APPLIED PHYSICS LETTERS **89**, 091905 (2006)

Effect of the misorientation of the 4*H*-SiC substrate on the open volume defects in GaN grown by metal-organic chemical vapor deposition

E. Tengborn,[a] M. Rummukainen, F. Tuomisto, and K. Saarinen[b]
Laboratory of Physics, Helsinki University of Technology, P.O. Box, 1100 FIN-02015 TKK, Finland

M. Rudzinski, P. R. Hageman, and P. K. Larsen
Experimental Solid State Physics III, RIM, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands

A. Nordlund
Nuclear Engineering, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

(Received 28 May 2006; accepted 5 July 2006; published online 28 August 2006)

Positron annihilation spectroscopy has been used to study GaN grown by metal-organic chemical vapor deposition on misoriented 4*H*-SiC substrates. Two kinds of vacancy defects are observed: Ga vacancies and larger vacancy clusters in all the studied layers. In addition to vacancies, positrons annihilate at shallow traps that are likely to be dislocations. The results show that the vacancy concentration increases and the shallow positron trap concentration decreases with the increasing substrate misorientation. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2338887]

Gallium nitride (GaN) is used in optoelectronic components. The large direct band gap and strong interatomic bonds enable the material to be used in short-wavelength and high power devices, such as blue light emitting diodes and high power transistors.[1] The crystal quality of GaN epilayers is often poor due to the lack of a native substrate which shortens the device lifetime. The lattice mismatch induces strain relaxes through the formation of extended defects, reaching dislocation densities in the 10^{10} cm^{-2} range.[1,2] The understanding of the defect formation is essential in order to produce better quality materials.

The high thermal conductivity and the relatively small lattice mismatch make SiC a promising substrate for high power applications.[3] With molecular beam epitaxy grown GaN, threading screw dislocations can be reduced by two orders of magnitude and edge dislocations by one order of magnitude using misoriented substrates, on which the growth changes to two-dimensional step-flow mode.[4,5] However, cracks are observed to form in layers grown on misoriented substrates using metal-organic chemical vapor deposition (MOCVD).[6]

In this letter we report on defects observed in GaN epilayers grown by MOCVD on misoriented 4*H*-SiC substrates at 1170 °C, as described earlier.[6] We studied three samples where the substrate was tilted by 0°, 3.4°, and 8° from $\langle 0001\rangle$ towards $\langle 11\bar{2}0\rangle$. The samples with a tilted substrate had cracks with average separations 50 and 15 μm for the misorientation angles 3.4° and 8°, respectively. A *p*-type Mg-doped GaN sample, free of defects observable by positron annihilation, was used as a reference.[7] The positron annihilation experiments were performed with a monoenergetic beam by measuring the Doppler broadening of the 511 keV annihilation radiation at temperatures 30–500 K. The Doppler spectra were analyzed with the conventional *S* and *W* parameters.[8] When a thermalized positron is trapped in an open volume defect it preferably annihilates with a low momentum electron leading to higher *S* and lower *W* values.

Figure 1 shows the *S* parameter measured in the samples at room temperature as a function of the positron implantation energy. At energies below 10 keV the *S* parameter is high, as positrons annihilate at the sample surface. At 10–20 keV *S* is fairly constant corresponding to annihilations solely in the GaN layer. At higher energies some of the positrons already reach the SiC substrate seen as a slight increase in the *S* parameter. In all the samples the *S* parameter is higher and the *W* parameter lower (not shown) than in the bulk GaN lattice (S_B=0.459), indicating the presence of vacancies. The *S* parameter is highest in the 8° off-axis sample, second highest in the 3.4° off-axis sample, and lowest in the on-axis sample.

