Dresselhaus effect in bulk wurtzite materials

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The spin-splitting energies of the conduction band for ideal wurtzite materials are calculated within the nearest-neighbor tight-binding method. It is found that ideal wurtzite bulk inversion asymmetry yields not only a spin-degenerate line (along the k_z axis) but also a minimum-spin-splitting surface, which can be regarded as a spin-degenerate surface in the form of $bk_z^2 - k_\parallel^2 = 0$ ($b \approx 4$) near the Γ point. This phenomenon is referred to as the Dresselhaus effect (defined as the cubic-in-k term) in bulk wurtzite materials because it generates a term $\gamma_{wz}(bk_z^2 - k_\parallel^2)(\sigma_x k_y - \sigma_y k_x)$ in the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2775038]

In recent years a great deal of research in semiconductor physics has been focused on an emerging field—spintronics. One of the most promising proposals is the spin transistor due to Datta and Das.[1] Recently, a different type of spin transistor, the resonant spin lifetime (RSL) transistor is proposed,[2,3] which is based on the special properties of the spin lifetime tensor due to the interplay between bulk inversion asymmetry (BIA) and structure inversion asymmetry (SIA) in the zinc-blende[4] or wurtzite[5] quantum wells (QWs). In the zinc-blende semiconductors, BIA yields a cubic-k term (called Dresselhaus effect)[6] and SIA leads to a linear-k term (named Rashba effect)[7] in the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian. The Dresselhaus and Rashba effects in zinc-blende semiconductors have been well understood because they have been studied intensively by many theoretical methods such as the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$, eight-band $\boldsymbol{k}\cdot\boldsymbol{p}$, and tight-binding [also known as the linear-combination-of-atomic-orbital (LCAO)] methods.[6–11] In bulk wurtzite semiconductors, there are two wurtzite bulk inversion asymmetry (WBIA) effects; one is the Dresselhaus effect which leads to a k^3 term in the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ model and the other is the wurtzite structure inversion asymmetry (WSIA) effect, which yields a linear-k term in the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ model.[12,13] The WSIA effect, which may also be called as the Rashba effect in bulk wurtzite, has been vigorously investigated since 1950s.[13] However, the Dresselhaus effect in bulk wurtzite is still unknown. In this letter, we shall investigate the Dresselhaus effect in bulk wurtzite within the nearest-neighbor LCAO method.[10,14] In the nearest-neighbor LCAO model, ideal wurtzite structure ($c/a = 0.633$ and $u = d_\parallel/c = 0.375$, where $d_\parallel$ is the length of the bonds parallel to the c axis) yields only the Dresselhaus effect, while deviations from ideal structure generate the WSIA effect.[12] Recently, Tsubaki *et al.*[15] and Lo *et al.*[16,17] independently observed a large spin-splitting energy in the two-dimensional electron gases (2DEGs) of GaN/AlGaN wurtzite heterostructures; moreover, the spin-splitting energy at Fermi surface can be changed dramatically from 0 to 10 meV, by varying the carrier concentrations or the gate voltages.[15,16] These imply that not only large spin splitting energies[12] but also a spin-degenerate surface[16] exists in the bulk wurtzite semiconductors. In this letter, we shall demonstrate that a cone-shaped minimum-spin-splitting (MSS) surface does exist in the ideal wurtzite Brillouin zone, due to the Dresselhaus effect. Near the Γ point, the MSS surface can be regarded as a spin-degenerate surface because its splitting energies are generally small. Such spin-degenerate surface can be described by an equation of $bk_z^2 - k_\parallel^2 = 0$ ($b \approx 4$), where $\mathbf{k}_\parallel = k_\parallel(\hat{x}\cos\theta + \hat{y}\sin\theta)$, $\mathbf{k}_x \parallel \boldsymbol{\Gamma}\mathbf{M}$, and $\mathbf{k}_y \parallel \boldsymbol{\Gamma}\mathbf{K}$.

