L-valley electron g factor in bulk GaAs and AlAs

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We study the Landé g-factor of conduction electrons in the L-valley of bulk GaAs and AlAs by using a three-band \( \mathbf{k} \cdot \mathbf{p} \) model together with the tight-binding model. We find that the L-valley g-factor is highly anisotropic, and can be characterized by two components, \( g_\perp \) and \( g_\parallel \). \( g_\perp \) is close to the free electron Landé factor but \( g_\parallel \) is strongly affected by the remote bands. The contribution from remote bands on \( g_\parallel \) depends on how the remote bands are treated. However, when the magnetic field is in the Voigt configuration, which is widely used in the experiments, different models give almost identical g-factor.

The knowledge to electron g-factor of semiconductors is of fundamental importance to investigate the spin-related problems. In the past decades, a lot of investigations have been carried out to understand the material and structure dependence of the g-factor. Experimentally, g-factor can be measured through the measurement of Lamour frequency by the techniques such as time resolved Faraday/Kerr rotation or through the measurement of the Zeeman splitting by electron spin resonance. Theoretical studies of the g-factor are carried out through various band structure calculations, such as \( \mathbf{k} \cdot \mathbf{p} \) model, tight-binding model and the \textit{ab initio} calculation. For zinc blende materials, most of the previous studies focus on the g-factors at \( \Gamma \) point. As recent investigations have been extended to the spin dynamics far away from equilibrium, the knowledge of g factor of higher valleys becomes important. For III-V semiconductors, the g-factor in the X-valley is believed to be close to the Landé factor of free electron, \( g_0 \), regardless of the materials due to the large band gap and the vanishing of the spin splitting at the X-point. By using two-band \( \mathbf{k} \cdot \mathbf{p} \) Kane-like model it is shown that the g-factor in the vicinity of the L-valley of IV semiconductors is highly anisotropic and can be characterized by \( g_\parallel \) and \( g_\perp \) which correspond to the g-factor along the directions parallel and perpendicular to the L-axis (i.e., along [111] direction for the [111] valley). However, the investigations of g-factor in the L-valley of III-V semiconductors are still to be carried out, especially for GaAs (Ga\(_{1-x}\)Al\(_x\)As), one of the most promising materials for realizing the spintronic device. In this paper, we present the g-factor of the L-valley of GaAs and AlAs by \( \mathbf{k} \cdot \mathbf{p} \) band structure calculation. With these two g-factors, one can further obtain the g-factor of Ga\(_{1-x}\)Al\(_x\)As by linear interpolation on \( x \), which is widely used in practice to get the material parameters of the semiconductor alloy.

Similar to the effective mass, the electron g-factor of a specific band is affected by the remote bands. The relevant bands in the vicinity of L-point in our calculation are shown in Fig. 1 and are identified by their symmetries.

The bands with \( L_\beta \) symmetry split to bands with \( L_{1,5} \) and \( L_6 \) symmetries due to the spin-orbit coupling. \( L_{1c} \) is the lowest conduction band at which we target. In addition to the top valence band \( L_{3v} \) included in the two-band Kane-like model we further include higher conduction bands \( L_{3c} \), as the gap between \( L_{1c} \) and \( L_{1c} \) bands is close to the gap between \( L_{3v} \) and \( L_{1c} \) in bulk GaAs/AlAs. In the calculation of \( g_\parallel \) we also include the remote band \( L_{2c} \). The other remote bands are neglected in the calculation for they are too far away from the conduction band to make any important effect. For the general information of the band structure and the symmetry of zinc-blende materials, one can refer to the literature, say Ref. 25.

