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Wave vector dependent Rashba coefficient and nonlinear Rashba spin splitting in AlGaN/GaN quantum wells

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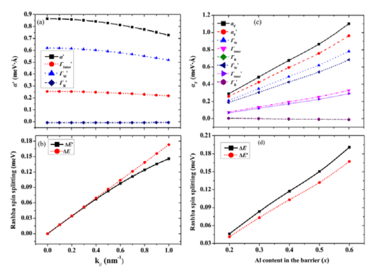
HIGHLIGHTS

- We study the wave vector dependent Rashba coefficient in AlGaN/GaN QWs.
- The nonlinear Rashba spin splitting in AlGaN/GaN QWs are calculated.
- The results obtained from the linear and nonlinear Rashba model are compared.
- The corrections to α and ΔE at the Fermi level in $Al_xGa_{1-x}N$/GaN QWs increase with x.

GRAPHICAL ABSTRACT

The corrected Rashba coefficient and Rashba spin splitting for the first subband of AlGaN/GaN QWs as a function of $k_{//}$ and x.



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ABSTRACT

By considering the energy dispersion of the conduction subband, we found the corrected Rashba coefficient (α') in AlGaN/GaN quantum wells (QWs) decreases with the in-plane wave vector $k_{//}$, and the corrected Rashba spin splitting ($\Delta E'$) increases nonlinearly as a function of $k_{//}$. Moreover, the correction to the Rashba spin splitting also increases with $k_{//}$, since the ratio of the kinetic energy in the effective band gap increases. The effect of energy dispersion on the correction to the Rashba spin splitting will be greater for large in-plane wave vectors and materials with narrow band gap. Although the band gap of the barrier increases with Al content (x), we found the corrections to the Rashba coefficient and Rashba spin splitting at the Fermi level in $Al_xGa_{1-x}N$/GaN QWs increase with x, since the expansion region of the envelope functions decrease, and the polarized electric field in the well increases rapidly.

1. Introduction

The use of the spin degree of freedom in the semiconductor technology is a most attractive idea for potential technological applications in spintronic devices. Since the proposal of the Datta–Das spin transistors [1], there are a large amount of experimental and theoretical investigations of spin related phenomena in artificial structures [2–13]. In combination with bulk inversion asymmetry (BIA) [14] and structural inversion asymmetry (SIA) [15] of semiconductor heterostructures, the spin–orbit interaction lift the spin degeneracy of the energy spectrum, namely, the zero field spin splitting [10].

It is known that the Rashba spin–orbit interaction due to SIA decreases as the band gap increases. However, theoretical work has shown that in a system with an asymmetric potential, the Rashba spin splitting at the Fermi level are related to the average electric field [12,15–17] and also the sheet carrier density (the Fermi wave vector) [3,6,7,10,18]. The strong polarization electric field and high density of 2DEG in wide-gap AlGaN/GaN heterostructures compensate for the relative smallness of the Rashba coefficient and make the Rashba spin splitting at the Fermi level in AlGaN/GaN QWs comparable to that of narrow-gap III–V materials, such as 1 meV for the InAlAs/InGaAs QW [10,19–21].

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According to the previous analytical models [12,17,22], the Rashba coefficient is not directly related to the in-plane wave vector $k_{//}$, and the Rashba spin splitting increases linearly with $k_{//}$, which is called linear Rashba model and has been used in describing the spin-related properties of semiconductor structures. However, recent numerical calculations and experiments found that the Rashba spin splitting in narrow-gap semiconductor QWs varies nonlinearly as a function of $k_{//}$ [9,23,24]. Yang and Chang proposed a nonlinear Rashba model which can reproduce the nonlinear Rashba spin splitting in various narrow-gap QWs, and found that this nonlinear behavior originates from the decrease of the interband coupling between the conduction band and the valence bands considering the energy dispersion of the conduction subband [25], and they also found that the strong nonlinear behavior of the Rashba spin splitting in HgTe QWs leads to the resonance of the spin Hall conductivity [26].

In recent years, many theoretical work calculated the Rashba spin–orbit (SO) parameters in the AlGaN/GaN heterostructures using the linear Rashba model, and the calculated Rashba spin splitting is a linear function of the wave vector [10,18,21]. In this paper, by considering the dispersion of conduction subband, we explore the wave vector dependent Rashba coefficient and the nonlinear Rashba spin splitting in the wide band gap AlGaN/GaN QWs, and study how the corrected Rashba coefficient and Rashba spin splitting at the Fermi level vary as a function of Al content in the barrier (x), and compare them with corresponding original results.