To study the Dresselhaus effect in bulk wurtzite, the band structures for ideal wurtzite materials AlN, ZnO, CdS, CdSe, and ZnS are calculated using the nearest-neighbor LCAO method. The LCAO Hamiltonian $H(\mathbf{k})$ can be written in the following form:

$$H(\mathbf{k}) = H_0(\mathbf{k}) + H_{SO}(\mathbf{k}) = \begin{bmatrix} H_0^{\uparrow\uparrow}(\mathbf{k}) & 0 \\ 0 & H_0^{\downarrow\downarrow}(\mathbf{k}) \end{bmatrix} + \begin{bmatrix} H_{SO}^{\uparrow\uparrow} & H_{SO}^{\uparrow\downarrow} \\ H_{SO}^{\downarrow\uparrow} & H_{SO}^{\downarrow\downarrow} \end{bmatrix}. \quad (1)$$

The Hamiltonian without the spin-orbit terms (i.e., $H_0^{\alpha\alpha}(\mathbf{k})$, $\alpha = \uparrow$ or $\downarrow$) has been given in Ref. 14, the tight-binding parameters are listed in Table I of Ref. 14, and the renormalized spin-orbit splittings of the anion and cation p states (e.g., $\Delta_N = 9$ meV and $\Delta_{Al} = 24$ meV) in $H_{SO}(\mathbf{k})$ have been reported in Refs. 10 and 11. In this letter, only the results for AlN will be shown as an example for studying the Dresselhaus effect.

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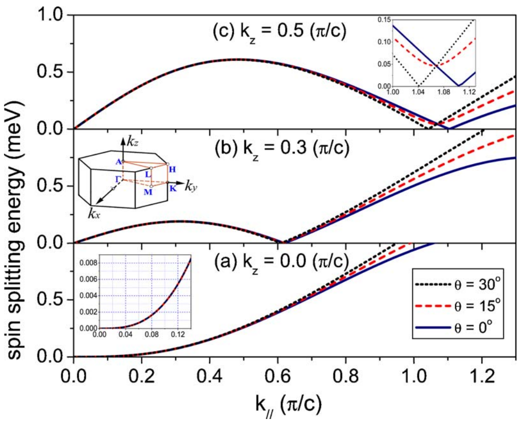

FIG. 1. (Color online) Spin-splitting energy as a function of $k_\parallel$ for $\theta=0°$, 15°, and 30° on the planes of (a) $k_z=0$, (b) $k_z=0.3\pi/c$, and (c) $k_z=0.5\pi/c$ using the LCAO method. The first Brillouin zone with symmetry points is shown in the inset of (b).

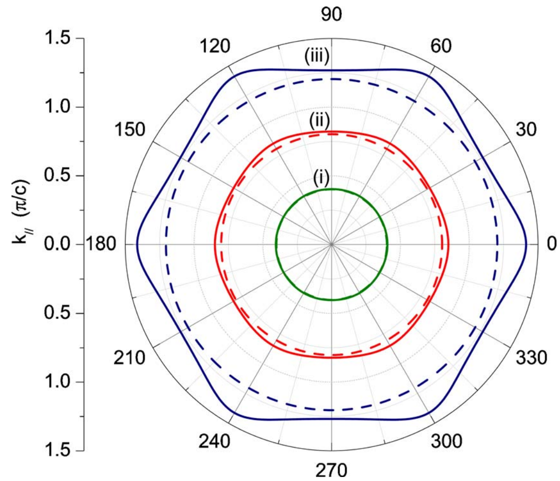

FIG. 2. (Color online) Projections of the minimum spin-splitting surface (solid lines) and the reference spin-degenerate surface $k_\parallel^2=4.028k_z^2$ (dash lines) onto the planes of (i) $k_z=0.2\pi/c$, (ii) $k_z=0.4\pi/c$, and (iii) $k_z=0.6\pi/c$.