The temperature dependence of positron trapping into defects can be used to identify the defects and estimate their concentration. In undoped GaN, vacancies have been shown

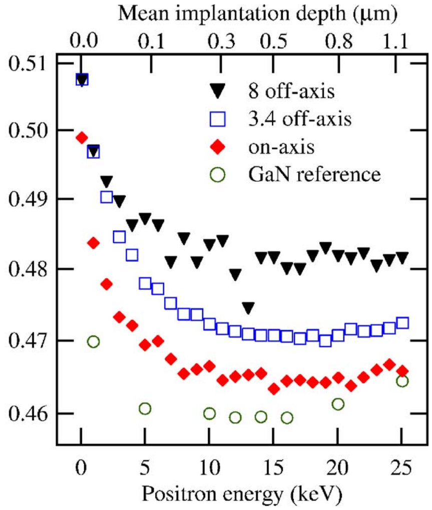

FIG. 1. (Color online) *S* parameter measured at room temperature as a function of the positron implantation energy. The mean implantation depth is indicated on the top axis.

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[a] Present address: Fundamental Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden; electronic mail: elisabeth.tengborn@chalmers.se

[b] Deceased.

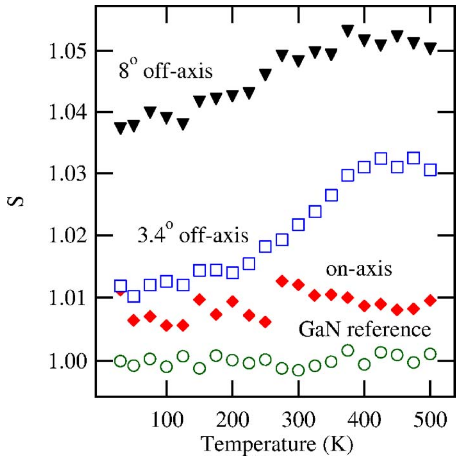

FIG. 2. (Color online) *S* parameter as a function of measurement temperature at 15 keV positron implantation energy.

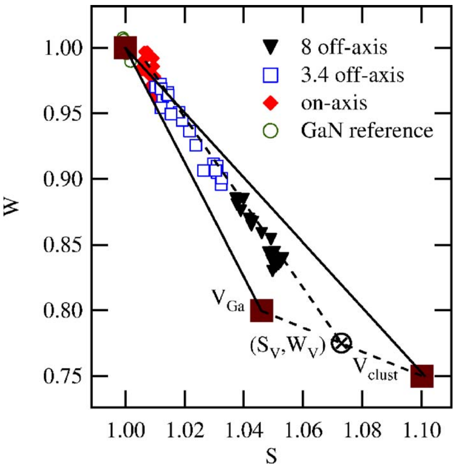

FIG. 3. (Color online) (*S*, *W*) parameters measured as a function of temperature in the GaN samples. The (*S*, *W*) values corresponding to the vacancy free GaN (S_B, W_B), the Ga vacancy ($S_{V,\mathrm{Ga}}$, $W_{V,\mathrm{Ga}}$), and a vacancy cluster (S_{clust}, W_{clust}) are shown. The dotted lines show the fitting procedure used to determine the relative concentrations of the Ga vacancies the vacancy clusters, the parameter S_V used to estimate the absolute defect concentrations.

to be in their negative charge state.[9] The positron trapping coefficient to negatively charged vacancies μ_{V^-} varies as $T^{-0.5}$.[8] Therefore, if only negatively charged vacancies are present, the *S* parameter will increase as the temperature decreases. At low temperatures, positrons can also be trapped by shallow positron traps, such as negatively charged ions or dislocations.[10,11] Above room temperature positrons are trapped by vacancies but the signal from the shallow traps vanishes as positrons are able to thermally escape from them. Hence the vacancy concentration can be determined from the measurement at high temperatures.

Figure 2 shows the *S* parameter as a function of the measurement temperature. The positron energy was kept at 15 keV, i.e., a mean implantation depth of 0.5 μm. At this depth all positrons annihilate in the epilayer. The misoriented samples have a constant *S* parameter at temperatures below 100 K. The *S* value increases with temperature in the range 150–400K, and above 400 K it becomes constant again. This behavior is typical when shallow traps and vacancies coexist in the sample, competing as positron traps.[8] The *S* parameter in the on-axis sample is constant at low temperatures up to 250 K, which suggests that we observe saturated trapping into shallow traps at these temperatures. This indicates that the *S* value measured at low temperatures in the on-axis sample is specific to the shallow trap. We thus obtain $S_{\mathrm{ST}}=0.462$, slightly higher than that of the bulk GaN.

