Temperature dependence of the electron Landé *g*-factor in cubic GaN

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(Received 16 October 2015; accepted 20 November 2015; published online 8 December 2015)

The temperature dependence of the electron Landé *g*-factor in bulk cubic GaN is investigated over an extremely broad temperature range from 15 K up to 500 K by time-resolved Kerr-rotation spectroscopy. The *g*-factor is found to be approximately constant over the full investigated temperature range. Calculations by $\mathbf{k}\cdot\mathbf{p}$-theory predict a negligible temperature dependence $g(T)$ in complete agreement with the experiment as a consequence of the large band-gap and small spin orbit splitting in cubic GaN. © *2015 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4937128]

I. INTRODUCTION

The electron Landé *g*-factor is a key parameter of a semiconductor as it depends sensitively on details of the band structure, like band gaps and interband matrix elements. The *g*-factor further governs the spin splitting in an external magnetic field, being of crucial importance for numerous spintronics concepts.[1] Low-temperature values of the *g*-factor are well-known for a broad variety of semiconductors from experiments by various techniques like electron spin resonance,[2–4] photoluminescence spin quantum beat spectroscopy,[5–7] or time-resolved Kerr-rotation (TRKR).[8–10] Theoretically, the low-temperature value of the *g*-factor is predicted with high accuracy for many semiconductors by $\mathbf{k}\cdot\mathbf{p}$-theory,[11] which is generally an extremely successful method for the description of semiconductor bandstructures, including spin orbit coupling (SOC).[12] Apart from low-temperature values of the *g*-factor, the full temperature dependence $g(T)$ up to at least room temperature is highly relevant not only for a deepened understanding of temperature effects on the bandstructure, but also for possible applications in spintronics. The temperature dependence of the *g*-factor is, however, experimentally studied only for few small-gap and medium-gap semiconductors, and its theoretical description within $\mathbf{k}\cdot\mathbf{p}$-theory is still a matter of controversy.[6,9,13] Initial work of Oestreich *et al*. had shown a strong discrepancy between the experimentally found temperature dependence of the *g*-factor and predictions of $\mathbf{k}\cdot\mathbf{p}$-theory.[5,14] Experimentally, an increase of the *g*-factor with temperature towards the free electron *g*-factor is found in GaAs,[5,8,14–16] CdTe,[9,14,17] InP,[14] and GaAsBi,[7] while first attempts to describe the temperature-dependent *g*-factor via $\mathbf{k}\cdot\mathbf{p}$-theory by including the temperature dependence of the band gaps predicted a decrease of the *g*-factor with temperature.[5,14,17] Later on, different approaches to the correct description of the observed temperature dependence were pursued, taking into account either only the dilatational change of the band gaps together with an energy dependence of the *g*-factor,[13,18] or the full change of the band gaps in combination with a pronounced temperature dependence of the interband matrix element.[6] Besides, a more phenomenological approach models $g(T)$ via a strongly temperature dependent contribution of remote bands.[9] All these studies concentrated, however, on the medium-gap semiconductors GaAs, CdTe, and InP.

Here, we experimentally determine the temperature dependence of the electron Landé *g*-factor in cubic GaN (c-GaN) over an extremely broad temperature range from 15 K up to 500 K by time-resolved Kerr-rotation. The investigation of the temperature dependence $g(T)$ in c-GaN allows to test the predictions of $\mathbf{k}\cdot\mathbf{p}$-theory for the extreme case of a wide-gap semiconductor with small spin orbit coupling. In addition, the knowledge of $g(T)$ in c-GaN is highly relevant for the design of possible spintronics devices as c-GaN is a promising material system for spintronics due to its very long electron spin lifetimes.[19–21]

II. EXPERIMENTAL

The c-GaN samples investigated were grown by plasma-assisted molecular beam epitaxy.[22] The 580 nm-thick c-GaN epilayers were grown on top of cubic AlN-barriers with a thickness of 30 nm and 15 nm for samples A and B, respectively, on 3C-SiC substrates.[23] Sample A was intentionally undoped, resulting in a background *n*-type doping density of $n_D = 1\times10^{17}$ cm^{-3}, while sample B was *n*-doped by Si with a doping density of $n_D = 1\times10^{18}$ cm^{-3}.