Figure 1 shows the absolute values of the spin-splitting energy (i.e., $|\delta E(k_\parallel,\theta,k_z)|$) as a function of $k_\parallel$ for $\theta=0°$, 15°, and 30° in the planes of (a) $k_z=0$, (b) $k_z=0.3\pi/c$, and (c) $k_z=0.5\pi/c$. It is seen that in each k_z plane, the three curves ($\theta=0°$, 15°, and 30°) are strongly θ dependent for $k_\parallel>0.9\pi/c$. However, as $k_\parallel$ decreases, they become less θ dependent. They even become nearly θ independent when $k_\parallel<0.6\pi/c$. These imply that the LCAO Hamiltonian exhibits a sixfold symmetry at large $k_\parallel$ but exhibits a circular-symmetry-like behavior at small $k_\parallel$. We refer to this phenomenon as the wurtzite rotation symmetry (WRS) effect. The most interesting phenomenon found in Fig. 1 is that each curve exhibits a MSS point located at $k_\parallel^{\mathrm{MSS}}(k_z,\theta)$ [note that $k_\parallel^{\mathrm{MSS}}(0,\theta)=0$]. This means that a cone-shaped MSS surface exists in the ideal wurtzite Brillouin zone. The MSS surface can be regarded as a spin-degenerate surface because the spin splitting on the MSS surface is generally very weak. For the spin degeneracy, specifically speaking, there are 12 spin-degenerate lines on the MSS surface and they appear only when θ equals 0° and integer multiples of 30° [see inset of Fig. 1(c)]. Totally, there are 13 spin-degenerate lines in the Brillouin zone if the spin-degenerate line $\overline{\Gamma A}$ ($k_\parallel=0$) due to time-reversal symmetry is also included.

Figure 2 shows the projections of the MSS surface (solid lines) and the spin-degenerate surface of $k_\parallel^2-4.028k_z^2=0=\delta E$ (dash lines) onto the planes of (i) $k_z=0.2\pi/c$, (ii) $k_z=0.4\pi/c$, and (iii) $k_z=0.6\pi/c$. It is seen that the projections of the spin-degenerate surface (dashed lines) exhibit a circular-symmetry behavior, while the projections of the MSS surface (solid lines) exhibit a wurtzite-rotation-symmetry behavior . It is also seen that the dash line and solid line are nearly identical at small k_z [see Fig. 2(i)] but have significant difference at large k_z [see Fig. 2(iii)]. These indicate that the hexagonal-cone-shaped MSS surface can be well described by a circular-cone-shaped spin-degenerate surface (i.e., $bk_z^2-k_\parallel^2=0=\delta E$, $b=4.028$) when k_z is not too large due to the WRS effect. The existence of the spin-degenerate surface $bk_z^2-k_\parallel^2=0$ implies that the spin-splitting energy δE near the Γ point can be written in the form of $\delta E=2\gamma_{\mathrm{wz}}k_\parallel(bk_z^2-k_\parallel^2)$, in which $\delta E=k_\parallel=0$ represents the spin-degenerate line $\overline{\Gamma A}$. When the spin directions are also taken into account,[7,18] the spin-orbit component of the two-band $\boldsymbol{k\cdot p}$ Hamiltonian H_{SO} (**k**) can be written as

$$H_{\mathrm{SO}}(\mathbf{k}) = \gamma_{\mathrm{wz}}(bk_z^2-k_\parallel^2)(\sigma_x k_y-\sigma_y k_x). \qquad (2)$$

Here the spin directions are determined by examining the conduction-band eigenvectors of the LCAO Hamiltonian. The value of γ_{wz} evaluated from the $k_\parallel^3$-dependent curve in the inset of Fig. 1(a) is about 0.74 meV Å^3. This confirms that in the nearest-neighbor LCAO model, ideal wurtzite structure yields the cubic-k terms of $\gamma_{\mathrm{wz}}(bk_z^2-k_\parallel^2)(\sigma_x k_y-\sigma_y k_x)$ in the two-band $\boldsymbol{k\cdot p}$ Hamiltonian. This phenomenon is referred to as the Dresselhaus effect in bulk wurtzite. Note that in the above equation [Eq. (2)], the high-order terms have been neglected. When the high-order terms are also taken into account, the spin-degenerate surface will become a MSS surface. The coefficients b for some other ideal wurtzite materials (b^β, β=ZnO, CdS, CdSe, and ZnS) were also calculated. It is interesting to find that $\sqrt{b}$ is nearly equal to the ratio of the average length of $\overline{\Gamma M}$ and $\overline{\Gamma K}$ to $\overline{\Gamma A}$ [see inset of Fig. 1(b)] for all the wurtzite materials (i.e., $\sqrt{b}\approx(\overline{\Gamma M}+\overline{\Gamma K})/(2\overline{\Gamma A})=2.032$). This means that the Dresselhaus effect mentioned above is valid for all the wurtzite materials.