Follow the standard \( \mathbf{k} \cdot \mathbf{p} \) calculation procedure, the anisotropic g factor of \( L_{1c} \) band can be expressed as

\[
g = g_0 + \frac{2}{m_0}\sum_{\mu \nu} \left\{ \left( E_{L_{1c}} - E_{\mu} \right) E_{L_{1c}} - E_{\nu} \right\} \left( h_{\mu \nu}(p_{\mu \nu} \times p_{\nu \sigma}) + h_{\mu \nu}(p_{\mu \nu} \times p_{\sigma \sigma}) + h_{\nu \nu}(p_{\nu \nu} \times p_{\mu \sigma}) \right). \tag{1}
\]

where \( p_{\mu \nu} \) is inter-band momentum matrix element between \( \mu \) and \( \nu \) bands. Noted that index “0” denotes \( L_{1c} \) band. \( h \) is the effective magnetic field from the spin-orbit coupling. \( g_0 \) and \( m_0 \) are the Landé factor and mass of free electron. In the coordinate system defined by the principle axes of the constant energy conduction band ellipsoid, i.e. \( z \)-axis parallels to \( \Gamma-L \) axis, the \( g \) matrix is diagonal, with \( g_{zx} = g_{yy} = g_\perp \) and \( g_{zz} = g_0 \). The contribution of the remote band is reverse proportional to the band distance. Therefore, the closest bands have most significant effects. However, for \( g_\perp \), there are no direct corrections from the closest \( L_{3v} \) and \( L_{3c} \) bands due to the symmetry. Instead, the corrections come from the indirect ones through the mediation of far-away remote bands. With the next closest \( L_{2c} \) band included, \( g_\perp \) reads

\[
g_\perp - g_0 = \text{Re} \sum_{\mu \nu} \left( \frac{E_{L_{1c}} - E_{\mu}}{E_{L_{1c}} - E_{L_{3c}}} \right) \left( \frac{E_{L_{3c}} - E_{\nu}}{E_{L_{3c}} - E_{L_{2c}}} \right) \langle L_{1c}|p_{\mu \nu}|L_{3c}\rangle \langle L_{2c}|p_{\nu \sigma}|L_{1c}\rangle. \tag{2}
\]
TABLE I: Band structure parameters and $g$ factors at $L$ point for GaAs and AlAs. The rows labeled “α” and “β” represent the results from three-band model by choosing the value of $\lambda$ to be corresponding value of $L$-point of Ge and the value at Γ-point.$^2$ The rows with “γ” denote the results from two-band model.

|            | $E_{L_{1c}}$ | $E_{L_{3c}}$ | $E_{L_{3\gamma}}$ | $\delta$ | $\delta'$ | $m_l$ | $m_t$ | $P$ | $P'$ | $g_L$ | $g_\parallel$ | $g_\perp$ | $g_z$ |
|------------|-------------|-------------|----------------|---------|---------|------|------|----|-----|-------|-----------|----------|------|
| GaAs       | 1.85$^a$   | -1.20$^a$  | 5.47$^a$      | 0.22$^a$| 0.08$^b$| 1.9$^{a,b}$ | 0.075$^a$ | 12.5 | 2.75 | 0.075$^a$ | 2.03 | 1.09 | 2.03 |
| AlAs       | 2.581$^c$  | -0.983$^c$ | 5.069$^c$     | 0.208$^c$ | 0.058$^c$ | 1.9$^{a,b}$ | 0.096$^{a,b}$ | 11.9 | 2.62 | 0.096$^{a,b}$ | 2.03 | 1.41 | 1.85 |

$^a$Ref. 27  $^b$Ref. 29  $^c$Ref. 30

It is expected that this value is small due to the large gap between $L_{1c}$ and $L_{2c}$ bands. In order to calculate the contribution of the remote bands quantitatively, one needs the matrix elements of $h$ and $p$ which are not accessible theoretically by the $k \cdot p$ calculation alone. In practice, these elements can be obtained by fitting the experiment data, such as effective masses and band gaps. In the framework of the $k \cdot p$ theory, the anisotropic effective mass $m^*$ of $L$-point is

$$m_0/m^* = 1 + 2 \sum_\mu (E_{L_{1c}}|p|\mu)(\mu|p|L_{1c})/E_{L_{1c}} - E_\mu.$$  (3)