Figure 3 shows the *W* parameters of the temperature dependent measurements as a function of *S*. Correlated changes in the (S,W) plane can be used to identify defects. The characteristic parameters for a Ga vacancy V_{Ga} and a vacancy cluster V_{clust} have been included in the figure.[9,12,13] All the measured parameters fall on a line between those joining the defect-free GaN to the V_{Ga} and the defect-free GaN to the V_{clust}. The annihilation parameters are superpositions of the parameters corresponding to positrons annihilating from different states. We can estimate the relative concentrations of the defects from the slope of the line in the (S,W) plane: about 50% of the observed defects are V_{Ga} and 50% are larger V_{clust}.

The positron trapping rate into vacancies κ_V can be estimated from the measurement points above 400 K as $\kappa_V = \tau_B^{-1}(S-S_B)/(S_V-S)$, where $\tau_B=160$ ps is the positron bulk lifetime,[14] *S* the measured parameter, S_B the parameter of the bulk, and S_V the parameter corresponding to 100% annihilations in vacancies. S_V can be extrapolated from the point where the line fitted to the measurement data intersects the line between the points of V_{Ga} and V_{clust} giving $S_V=0.493$. The vacancy concentration c_V is $c_V=\kappa_V N_{\mathrm{at}}/\mu_V$, where μ_V is the positron trapping coefficient and $N_{\mathrm{at}}=8.8\times10^{22}\ \mathrm{cm}^{-3}$ the atomic density. For μ_V we use the typical value for vacancies in semiconductors at high temperatures, i.e., $2\times10^{15}\ \mathrm{s}^{-1}$.[8] Table I presents the estimated total vacancy concentrations. The concentrations vary from $4\times10^{16}\ \mathrm{cm}^{-3}$ in the on-axis sample to $7\times10^{17}\ \mathrm{cm}^{-3}$ in the 8° off-axis sample. This increase with increasing angle of misorientation correlates with the increase of the free electron concentration,[6] as expected for negative vacancies.

The trapping rate to shallow traps κ_{ST} can be estimated from the low temperature data where no detrapping from shallow traps occurs.[8] We estimate the value of κ_V at 50 K from the high-temperature trapping rate, using the $T^{-0.5}$ dependence of the trapping coefficient for negative vacancies. The obtained values of κ_{ST} at 50 K are presented in Table I. Since all the positrons annihilate as they are trapped in the shallow traps in the on-axis sample, only an estimate of the lower limit for the trapping rate is presented. The data clearly show that the trapping rate to the shallow traps decreases with the increasing misorientation angle.

The observed shallow positron traps are likely to be dislocations. They contain a small open volume whereas the *S* parameter corresponding to negative ions is the same as in the GaN lattice.[11] Notice that these shallow traps are not associated with the cracks described by Rudzinski *et al.*,[6] since these are separated by 15 μm while the positron diffu-

TABLE I. Total vacancy concentrations ($[V_{\mathrm{Ga}}+V_{\mathrm{clust}}]$) and the trapping rates into the shallow traps (κ_{ST}) at 50 K in the GaN samples.

Substrate orientation	$[V_{\mathrm{Ga}}+V_{\mathrm{clust}}]$ (cm^{-3})	κ_{ST} (s^{-1})
0° on axis	4×10^{16}	$\geqslant 2\times10^{11}$
3.4° off axis	2×10^{17}	1×10^{11}
8° off axis	7×10^{17}	5×10^{10}

sion length is less than 100 nm. As the trapping rates are proportional to the defect densities, we can conclude that the dislocation density is higher in layers with the less misoriented substrate. This result is in good agreement with the results obtained by defect-selective etching experiments.[6]

In conclusion, a significant concentration of vacancy-type defects, identified as 50% Ga vacancies and 50% vacancy clusters, was detected in all the samples. The composition of the vacancies is similar in all the samples, and the concentration of vacancy-type defects increases from 4×10^{16} to 7×10^{17} cm^{-3} with the misorientation angle. Shallow positron traps, likely dislocations, were observed and their concentration is shown to decrease with increasing angle of misorientation.

M. Rudzinski is grateful for the financial support from Philips Semiconductors B.V. Nijmegen.

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