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

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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 k · 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 k · 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 k · 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 k · p-theory.⁵,¹⁴ Experimentally, an increase of the g-factor with temperature towards the free electron g-factor is found in GaAs,⁵,⁶,¹⁴-¹⁶ CdTe,⁹,¹⁴,¹⁷ InP,¹⁴ and GaAsBi,⁷ where first attempts to describe the temperature-dependent g-factor via k · 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.⁵ 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 k · 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.³³ Sample A was intentionally undoped, resulting in a background n-type doping density of n_D ≈ 1 × 10¹⁷ cm⁻³, while sample B was n-doped by Si with a doping density of n_D = 1 × 10¹⁸ 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
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 \( \omega_L \) is extracted by damped-cosine fits of the form \[ A_1 \exp(-t/\tau_x) + A_2 \exp(-t/\tau_x) \cos(\omega_L(t - t_0)) \] to the TRKR transients, where \( \tau_x \) 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 of the Landé \( g \)-factor for samples A and B.

![Figure 1](image1.png)

**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.

![Figure 2](image2.png)

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

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. 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. 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 \( \Delta g \) of the \( g \)-factor \( g^* \) at the bottom of the conduction band from the free-electron \( g \)-factor \( g_0 = 2.0023 \), corresponding to

\[
\frac{g^*}{g_0} = 1 + \Delta g.
\]

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 \( g(E) \) 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. 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 \( P_{\text{pump}} \), 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. in a three-level model by...
The inclusion of $\Delta$ 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\(^{32}\)

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

with $E_0^B = 3.351$ eV, $g_p^B = 0.126$ 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\(^{23}\) derived from the low-temperature value of the $g$-factor (see Table I). No values are available for the interband coupling $\Delta$ 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 $k \cdot p$-models. In the initial approach, which we will refer to as Model I in the following, the temperature dependence $g_T(T)$ 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 $g^T(T = 0)$, 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.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Set I</th>
<th>Set II</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$ (eV)</td>
<td>6.5</td>
<td>5.5</td>
</tr>
<tr>
<td>$\Delta_0$ (eV)</td>
<td>0.59</td>
<td>0.08 ± 0.02</td>
</tr>
<tr>
<td>$E_{P0}$ (eV)</td>
<td>15.4</td>
<td>28 ± 2</td>
</tr>
<tr>
<td>$E_{P1}$ (eV)</td>
<td>4.2</td>
<td>11.2</td>
</tr>
<tr>
<td>$\Delta$ (meV)</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$C'$ (eV)</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

FIG. 3. Schematic band structure of c-GaN at the center of the Brillouin zone for the five-level $k \cdot p$-model. The zero of energy is chosen at the bottom of the $\Gamma_8$ band. The interband matrix elements $P_0$ and $P_1$ as well as the interband coupling $\Delta$ are schematically indicated. The constant $C'$ summarizes remote-band contributions.

FIG. 4. Schematic band structure of c-GaN at the center of the Brillouin zone for the five-level $k \cdot p$-model. The zero of energy is chosen at the bottom of the $\Gamma_8$ band. The interband matrix elements $P_0$ and $P_1$ as well as the interband coupling $\Delta$ are schematically indicated. The constant $C'$ summarizes remote-band contributions.
predicted weak temperature dependence results obviously from the combination of a large fundamental gap \( E_0 \) and a small spin orbit splitting \( \Delta_0 \) in the leading term of \( \Delta g \) in Eq. (3). We note that the \( g \)-factor according to the Roth formula Eq. (2) shows a completely analogous temperature dependence. Inclusion of \( \Lambda \) in Eq. (4) leads again only to a minute temperature dependence with an overall change of the \( g \)-factor of approximately \( \pm 0.006 \) from 0 K to 500 K for a rough estimate of the interband coupling \( |\Lambda| = 30 \) 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 \( \Delta E_g^{\text{II}}(T) \) of the fundamental band gap only due to the lattice dilatation is given by\(^{13}\)

\[
\Delta E_g^{\text{II}}(T) = -3B \left( \frac{\partial E_0}{\partial P} \right)_T \int_0^T \frac{d\theta}{T} dT,
\]

with \( B \) as the bulk modulus, \( \partial E_0/\partial P \) as the pressure-induced shift of the band gap, and \( \partial \theta/T \) as the temperature-dependent linear thermal expansion coefficient. Using \( B = 201 \) GPa,\(^{43}\) \( \partial E_0/\partial P = 43 \) meV/GPa,\(^{44}\) and \( \partial \theta/T \) 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 \( P_0 \propto a^{-3} \) 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 \( E_g^{\text{II}}(T) \) 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.](image)

![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).](image)
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.\textsuperscript{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.\textsuperscript{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 $k \cdot p$-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,\textsuperscript{50} strain fluctuations makes cubic GaN a promising material system for spintronics.

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26The interband coupling is estimated via $\Delta_2$, $\Delta_2$ and the atomic spin orbit splittings as described in Ref. 31.


33Note that the same absolute temperature dependence is assumed for $E_{P2}$ and $E_{P3}$ in Ref. 6, corresponding to an extreme relative change of $E_{P1}$.