For the longitudinal mass,

$$m_0/m_l = m_0/m_{zz} = 1 + 2 \sum_\mu (E_{L_{1c}}|p_z|L_{2c})^2/E_{L_{1c}} - E_{L_{2c}}.$$  (4)

The $L_{3\gamma}$ spin-orbit split off band gap $\delta = 2\epsilon(L_{3\gamma}|h_z|L_{3\gamma})$. By assuming that all the non-vanishing $p$ elements in Eq. 2 and 4 are the same, and all of the non-vanishing $h$ elements are equal to each other, $g_\perp$ can be expressed as

$$g_\perp - g_0 \cong -\delta(m_0/m_l - 1)/(E_{L_{1c}} - E_{L_{3\gamma}}).$$  (5)

Using the experiment data of $m_l$ and $\delta$, one can justify that the correction to $g_\perp$ is rather small for both GaAs and AlAs due to the large gap between $L_{1c}$ and $L_{3\gamma}$. As a result, $g_\perp$ differs from $g_0$ by only 2%. The closeness of $g_\perp$ to $g_0$ at $L$-point is not limited to GaAs but rather universal property of semiconductor with diamond and zinc-blende structures, in which the symmetry eliminates the direct correction from the closest bands.

The parallel component $g_\parallel = g_{zz}$ is very different. It reads

$$g_\parallel - g_0 = Re\left(\sum_\mu \frac{\langle L_{1c}|p_x|L_{3\gamma} \rangle}{(E_{L_{1c}} - E_{L_{3\gamma}})(E_{L_{1c}} - E_{L_{3\gamma}})} \times\langle L_{3\gamma}|h_z|L_{3\gamma} \rangle\langle L_{3\gamma}|p_y|L_{1c} \rangle\right).$$  (6)

FIG. 1: Schematic of band structure near $L$ point for zinc-blende crystal.

With the modifications from $L_{3\gamma}$ and $L_{3\gamma}$ bands, it can be written as

$$g_\parallel - g_0 = -2m_0/\hbar^2 [P^2(E_\delta(E_\delta + \delta) + P^2(E_\delta E_\delta')].$$  (7)

Here $E_\delta = E_{L_{1c}} - E_{L_{3\gamma}}$ and $E_\delta' = E_{L_{3\gamma}} - E_{L_{1c}}$ are the band gaps. $\delta'$ is the spin-orbit splitting of the $L_{3\gamma}$ conduction band. $-im_0P'(P')/\hbar$ is the non-vanishing inter-band momentum matrix element between $L_{1c}$ and $L_{3\gamma}$ bands. Among these parameters, the band gaps and the spin-orbit splittings can be measured directly or obtained through band structure calculations. In our calculation, we use the experiment data from Refs. 27 and 29 when available. For the parameters without experiment data, theoretical results from the tight-binding model are used. Since there is no value of $\delta'$ in the literature, we calculate it using the tight-binding model with the tight-binding parameters taken from Ref. 30. All the parameters in Eq. 7 are listed in Table I except $P$ and $P'$. However, there are neither direct experimental data nor theoretical results from three band model on $P$ and

$^a$Ref. 27  $^b$Ref. 29  $^c$Ref. 30
$P'$. In $k \cdot p$ band structure calculation, both are determined by fitting other experimentally measurable parameters. Here we use the transversal effective mass as a fitting target. From Eq. (3), the transversal effective mass $m_1 = m_{xx}$ reads:

$$m_0 - 1 = \frac{m^2}{m_1} \left[ P^2 \left( \frac{\delta}{E_{p_g}} + \frac{1}{E_{p_g}} \right) - P'^2 \left( \frac{\delta}{E_{p_g}} + \frac{1}{E_{p_g}} \right) \right].$$