From the above discussions, we conclude that the Dresselhaus effect yields the cubic-k terms shown in Eq. (2), and therefore, produces a cone-shaped MSS surface in the Brillouin zone. When the WSIA effect is also taken into account in Eq. (2), the two-band $\boldsymbol{k\cdot p}$ Hamiltonian becomes $H_{\mathrm{SO}}(\mathbf{k})=[\alpha_{\mathrm{wz}}-\gamma_{\mathrm{wz}}(k_\parallel^2-bk_z^2)](\sigma_x k_y-\sigma_y k_x)$, where α_{wz} is the WSIA coefficient. This explains why the WSIA effect (s-p_z mixing at $k=0$) can change the shape of the MSS surface. As shown in Fig. 3, the MSS surface for real wurtzite AlN has a shape of hexagonal hyperboloid of two sheets [Fig. 3(b)], but the MSS surface for ideal wurtzite AlN has a shape of hexagonal cone [Fig. 3(a)]. Here the band structures for real wurtzite AlN are obtained by differentiating the bond in the [001] direction from three other bonds.[19] Certainly, the MSS surface will have a shape of hexagonal hyperboloid of one sheet if $\alpha_{\mathrm{wz}}/\gamma_{\mathrm{wz}}>0$ [Please refer to Fig. 1(a) of Ref. 16.]. If the WSIA effect (e.g., strain induced WSIA effect) is extremely strong, the MSS surface may be completely eliminated. The strong coupling between the conduction bands (e.g., $\Delta_{C1}-\Delta_{C3}$ coupling[12] in GaN) should also have significant influence on the shape of the MSS surface. Its influence

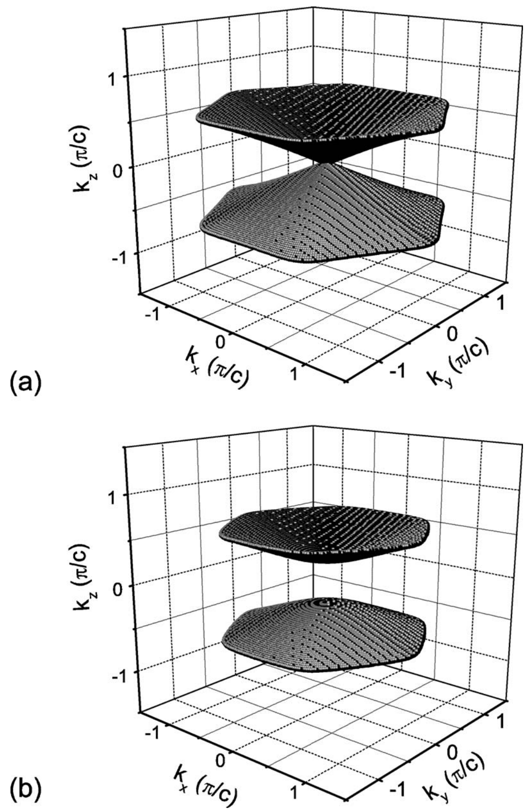

FIG. 3. Three-dimensional plot of the minimum spin-splitting surface for (a) ideal wurtzite and (b) real wurtzite in k space for various k_z's.

is currently under investigation using the second-nearest-neighbor LCAO method and will be reported in the near future. The spin splitting energies for real wurtzite AlN were also calculated using the local-density approximation (LDA) of the density-functional theory (DFT). The DFT-LDA results confirm the fact that the MSS surface for real wurtzite AlN has a shape of hexagonal hyperboloid of two sheets.

