Spin splitting in bulk wurtzite AlN under biaxial strain


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Spin splitting in bulk wurtzite AlN under biaxial strain

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The spin-splitting energies in biaxially strained bulk wurtzite material AlN are calculated using the linear combination of atomic orbital (LCAO) method, and the equi-spin-splitting distributions in \( k \)-space near the minimum-spin-splitting (MSS) surfaces are illustrated. These data are compared with those derived analytically by two-band \( \mathbf{k} \cdot \mathbf{p} \) (2KP) model. It is found that the results from these two methods are in good agreement for small \( k \). However, the ellipsoidal MSS surface under biaxial compressive strain does not exist in the 2KP model, because the data points are far from the \( \Gamma \) point. Instead, three basic shapes of the MSS surface occur in the wurtzite Brillouin zone: a hyperboloid of two sheets, a hexagonal cone, and a hyperboloid of one sheet, evaluated from the LCAO method across the range of biaxial strains from compressive to tensile. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4720469]

I. INTRODUCTION

Spintronics has received considerable attention in the field of semiconductor research in recent years. Several types of transistors utilizing spin properties of semiconductors have been proposed.1–3 One of these proposed spin devices, the resonant spin lifetime (RSL) transistor, is based on the special properties of the spin lifetime tensor arising from the interplay between bulk inversion asymmetry (BIA) and structure inversion asymmetry (SIA) in zinc-blende4 or wurtzite5 quantum wells (QWs). In zinc-blende semiconductors, unstrained BIA yields a cubic-\( k \)-term (called the Dresselhaus effect),6 while strain7,8 and SIA lead to a linear-\( k \) term (named the Rashba effect)9 in the two-band \( \mathbf{k} \cdot \mathbf{p} \) (2KP) Hamiltonian. In bulk wurtzite semiconductors, there are also two types of wurtzite bulk inversion asymmetry (WBIA) effects.10,11 In the nearest-neighbor linear combination of atomic orbitals (LCAO) model, the ideal wurtzite structure yields only the type-II WBIA effect (called the Dresselhaus effect in Ref. 10), while deviations from the ideal structure caused by the crystal field or strain yield the type-I WBIA effect (called the Rashba effect in Ref. 11). The type-II WBIA effect induces a cone-shaped minimum-spin-splitting (MSS) surface in the ideal wurtzite Brillouin zone. Since the spin splitting on the MSS surface is generally very weak, it can be regarded as a spin-degenerate surface.10 When the crystal field and strain are taken into account, the type-I WBIA effect induces a shape-controllable MSS surface (i.e., a MSS surface that can become a hyperboloid of two sheets, a hexagonal cone, or a hyperboloid of one sheet) in the real wurtzite Brillouin zone. Such a shape-controllable MSS surface also makes the wurtzite material a potential candidate for spintronic devices.5,10,11 Based on the mechanics of spin-orbit interaction, the interplay between Rashba and Dresselhaus effects will determine the shape of MSS surface of wurtzite aluminum nitride (AlN), which is crucial information in the band-engineering of AlN-based materials for spintronic application. Consequently, the role of biaxial strain and its influence on the MSS surface have to be solved when one wants to engineer the AlN-based materials for spintronic devices.

However, the shape of the MSS surface still has not been studied under biaxial compressive strain. It requires a better understanding of the change of spin-splitting energies near the MSS surface in order to design spintronic devices, such as the RSL transistor. Therefore, it is important to study the equi-spin-splitting (ESS) distribution near the MSS surface, as well. However, the ESS distribution near the MSS surface under different strains is still unknown. In this paper, we shall investigate from biaxial compressive to biaxial tensile strains on the shapes of the MSS surfaces and the ESS distribution near these MSS surfaces by using the LCAO method, and compare these results to those obtained with the 2KP model. We show that the MSS and ESS surfaces calculated by the 2KP model are in good agreement with LCAO calculations for small \( k \), but inconsistent for large \( k \). It is also shown that the ellipsoidal MSS surface predicted by the 2KP model under biaxial compressive strain does not exist, because the MSS data points are far from the \( \Gamma \) point in this case.