The setup as described in Ref. 24 was used for the TRKR measurements. The energy of pump and probe beam was varied from 3.280 eV at 15 K to 3.113 eV at 500 K, following the red-shift of the band gap for increasing temperature. The average power of pump and probe was set to 10 mW and 1 mW, respectively. The samples were mounted in a specifically designed cryostat allowing for temperatures from 15 K up to 500 K. An external magnetic field B_{ext} was applied in the sample plane. The external magnetic field at the sample position was calibrated via a Hall sensor.

III. RESULTS AND DISCUSSION

Figure 1 shows typical TRKR transients for sample B at temperatures of 150 K and 500 K, respectively. The TRKR transients show oscillations due to spin Larmor precession around the external magnetic field, with the Larmor

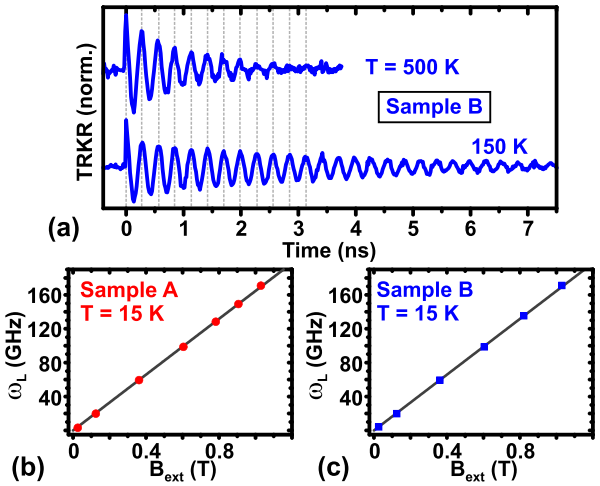

FIG. 1. (a) TRKR transients for sample B at a temperature of 150 K and 500 K, respectively, in an external magnetic field $B_{\text{ext}} = 0.1$ T. The vertical dashed lines indicate the phase relation between the Larmor oscillations at both temperatures. (b) and (c) Magnetic field dependence $\omega_L(B_{\text{ext}})$ of the Larmor precession frequency for samples A and B at $T = 15$ K. The very good agreement with linear fits (solid lines) clearly demonstrates a perfectly linear magnetic field dependence.

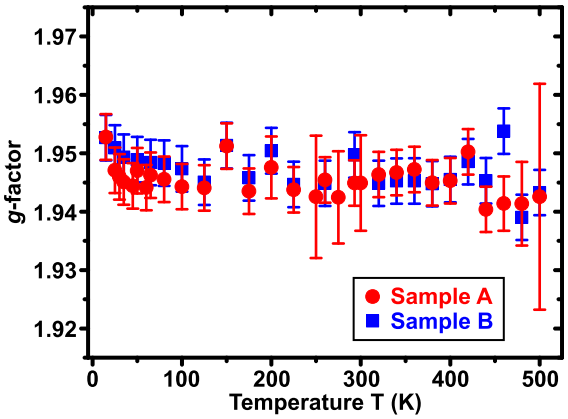

FIG. 2. Temperature dependence of the Landé g-factor for samples A and B from 15 K up to 500 K.

precession frequency $\omega_L = (\mu_B B_{\text{ext}}/\hbar)g$ as a direct measure of the Landé g-factor. The Larmor oscillations are almost completely in phase for the transients at 150 K and 500 K as indicated by the dashed vertical lines in Fig. 1(a), which clearly hints at a weak temperature dependence of the g-factor. The Larmor precession frequency ω_L is extracted by damped-cosine fits of the form[25] $[A_1 \exp(-t/\tau_c) + A_2]\exp(-t/\tau_s)\cos[\omega_L(t - t_0)]$ to the TRKR transients, where τ_c is a carrier lifetime. We note that the long spin relaxation times in c-GaN allow for the observation of numerous Larmor oscillations even at high temperatures and small external magnetic fields, thus enabling us to precisely determine the temperature dependence $g(T)$ up to 500 K. Figures 1(b) and 1(c) show the magnetic field dependence $\omega_L(B_{\text{ext}})$ of the Larmor precession frequency for samples A and B at a temperature of $T = 15$ K. We find a perfectly linear dependence of the Larmor precession frequency on the external magnetic field as demonstrated by linear fits [solid lines in Figs. 1(b) and 1(c)]. This linear magnetic field dependence excludes possible excitonic effects in the determination of the g-factor, as the electron-hole exchange interaction δ would lead to a hyperbolic magnetic field dependence $\omega_{L,X} = \sqrt{(g\mu_B B_{\text{ext}})^2 + \delta^2}/\hbar$ of the Larmor precession frequency $\omega_{L,X}$ for excitons.[26] We further find short radiative decay times $\tau_r < 40$ ps from time-resolved photoluminescence measurements (not shown), demonstrating a fast decay of initially created excitons, which, therefore, do not affect the determination of the g-factor.

