c is the c-lattice constant of GaN, then the average density of the charges from the dislocations with a density of 10^8 cm^{-2} becomes $\sim4\times10^{15}$ cm^{-3}. With the assumption of the same Coulombic potentials for impurities and charges from dislocations, this crude calculation leads to the conclusion that for an impurity density higher than $\sim4\times10^{15}$ cm^{-3} the impurity scattering is comparable to, or outweighs the dislocation scattering for a dislocation density of 10^8 cm^{-2}. It is interesting to note that in the very low 2DEG density region ($<2\times10^{12}$ cm^{-2}) the RT-mobility [Fig. 3(a)] shows that the samples grown on the bulk wafers have systematically lower mobilities than the ones on the template substrates, which might imply that the samples grown on the bulk wafers contain relatively more impurities.[31] To unveil the true impact of dislocations on the mobility, further chemical analysis such as SIMS, and extended temperature-dependent transport measurements, especially magnetotransport measurements extending to very low temperatures, where acoustic phonons are frozen out and the mobility is a direct measure of defect scattering is necessary, and is suggested for future work.

To summarize, it is found that surprisingly, a variation of dislocation densities over 4 orders of magnitude has no discernible effect on the low-temperature (77 K) mobility of low-density 2DEGs at AlGaN/GaN heterostructures. This indicates that scattering mechanisms other than dislocations

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may be responsible for limiting the low-temperature mobility in such heterostructures. Further growth and characterization studies are therefore necessary to deconvolute the role of the scattering mechanisms and to understand the true effects of dislocation density on the mobility, and to achieve higher low-temperature mobilities in low-density nitride 2DEGs in the future.

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[31] The thickness of the buffer layer did not measurably impact the mobility. We have grown a separate sample set with much thicker GaN buffer and cap layers in order to minimize impurity scattering: 100 nm GaN/21 nm $Al_xGa_{1-x}N$ (x=0.15)/1,000 nm GaN buffer. The sample grown on the bulk and template substrate

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show a 77 K-mobility of 17,300 cm^2/Vs and 16,700 cm^2/Vs, respectively, very close to the ones of the similar sample structures with much thinner GaN buffer and cap layers in Fig.3(b): 16,800 cm^2/Vs for the bulk sample and 15,600 cm^2/Vs for the template sample. Nevertheless, careful SIMS measurements are needed to understand the role of background impurity scattering on the low temperature mobility.

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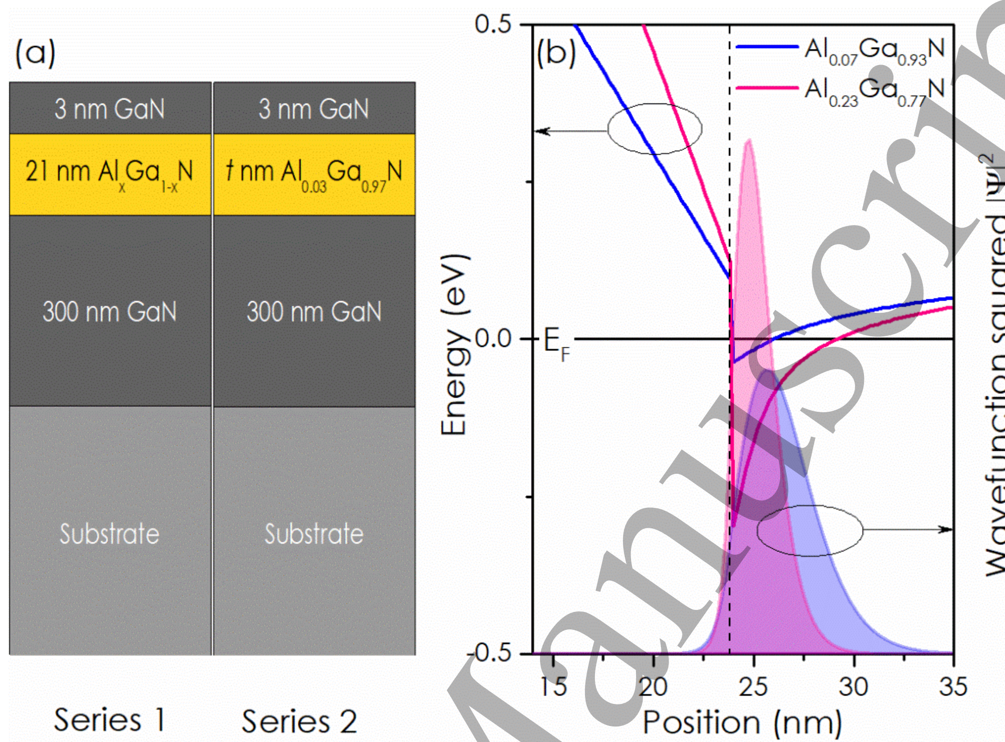

Fig. 1 (a) Schematic sample structures of series 1 and 2. (b) Calculated conduction band diagram and electron wavefunction squared at the ground state for two different Al compositions x= 0.07 and 0.23 in 3 nm GaN/21 nm $Al_xGa_{1-x}N$/300 nm GaN. The dashed line indicates the interface between the AlGaN and GaN where 2DEG is formed. Note that the centroid of the 2DEG is closer to the interface with higher Al composition.