II. METHODS AND RESULTS

To calculate the spin-splitting energies in bulk wurtzite materials, the band structures for both unstrained and biaxially strained wurtzite AlN are computed using the \( \text{sp}^3 \) LCAO method with spin-orbit coupling. The Hamiltonian \( H(\mathbf{k}) \) can be written in the form,
where $H_0^{\alpha \beta} (\vec{k})$ is the Hamiltonian without the spin-orbit terms ($\alpha = \uparrow$ or $\downarrow$), where $\vec{k} = \vec{k}_f + \vec{k}_g = k_f (\cos \theta + \tilde{y} \sin \theta) + 2k_z$, $\vec{k}_f / \vec{\Gamma}_f$, and $\vec{k}_g / \vec{\Gamma}_g$. The renormalized spin-orbit splitting of the anion and cation $p$ states (e.g., $\Delta_{\text{N}} = 9 \text{ meV}$ and $\Delta_{\text{Al}} = 24 \text{ meV}$) in $H_{SO}^{\alpha \beta}$ ($\alpha, \beta = \uparrow$ or $\downarrow$) is given in Refs. 14 and 15. The LCAO parameters are listed in Table I of Ref. 16. When the crystal field is taken into account, the band structure of the unstrained wurtzite material is obtained by differentiating the bond in the [001] direction from the three other bonds.15 The corresponding LCAO parameters used in these strained cases are obtained through Harrison’s $d^{-2}$ rule and modification of the Slater-Koster coefficients from those of the ideal wurtzite structure.16 The spin-splitting energies of the lowest conduction band are obtained from the eigenvalues of the above Hamiltonian $H(\vec{k})$.

In the 2KP Hamiltonian, the spin-orbit component induced by the type-II WBIA effect is $H_{SO}^{\alpha \beta} (\vec{k}) = (-\gamma_0 k_{f f}^{\alpha \beta} + \lambda_0 k_{g g}^{\beta \alpha}) (\sigma_x k_y - \sigma_y k_x)$, where $\gamma_0$ and $\lambda_0$ are the type-II WBIA coefficients, and $\lambda_0/\gamma_0 \approx 4$.10 As the crystal field and biaxial strain24 are taken into account, a perturbation term $H_{SO}^{\alpha \beta} (\vec{k}) = (\sigma_x k_y - \sigma_y k_x)$ induced by the type-I WBIA effect is added to the spin-orbit component, where $\sigma_{xx}$, $\gamma'$, and $\lambda'$ are the type-I WBIA coefficients.9-11 As a result, the spin-orbit component of the 2KP Hamiltonian can be written as $H_{SO}^{\alpha \beta} (\vec{k}) = H_{SO}^{\alpha \beta} + H_{SO}^{\beta \alpha}$, where $\gamma_{xx}$ and $\lambda_{xx}$ are the WBIA coefficients, as well as the LCAO parameters. Here, $\gamma_{xx} = 4 \gamma$, and $\lambda_{xx} = 3 \lambda$.10,11 The spin-splitting energy ($\delta E$) can be described by the following equation:

$$\delta E = 2k_{\parallel} (\sigma_x k_y - \sigma_y k_x) + \frac{\lambda_{xx} k_y^2 + \lambda_{xx} k_x^2}{\sqrt{-2 \lambda_{xx} k_y}}.$$  

To calculate the MSS and ESS surfaces in $k$-space analytically using the 2KP model, we write $2\gamma_{xx} k_{\parallel}^2 = 2(\gamma_{xx} + \lambda_{xx}) k_{y} k_{y} + \delta E = 0$. Therefore, by calculating $k_{\parallel}$ for the MSS and ESS surfaces, the analytical solution as a function of $k_{\parallel}$ with the 2KP model can be written as

$$k_{\parallel} = \pm \frac{\sqrt{-2 \lambda_{xx} k_y}}{\sqrt{-2 \lambda_{xx} k_y}}.$$  