Figure 2 shows the temperature dependence of the g-factor $g = \hbar\omega_L/\mu_B B_{\text{ext}}$ resulting from the calibrated external magnetic field $B_{\text{ext}} = 0.1$ T and the ω_L obtained from the fitting procedure for samples A and B from 15 K up to 500 K. The error bars in Fig. 2 include the uncertainties from the fitting procedure as well as from the stability and programming accuracy of the magnet power supply. The g-factor is within the experimental error identical for both samples, and shows only a negligible temperature dependence over the full investigated temperature range. This robustness of the g-factor against temperature variations is clearly beneficial for possible applications in spintronics, as it would guarantee robust operation insusceptible to temperature fluctuations. We note that electron localization at donors for low temperatures does not have a spurious influence on the determination of the g-factor as the g-factor of donor-bound electrons generally shows only a minute deviation from the g-factor of free conduction band electrons.[2,27] In addition, the polarization of the pump beam was modulated between left and right circularly polarized at a frequency of 50 kHz in our measurements, thus suppressing optical pumping of nuclear spins via dynamic nuclear polarization.[10] Artifacts in the determination of the g-factor due to Overhauser fields can therefore also be excluded.

In the following, we will compare the experimentally observed negligible temperature dependence of the g-factor to predictions of $\mathbf{k}\cdot\mathbf{p}$-theory. Generally, spin orbit coupling leads to a deviation Δg of the g-factor g^* at the bottom of the conduction band from the free-electron g-factor $g_0 = 2.0023$, corresponding to

$$\frac{g^*}{g_0} = 1 + \Delta g\,. \tag{1}$$

It has to be noted that the g-factor measured in the experiment is not the bare g-factor g^* at the bottom of the conduction band, but an energetically averaged g-factor $\langle g\rangle$ as a consequence of the energy dependence $g(E)$ and the thermal distribution of the electron energies. In c-GaN, the energy dependence $g(E)$ of the g-factor is not known. We assume, however, a negligible energy dependence in the following and compare directly the measured g-factor and the theoretically predicted g^*, as an estimate based on an expression originally derived for narrow-gap semiconductors gives only a minute energy dependence.[16] Further support for this approximation comes from the pump power dependence of the g-factor shown in Fig. 3. The g-factor is within the experimental error independent of the pump power P_{pump}, indicating again a very weak energy dependence.

The initial $\mathbf{k}\cdot\mathbf{p}$-description of the g-factor was given by Roth *et al.*[28] in a three-level model by

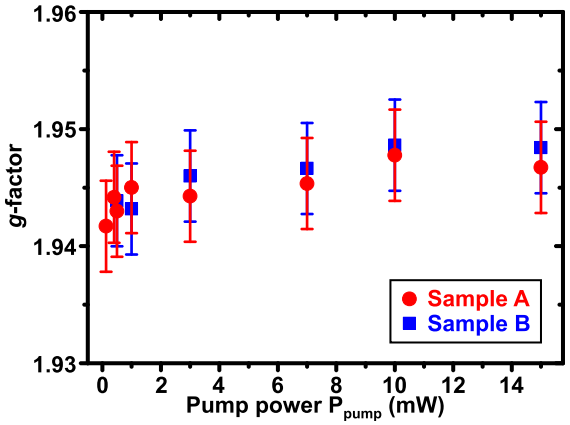

FIG. 3. Pump power dependence of the Landé g-factor for samples A and B at $T = 80$ K.

$$\Delta g = \frac{E_{P0}}{3}\left(\frac{1}{E_0} - \frac{1}{E_0 + \Delta_0}\right), \tag{2}$$

where $E_{P0} = (2m_0/\hbar^2)P_0^2$ is the Kane energy corresponding to the interband matrix element P_0. The band gaps E_0 and Δ_0 are defined in Fig. 4, following the convention of Ref. 13. Hermann and Weisbuch[29] later derived the expression

$$\Delta g = \frac{E_{P0}}{3}\left(\frac{1}{E_0} - \frac{1}{E_0 + \Delta_0}\right) + \frac{E_{P1}}{3}\left(\frac{1}{E_1 + \Delta_1} - \frac{1}{E_1}\right) + C', \tag{3}$$

within a five-level model, with the band gaps as defined in Fig. 4 and the Kane energy $E_{P1} = (2m_0/\hbar^2)P_1^2$ corresponding to the interband matrix element P_1. The constant C' accounts for the influence of remote bands. The model of Hermann and Weisbuch was further extended[6,13,30] by inclusion of the interband coupling $\bar{\Delta}$