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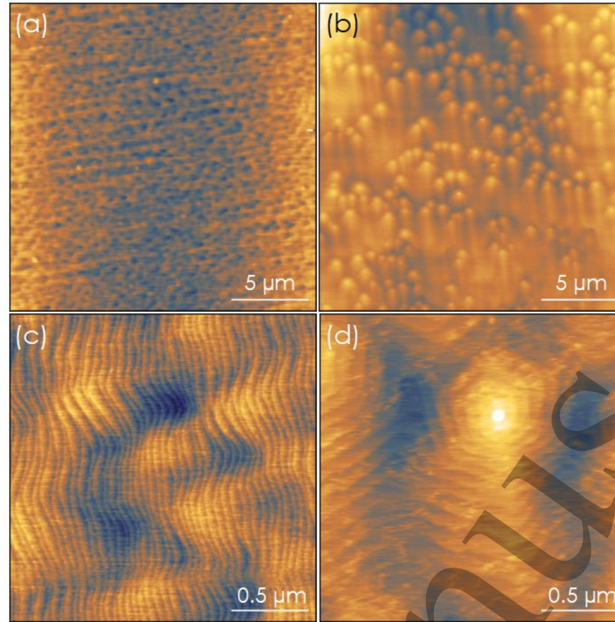

Fig. 2 [(a) and (b)] 20×20 μm^2 and [(c) and (d)] 2×2 μm^2 AFM micrographs of (Al,Ga)N/GaN structures grown on GaN bulk wafers [(a) and (c)] and GaN template substrates [(b) and (d)]. The root-mean-square roughness of the images are (a) 0.364, (b) 1.34, (c) 0.17 and (d) 0.53 nm. Note that spiral hillocks are observed only on the samples grown on GaN templates [(b) and (d)].

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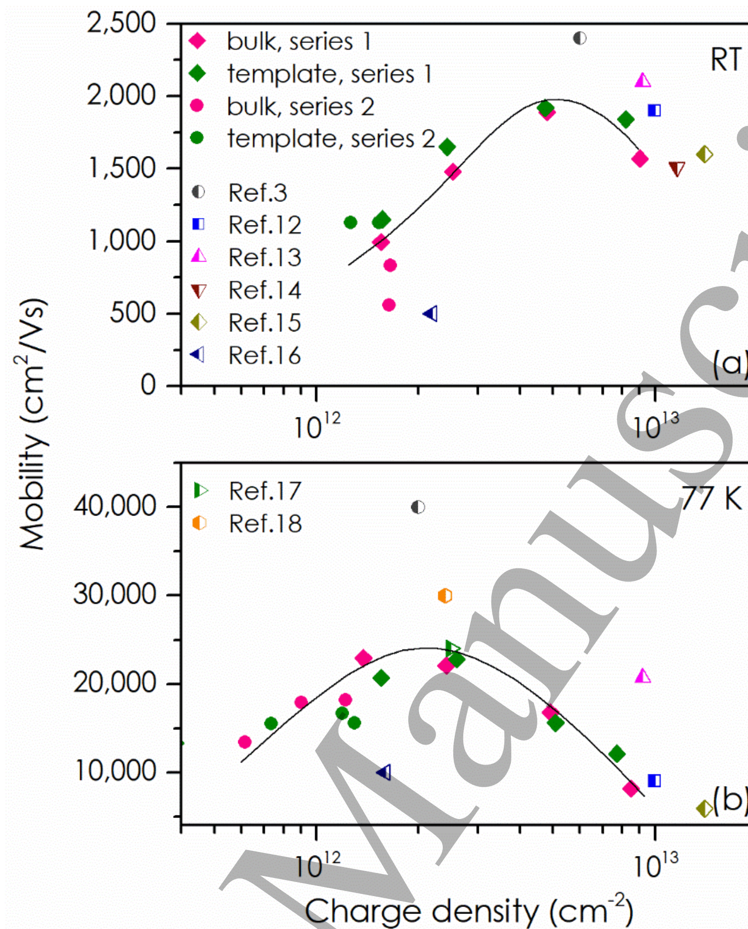

Fig. 3 2DEG Hall-effect Mobility versus charge density of series 1 and 2 at (a) room temperature (RT) and (b) 77 K. The lines are guides to the eye. The half-filled symbols are from the literature at the corresponding temperatures. References 13, 14 and 15 are AlGaN/AlN/GaN, AlInN/AlN/GaN, and AlN/GaN structures, respectively. The other references are AlGaN/GaN heterostructures. The surprising finding is the *absence* of a discernible difference in the low 2DEG density 77 K mobilities between heterostructures grown on substrates with 4 orders of magnitude difference in dislocation densities. There is a discrepancy in the number of data points between (a) and (b) as the presence of 2DEG at RT is not obvious for very low 2DEG density ($<1\times10^{12}$ cm^{-2}).

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