**TABLE I.** The 2KP parameters under different strains for wurtzite AlN used in this paper.

<table>
<thead>
<tr>
<th>Strain%</th>
<th>$\varepsilon_{xx} = -3.00%$</th>
<th>$\varepsilon_{xx} = 0%$</th>
<th>$\varepsilon_{xx} = +1.43%$</th>
<th>$\varepsilon_{xx} = +3.00%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2KP parameters</td>
<td>$\gamma_{xx} = 2.02455$</td>
<td>$\gamma_{xx} = 0.77011$</td>
<td>$\gamma_{xx} = 0.00720$</td>
<td>$\gamma_{xx} = -0.93568$</td>
</tr>
<tr>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td></td>
</tr>
<tr>
<td>$\lambda_{xx} = 4.31701$</td>
<td>$\lambda_{xx} = -2.25910$</td>
<td>$\lambda_{xx} = -6.22200$</td>
<td>$\lambda_{xx} = -11.18130$</td>
<td></td>
</tr>
<tr>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td></td>
</tr>
<tr>
<td>$\lambda_{xx} = -37.57961$</td>
<td>$\lambda_{xx} = -28.40268$</td>
<td>$\lambda_{xx} = -23.11324$</td>
<td>$\lambda_{xx} = -16.44389$</td>
<td></td>
</tr>
<tr>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td>(meV·Å)</td>
<td></td>
</tr>
</tbody>
</table>
for wurtzite AlN under different strain are obtained by fitting the spin-splitting energy data from the LCAO method and are listed in Table I. The signs of the 2KP parameters and the spin-splitting energy data from the LCAO method and are listed in Table I. The signs of the 2KP parameters and the spin-splitting energy data from the LCAO method and are listed in Table I. The signs of the 2KP parameters and the spin-splitting energy data from the LCAO method and are listed in Table I. The signs of the 2KP parameters and the spin-splitting energy data from the LCAO method and are listed in Table I. The signs of the 2KP parameters and the spin-splitting energy data from the LCAO method and are listed in Table I. The signs of the 2KP parameters and the spin-splitting energy data from the LCAO method and are listed in Table I.

Figure 1 shows the spin splitting as a function of $k_{//}$ under various external strains in bulk wurtzite AlN for (a) biaxial strain with $\varepsilon_{xx} = -3.00\%$, (b) biaxial strain with $\varepsilon_{xx} = 1.43\%$, and (c) biaxial strain with $\varepsilon_{xx} = 3.00\%$, as calculated for various values of $k_z$ using the LCAO method. For a biaxially strained wurtzite material with $\varepsilon_{xx} = -3.00\%$, it is seen that the shape of the MSS surface is a hyperboloid of two sheets or a hexagonal cone, respectively. The shapes of the ESS distribution near these MSS surfaces have two basic forms: a hyperboloid of one sheet, and an approximate, asymmetric hyperboloid surface [see Figs. 2(a) and 2(b)].

Figure 2 shows the ESS distribution near the MSS surface in bulk wurtzite AlN under various external strains, as calculated with the LCAO method. For a biaxially strained wurtzite material with $\varepsilon_{xx} = -3.00\%$ or $\varepsilon_{xx} = 1.43\%$, it can be seen that the sign of the MSS surface is a hyperboloid of two sheets or a hyperboloid of one sheet, and an approximate, asymmetric hyperboloid surface, and an opposing hyperboloid of one sheet [see Fig. 2(c)]. When $k_{//} = 0$, the high symmetry of the bulk material results in zero spin-splitting energy (spin degeneracy) along the [001] direction, due to time-reversal symmetry. Note that one type of the ESS distribution is an approximate, asymmetric hyperboloid surface not only near the MSS surface but also near this spin-degenerate line (when $k_{//} = 0$).