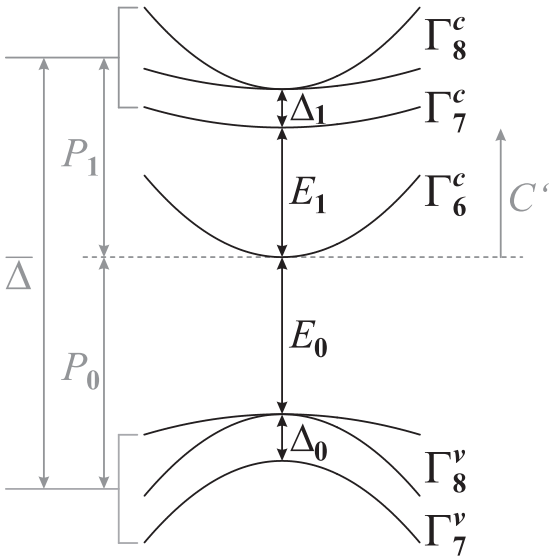

FIG. 4. Schematic band structure of c-GaN at the center of the Brillouin zone for the five-level $\mathbf{k}\cdot\mathbf{p}$-model. The zero of energy is chosen at the bottom of the Γ_6^c-band. The interband matrix elements P_0 and P_1 as well as the interband coupling $\bar{\Delta}$ are schematically indicated. The constant C' summarizes remote-band contributions.

$$\Delta g = \frac{E_{P0}}{3}\left(\frac{1}{E_0} - \frac{1}{E_0 + \Delta_0}\right) + \frac{E_{P1}}{3}\left(\frac{1}{E_1 + \Delta_1} - \frac{1}{E_1}\right) - \frac{2}{9}\bar{\Delta}\sqrt{E_{P0}E_{P1}}\left(\frac{2}{E_1(E_0 + \Delta_0)} + \frac{1}{E_0(E_1 + \Delta_1)}\right) + C'. \tag{4}$$

The inclusion of $\bar{\Delta}$ contributes significantly to the g-factor in, e.g., GaAs and InP.[30,31]

While the band parameters required for the calculation of the g-factor via Eqs. (2)–(4) are well-established for GaAs and other deeply studied semiconductors, only sparse information is available for c-GaN. We will therefore give a brief overview over available data for the band parameters in the following. The fundamental gap E_0 and its temperature dependence $E_0(T)$ are experimentally well-established and described by the Viña relation[32]

$$E_0(T) = E_0^B - \alpha_0^B\left(1 + \frac{2}{e^{\Theta_0/T} - 1}\right), \tag{5}$$

with $E_0^B = 3.351$ eV, $\alpha_0^B = 0.126$ eV, and $\Theta_0 = 607$ K.[33] For the spin orbit splitting, a temperature-independent experimental value of $\Delta_0 = 17$ meV is agreed on.[34] The values for the higher band gaps and interband matrix elements differ, however, considerably in the literature.[35–40] We restrict ourselves therefore to two consistent parameter sets[2,3] derived from the low-temperature value of the g-factor (see Table I). No values are available for the interband coupling $\bar{\Delta}$ in the literature.

In the remaining, we will discuss the predictions of the different approaches to incorporate the temperature dependence of the g-factor into $\mathbf{k}\cdot\mathbf{p}$-models. In the initial approach, which we will refer to as Model I in the following, the temperature dependence $g^*(T)$ was ascribed to the full temperature dependence $E_0(T)$ of the fundamental gap.[5,14] The corresponding temperature dependence of the g-factor according to Eq. (3) is shown by the dashed-dotted lines for parameter sets I and II, respectively, in comparison with the experimental data in Fig. 6 and on an enlarged scale in Fig. 7. The main difference resulting from the two parameter sets is a slightly different zero-temperature value $g^*(T = 0)$, while the temperature dependence is approximately the same. We will therefore concentrate only on parameter set I in the following. Although Model I completely fails for GaAs and CdTe,[5,14] its prediction is compatible with the negligible temperature dependence found in c-GaN. The

TABLE I. Consistent sets of band parameters for c-GaN from literature.