Besides this, one more relation, i.e., $P'/P$, is required in order to obtain $P$ and $P'$. There are three possible ways to estimate the value of $\lambda = P'/P$. The first is based on the assumption that this ratio at the same symmetry point is an universal constant for different materials. From the experiment data of Ge given in Refs. 16 and 27, i.e., $E_{L_{x_g}} = 0.744$ eV, $E_{L_{y_g}} = -1.53$ eV, $E_{L_{z_g}} = 4.3$ eV, $\delta = 0.23$ eV, $\delta' = 0.27$ eV, $m_1 = 0.0791 m_0$ and $g_0 = 0.82$, we obtain $\lambda = 0.22$ at $L$-point from Eqs. (16) and (18). With this value, one finds that $g_0 = 1.09$ and 1.41 for GaAs and AlAs respectively. This set of parameters are listed in Table I with rows labeled “$\alpha$”. The second way is to assume that $\lambda$ at different valleys are the same. In this way, we can use the value of $\lambda$ at $\Gamma$-point where the band structure is well studied. For GaAs (AlAs), $\lambda = 0.456 (0.533)$, which give $g_0 = 0.89 (0.93)$. These values are listed in Table I in the rows labeled “$\beta$”. The third way to choose $\lambda$ is to set it to be zero and thus reduce the three-band model to two-band one. The corresponding results are shown in Table I with rows labeled “$\gamma$”. From the table, one can see that the remote bands have significant effect on $g_0$. However, the contribution of the remote bands strongly depends on how the remote bands are treated. We comment that all the three estimations of $\lambda$ above have their reasonings. However, one has no way to judge which one is the best without experiments. Fortunately, there is certain important case where the corresponding $g$-factor does not depend on the model one uses, which we address in the following.

From the table, one finds that $g$-factor in $L$-valley is highly anisotropic. When an applied magnetic field departs from the principle axis, the corresponding $g$-factor is a combination of $g_\parallel$ and $g_\perp$. Moreover, different valleys also contribute differently. The overall $g$-factor should be averaged over the four $L$-valleys. However, when the magnetic field is along some highly symmetric crystal axis, such as [100] direction (i.e., in Voigt configuration), all the four $L$-valleys have the same overall $g$-factor. In this case, the $g$-factor can be expressed as

$$g_x = \sqrt{(g_\parallel^2 + g_\perp^2 \sin^2 \theta + g_\perp^2 \cos^2 \theta)/2},$$

with $\cos^2 \theta = 1/3$ for [100] direction. $g_x$ is also listed in Table I. One finds that the values of $g_x$ obtained from the three different choices of $\lambda$ are very close to each other. The difference in $g_x$ given by different models is less than 5%, even though the difference in $g_0$ can be as large as 20-30%. The closeness of $g_x$ from the three results is not a coincidence. One can see from Eq. (4) that under the Voigt configuration, the contribution of $g_\parallel^2$ to $g^2_\perp$ is more than twice as that of $g_\parallel^2$. Moreover, the remote bands have marginal effect on $g_\parallel$. As a result, $g_x$ is model insensitive. This result is of particular interest, since the applied magnetic field is exactly along the [100] direction in the Voigt configuration, which is widely used in the Kerr rotation experiments. We believe that the obtained $g_x$ is reliable in studying the spin dynamics in $L$-valley in Voigt configuration.

In summery, we have investigated the $L$-valley Landé $g$-factor in bulk GaAs and AlAs using a three-band $k \cdot p$ model. The parameters used in the calculation are from experiment data if available, or from the tight-binding calculation otherwise. The $g$-factor in the $L$-valley is highly anisotropic and can be characterized by two components: the transversal one $g_\perp$, corresponding for the magnetic field perpendicular to the $L$-axis, and the longitudinal one $g_\parallel$, for the magnetic field parallel to the $L$-axis. The transversal component is close to the free electron $g$-factor due to symmetry. Whereas the longitudinal component is shown to be strongly affected by the remote bands. The contribution of the remote bands depends on how these bands are treated, and the results are quite different. It is hard to judge which one is more reasonable without the justification of the experiments. However, when the magnetic field is in Voigt configuration (i.e., along [100] axis) which is widely used in experiments investigating spin dynamics, different methods used in this investigation give almost identical Landé factors: $g_x \approx 1.77$ for GaAs and 1.85 for AlAs.

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