Figure 3 shows the ESS surface near the MSS surface under different biaxial strains, as calculated by using both the 2KP model and the LCAO method. For a biaxially strained wurtzite structure with $\varepsilon_{xx} = -3.00\%$, the shape of the ESS ($\delta E = 0.1\, \text{meV}$) surface calculated by the 2KP model is ellipsoidal and is inconsistent with that calculated by the LCAO method [see Fig. 3(a)]. We note that the ellipsoidal MSS surface under biaxial compressive strain predicted by the 2KP model does not exist, since the MSS data points in this case are far from the $\Gamma$ point. We also note that the 2KP model predicts that a sharp rise in $k_z$ takes place in the range of small $k_{//}$ on the ESS surfaces; this result is consistent with that calculated by the LCAO method.

For the unstrained wurtzite material with $\varepsilon_{xx} = 0\%$, it is seen that the shape of the ESS ($\delta E = 0.1\, \text{meV}$) surface calculated method exhibits a linear behavior [see Figs. 1(a) and 1(b)]. These results imply that the type-I WBAE effect dominates the spin splitting in both compressively strained and unstrained wurtzite materials, due to the dominance of the linear-$k$ term. For the tensely strained ($\varepsilon_{xx} = 3.00\%$) wurtzite structure, a spin-degenerate surface exists on the $k_z = 0.0$ ($\pi/c$) plane in the wurtzite Brillouin zone [see Fig. 1(c)]. This is because in this case, the interplay between the linear-$k_{//}$ and cubic-$k_{//}$ terms generates spin-degenerate points in the plane of $k_z = 0.0$ ($\pi/c$) in the tensely strained wurtzites. The results predicted by the 2KP model are in good agreement with those from the LCAO method. Conversely, in the tensile strain, for large $k_{//}$, the spin splitting predicted by the 2KP model is much larger than that using by the LCAO method. Note that the ellipsoidal MSS surface under biaxial compressive strain predicted by the 2KP model does not exist, since the MSS data points in this case are far from the $\Gamma$ point.
by the 2KP model is a hyperboloid of one sheet and is in good agreement with that calculated by the LCAO method for small $k$ ($k_\parallel < 0.15 \pi/c$). Also, the shape of the MSS ($\delta E = 0.0 \text{ meV}$) surface calculated by the 2KP model is a hyperboloid of two sheets and agrees with that calculated by the LCAO method [see Fig. 3(b)]. On the ESS surface, the change of $k_z$ is dramatically large in the range of small $k_\parallel$, but shows a linear behavior for large $k_\parallel$ that is predicted by the 2KP model, consistent with the result calculated by the LCAO method. For a biaxially strained wurtzite material with $\varepsilon_{xx} = 1.43\%$, the shape of the MSS ($\delta E = 0.0 \text{ meV}$) surface calculated by the 2KP model is a hexagonal cone and is in good agreement with that calculated by the LCAO method. The shape of the ESS ($\delta E = 0.1 \text{ meV}$) surface calculated by the 2KP model is a hyperboloid of one sheet and agrees with that calculated by the LCAO method. However, for

![Graphs showing MSS and ESS curves under various external strains](image)

**TABLE II.** The signs of the 2KP parameters and the shapes of the MSS surface predicted by the 2KP and LCAO methods under different strains for wurtzite AlN.