In the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ model, the 2D wurtzite Hamiltonian can be written as[7,18]

$$H_{\mathrm{IA}}(\mathbf{k}) = [\alpha_{\mathrm{IA}} - \gamma_{\mathrm{wz}}k_{\parallel}^2](\sigma_x k_y - \sigma_y k_x), \tag{3}$$

and the effective spin splitting becomes $\delta E(k)=2[\alpha_{\mathrm{IA}}k_{\parallel} - \gamma_{\mathrm{wz}}k_{\parallel}^3]$. Here $\alpha_{\mathrm{IA}}=\alpha_R+\alpha_{\mathrm{BIA}}$, $\alpha_{\mathrm{BIA}}=\alpha_{\mathrm{wz}}+\gamma_{\mathrm{wz}}b\langle k_z^2\rangle$, and α_R is the Rashba coefficient. Clearly, a spin-degenerate Fermi surface given by $\alpha_R+\alpha_{\mathrm{BIA}}-\gamma_{\mathrm{wz}}k_F^2=0$ can be achieved in 2DEGs of wurtzite heterostructures by varying $k_{\parallel}$ (e.g., carrier concentration), α_R (e.g., gate voltage), α_{wz} (e.g., crystal field or strain), and $b\langle k_z^2\rangle$ (e.g., quantum well width). These phenomena indeed have been partly observed in the experiments.[15,16] The 2D [001]-grown wurtzite Hamiltonian is indeed very similar to the 2D [111]-grown zinc-blende Hamiltonian, except that the former does not have the σ_z component of the k^3 terms [i.e., $\gamma(3k_x^2-k_y^2)k_y\sigma_z/\sqrt{6}$ as shown in Eq. (9) of Ref. 4, where z is oriented along the growth direction]. The Dresselhaus effect yields a σ_z component of the k^3 terms in 2D [111] zinc-blende Hamiltonian but not in 2D [001] wurtzite Hamiltonian because the wurtzite crystals have a sixfold rotation [001]-axis symmetry but the zinc-blende crystals have a threefold rotation [111]-axis symmetry. Thus, we suggest that the [001] wurtzite QWs (e.g., GaN/AlN) are also the potential candidates for spintronic devices such as the RSL transistor,[2,3] in addition to the [111] zinc-blende QWs.[4,5] Note that, due to our calculations, the three spin lifetime components all show a resonant behavior in [001] wurtzite QWs, when the Fermi surface is spin degenerate.[5] This reveals the importance of the Dresselhaus effect, because it generates a spin-degenerate surface near the Γ point in the wurtzite Brillouin zone. The spin-degenerate Fermi surface, which has been observed in the n-type GaN QWs,[16] is also expected to be observed experimentally in the p-type GaAs QWs.[20]

In conclusion, the Dresselhaus effect in ideal bulk wurtzite has been investigated using the nearest-neighbor scheme of the LCAO method. It is demonstrated that the Dresselhaus effect yields a hexagonal-cone-shaped MSS surface in the ideal wurtzite Brillouin zone. The hexagonal-cone-shaped MSS surface can be regarded as circular-cone-shaped spin-degenerate surface in the vicinity of the Γ point. This indicates that the k^3 terms generated by the Dresselhaus effect can be written as $\gamma_{\mathrm{wz}}(bk_z^2-k_{\parallel}^2)(\sigma_x k_y-\sigma_y k_x)$ $(b\approx 4)$ in the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian. The Dresselhaus effect yields a spin-degenerate surface in bulk wurtzite but not in bulk zinc blende, simply because the wurtzite crystals (sixfold rotation [001] axis) have a higher rotation symmetry than the zinc-blende crystals (threefold rotation [111] axis). The existence of the spin-degenerate surface makes the [001]-wurtzite QW (e.g., GaN/AlN) a potential candidate for spintronic devices such as the RSL transistor.

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