Parameter	Set I Reference 2	Set II Reference 3
E_1 (eV)	6.5	5.5
Δ_1 (eV)	0.59	0.08 ± 0.02
E_{P0} (eV)	15.4	28 ± 2
E_{P1} (eV)	4.2	11.2
$\bar{\Delta}$ (meV)	…	…
C' (eV)	…	…

predicted weak temperature dependence results obviously from the combination of a large fundamental gap E_0 and a small spin orbit splitting Δ_0 in the leading term of Δg in Eq. (3). We note that the g-factor according to the Roth formula Eq. (2) shows a completely analogous temperature dependence. Inclusion of $\bar{\Delta}$ in Eq. (4) leads again only to a minute temperature dependence with an overall change of the g-factor of approximately ± 0.006 from 0 K to 500 K for a rough estimate of the interband coupling $|\bar{\Delta}| = 30$ meV.[41]

An alternative approach, referred to as Model II, takes only the dilatational change instead of the total change of the band gaps into account,[13,16,18] in analogy to the temperature dependence of the electron effective mass.[42] The change $\Delta E_0^{\mathrm{dl}}(T)$ of the fundamental band gap only due to the lattice dilatation is given by[13]

$$\Delta E_0^{\mathrm{dl}}(T) = -3B\left(\frac{\partial E_0}{\partial P}\right)_T \int_0^T \alpha_{th}(\tilde{T})d\tilde{T}\,, \tag{6}$$

with B as the bulk modulus, $\partial E_0/\partial P$ as the pressure-induced shift of the band gap, and $\alpha_{th}(T)$ as the temperature-dependent linear thermal expansion coefficient. Using $B = 201$ GPa,[43] $\partial E_0/\partial P = 43$ meV/GPa,[44] and $\alpha_{th}(T)$ according to Ref. 45, Eq. (6) gives the dilatational temperature dependence of the fundamental gap shown in Fig. 5(a). The corresponding temperature dependence $g^*(T)$ according to Eq. (3) is shown by the solid black line in Fig. 6, clearly demonstrating complete agreement with the experimental data.

In a third approach, which will be referred to as Model III in the following, the temperature dependence of the g-factor is modeled by the full temperature dependence of the band gaps in combination with strongly temperature dependent interband matrix elements as proposed in Ref. 17 and worked out in Ref. 6. The interband matrix element $P_0 \propto a^{-1}$ is inversely proportional to the interatomic distance a of the crystal atoms.[46] A weak decrease of P_0 with temperature hence arises from the thermal lattice expansion. In addition to the thermal lattice expansion, an increase of the averaged effective atomic distance due to the stretching of the crystal lattice by acoustic phonons is taken into account in Ref. 6. The electrons are assumed to follow these lattice expansions adiabatically, leading to a stronger decrease of the matrix element P_0 than by only the thermal expansion of the lattice. Estimating the corresponding decrease of P_0 along the lines of Ref. 47 gives the temperature dependence of the corresponding Kane energy E_{P0} shown in Fig. 5(b). The same relative change with temperature is also assumed for E_{P1}.[48]

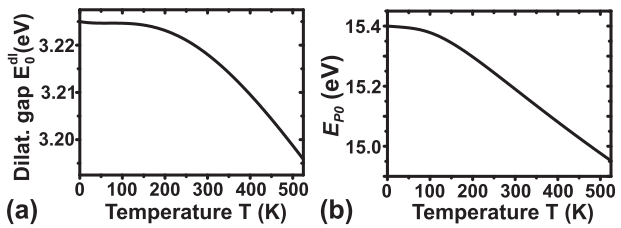

FIG. 5. (a) Dilatational temperature dependence $E_0^{\mathrm{dl}}(T)$ of the fundamental band gap used in Model II and (b) estimated temperature dependence of the Kane energy E_{P0} for use in Model III.