<table>
<thead>
<tr>
<th>Strain (%)</th>
<th>$-5.00% \leq \varepsilon_{xx} \leq -1.00%$</th>
<th>$-1.00% &lt; \varepsilon_{xx} \leq +1.43%$</th>
<th>$+1.43% &lt; \varepsilon_{xx} \leq +5.00%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2KP$</td>
<td>$x_{xz} &gt; 0$</td>
<td>$x_{xz} &lt; 0$</td>
<td>$x_{xz} &lt; 0$</td>
</tr>
<tr>
<td></td>
<td>$\gamma_{xz} &gt; 0$</td>
<td>$\gamma_{xz} &lt; 0$</td>
<td>$\gamma_{xz} &lt; 0$</td>
</tr>
<tr>
<td></td>
<td>$\lambda_{xz} &lt; 0$</td>
<td>$\lambda_{xz} &lt; 0$</td>
<td>$\lambda_{xz} &lt; 0$</td>
</tr>
<tr>
<td></td>
<td>$x_{xz}/\gamma_{xz} &gt; 0$</td>
<td>$x_{xz}/\gamma_{xz} &lt; 0$</td>
<td>$x_{xz}/\gamma_{xz} &lt; 0$</td>
</tr>
<tr>
<td></td>
<td>$x_{xz}/\lambda_{xz} &lt; 0$</td>
<td>$x_{xz}/\lambda_{xz} &lt; 0$</td>
<td>$x_{xz}/\lambda_{xz} &gt; 0$</td>
</tr>
</tbody>
</table>

Shape of MSS surface predicted by 2KP
- ellipsoid
- a hyperboloid of two sheets
- a hyperboloid of one sheet

Shape of MSS surface predicted by LCAO
- a hyperboloid of two sheets
- a hyperboloid of two sheets
- a hyperboloid of one sheet
$k_{||} < 0.32 \pi/c$, the ESS data points ($\delta E = 0.1\text{ meV}$) predicted by the 2KP model do not exist, due to the lack of an analytical solution for $k_z$ when $(-\delta E + 2\alpha_{ww} k_{||} - 2\gamma_{ww} k_z^2) < 0$ [see Fig. 3(c)]. For a biaxially strained wurtzite with $\varepsilon_{xx} = 3.00\%$, for $k_{||} < 0.1 \pi/c$, the shape of the ESS ($\delta E = -0.1\text{ meV}$) surface calculated by the 2KP model is an opposing hyperboloid of one sheet and is in good agreement with that calculated by the LCAO method for $k_z < 0.25 \pi/c$. However, the shape of the MSS ($\delta E = 0.0\text{ meV}$) surface calculated by the 2KP model disagrees with that calculated by the LCAO method, since the MSS data points in this case are far from the $\Gamma$ point. In this case, the MSS (ESS) surface for $0.1 \pi/c < k_{||} < 0.5 \pi/c$ predicted by the 2KP model does not exist, due to the lack of an analytical solution for $k_z$ when $(-\delta E + 2\alpha_{ww} k_{||} - 2\gamma_{ww} k_z^2) < 0$ [see Fig. 3(d)]. These results show that over the range of biaxial strains, from tensile to compressive, the spin splitting in wurtzite structures can be well described by the 2KP model near the zone center.

III. CONCLUSIONS

We have determined the ESS distribution near the MSS surface of wurtzite AlN under different biaxial strains by using the LCAO method and have compared them with those calculated by using the 2KP model. LCAO calculations in the wurtzite Brillouin zone show that the MSS surface can be described, over the range of biaxial strains from tensile to compressive, by just three basic shapes: a hyperboloid of two sheets, a hyperboloid, and a hyperboloid of one sheet. It is also found that under biaxial compressive strain, the ellipsoidal MSS surface predicted by the 2KP model does not exist, as the MSS data points are far from the $\Gamma$ point in this case. Moreover, we have demonstrated that the MSS and ESS surfaces calculated by the 2KP model with an analytical formula are in good agreement with LCAO calculations for small $k$, but disagree with LCAO calculations for large $k$. Specifically, the analytical solution of the 2KP model can identify the interplay between the types-I and II WBIA effects, investigate the ESS and the MSS surfaces, and accurately determine the spin splitting near the zone center in wurtzite structures.

Therefore, the 2KP model is still valid and effective for the study of spintronics in wurtzite semiconductors.

ACKNOWLEDGMENTS

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