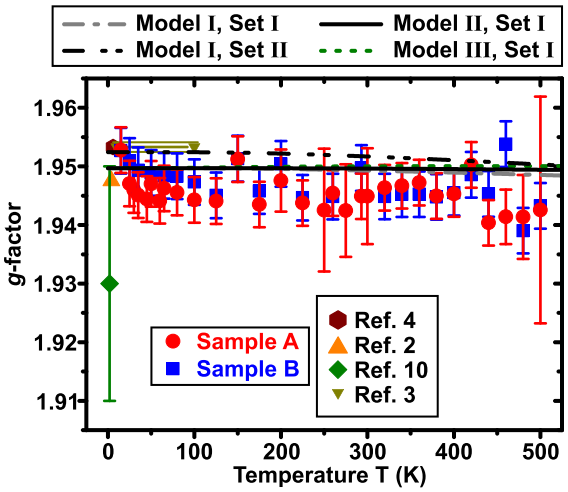

FIG. 6. Temperature dependence of the g-factor for samples A and B compared with predictions of $\mathbf{k}\cdot\mathbf{p}$-theory. The dashed-dotted lines show the predictions of Model I, which includes the full temperature dependence of the fundamental gap. The solid line shows the temperature dependence for only the dilatational change of the fundamental gap according to Model II. The dotted line refers to the prediction of Model III for strongly temperature dependent interband matrix elements. Also shown are low-temperature values from the literature.

Using the full temperature dependence of the fundamental gap and the estimated temperature dependencies of E_{P0} and E_{P1}, the temperature dependence $g^*(T)$ shown by the dotted line in Fig. 6 is obtained, which is again in complete agreement with the experimentally found temperature dependence.

All three approaches to incorporate the temperature dependence of the g-factor in the $\mathbf{k}\cdot\mathbf{p}$-models are thus fully compatible with the experimental data as discussed before. A detailed comparison of the predicted temperature dependencies (cf. Fig. 7) shows, however, different trends of the three models. Generally, the g-factor tends towards the free-electron g-factor g_0 for high electron energies, if one neglects the effect of bulk inversion asymmetry.[13,49] Model I, where the full temperature dependence of the fundamental gap enters, contradicts this trend, just like it does for GaAs

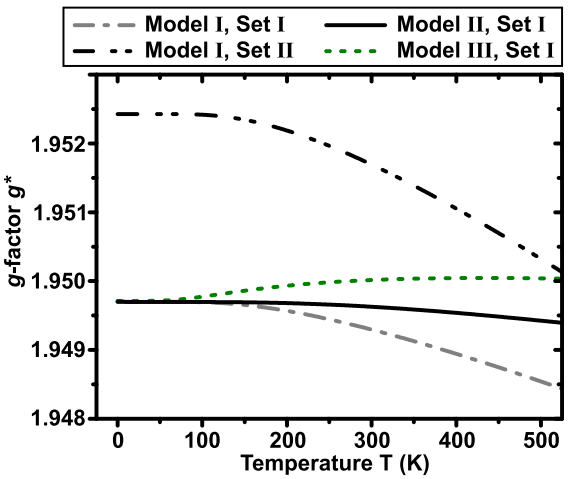

FIG. 7. Predicted temperature dependence $g^*(T)$ according to Model I (dashed-dotted lines) for parameter sets I and II, respectively, for Model II (solid line) and for Model III (dotted line).

and CdTe. Model II, which takes only the dilatational change of the fundamental gap into account, shows an extremely weak decrease of g^* with temperature, where it can, however, be assumed that inclusion of a weak energy dependence of the g-factor would lead to the expected high-energy behavior.[13,16] We note that the extremely weak temperature dependence of the g-factor in c-GaN is expected if the energy dependence of the g-factor plays a key role for its temperature dependence $g(T)$, as argued by Pfeffer and Zawadzki.[13] The zero-temperature g-factor $g(T=0)$ in c-GaN is already very close to the free-electron g-factor g_0, and a minute temperature dependence is therefore anticipated. Finally, Model III with the assumption of temperature-dependent interband matrix elements shows the expected trend towards g_0 already for the g-factor g^* at the bottom of the conduction band.

IV. CONCLUSION

In conclusion, we have experimentally investigated the temperature dependence of the electron Landé g-factor in bulk cubic GaN for temperatures from 15 K up to 500 K. The g-factor is approximately independent of the temperature over the full investigated temperature range. Calculations by $\mathbf{k}\cdot\mathbf{p}$-theory reproduce this negligible temperature dependence very well as a consequence of the large band gaps and small spin orbit splitting in cubic GaN. The robustness of the g-factor against temperature fluctuations and, as previously reported,[50] strain fluctuations makes cubic GaN a promising material system for spintronics.

ACKNOWLEDGMENTS

We gratefully acknowledge financial support by the German Science Foundation (DFG priority program 1285 "Semiconductor Spintronics" and DFG graduate program GRK 1464 "Micro- and Nanostructures in Optoelectronics and Photonics").

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