2. Theory and model

By eliminating the three valence band components of the envelope functions, the eight-band Kane Hamiltonian is projected into the 2×2 conduction band space [21,22], and the Rashba coefficient for the nth subband of the QWs can be written as [10,27–29]

$$\alpha_n = P_1P_2\left\langle \frac{\partial \beta}{\partial z}\right\rangle = P_1P_2[\Phi_n^2(0)(\beta_W-\beta_L)-\Phi_n^2(L)(\beta_W-\beta_R) + \langle n|B_LF_L|n\rangle_L + \langle n|B_WF_W|n\rangle_W + \langle n|B_RF_R|n\rangle_R], \tag{1}$$

$$\beta = \frac{\Delta_3}{(E_v-\varepsilon_n)(E_v-\varepsilon_n+\Delta_1-\Delta_2)-2\Delta_3^2}, \quad B = \frac{\Delta_3[2E_g+\Delta_1+3\Delta_2+2(\varepsilon_n-V)]}{\{(E_v-\varepsilon_n)(E_v-\varepsilon_n+\Delta_1-\Delta_2)-2\Delta_3^2\}^2}. \tag{2}$$

E_c and E_v are the conduction edge and the valence edge at Γ point after the strain, respectively [21]. V includes the conduction band offsets and the electrostatic potential, and F is the space-dependent electric field. 0 and L denote the positions of the left and right heterointerfaces, respectively. The confined energy level ε_{n0} and the envelope function Φ_n are determined by solving the Schrodinger and Poisson equations with the finite difference method [30]. Δ_1 [(22–80x) meV] is the spin–orbit split-off energy [31], and $\Delta_{2,3}$ (6.0 meV) are the crystal-field split energy [32]. P_1 and P_2 are interband momentum matrix elements, and $P_1=P_2=\hbar\sqrt{E/2m_0}$ (E=20 eV) [10]. Finally, the magnitude of the Rashba spin splitting for the nth subband can be written as $\Delta E_n = 2\alpha_n k_{//}$ [10].

If we set $\varepsilon - V = 0$ and ignore the wave function penetration into the barriers, we will obtain the Rashba coefficient contributing from the well [10,18]

$$\alpha = \frac{P_1P_2\Delta_3[2E_g+\Delta_1+3\Delta_2]e\langle E\rangle}{\{(E_g+\Delta_1+\Delta_2)(E_g+2\Delta_2)-2\Delta_3^2\}^2}. \tag{3}$$

Further, if we adopt the parameters of the zinc-blende structure ($\Delta_1=0,\ \Delta_2=\Delta_3=\frac{1}{3}\Delta,\ m_t^*=m_z^*=m^*,\ P_1=P_2$), we recover the Rashba coefficient of the zinc-blende structure in Ref. [12]

$$\alpha = \frac{\hbar^2}{2m^*}\frac{\Delta}{E_g}\frac{2E_g+\Delta}{(E_g+\Delta)(3E_g+2\Delta)}eE. \tag{4}$$

Both the Rashba coefficient in Eqs. (3) and (4) are independent of $k_{//}$. Moreover, if the energy of electrons (ε_n) in Eq. (2) is substituted by the subband edge ε_{n0} [10,18,21], the Rashba coefficient (α) will also be independent of $k_{//}$, and the Rashba spin splitting (ΔE) will increase linearly as a function of $k_{//}$. However, if we consider the energy dispersion of the conduction subband and take $\varepsilon_n = \varepsilon_{n0} + (\hbar^2 k_{//}^2/2m^*)$ in Eq. (2), the corrected Rashba coefficient (α') will depend on $k_{//}$, and the corrected Rashba spin splitting ($\Delta E'$) will increase nonlinearly as a function of $k_{//}$.

We can see from Eq. (2) that it is the effective band gap $E_g^{eff} = E_g + \varepsilon_n$, instead of the bare band gap E_g that directly determining the magnitude of the Rashba spin splitting. Therefore, strictly speaking, the Rashba spin splitting is intrinsically a nonlinear function of $k_{//}$ [25]. If the energy dispersion of subband is neglected, the Rashba coefficient and the Rashba spin splitting will be overestimated, especially for large $k_{//}$ and materials with narrow band gap.

3. Results and discussion

In this section, to explore the effect of the energy dispersion of the conduction subband or the kinetic energy of electrons on the Rashba SO interaction in QWs, first we calculate the corrected Rashba coefficient and Rashba spin splitting in the $Al_{0.5}Ga_{0.5}N/GaN$

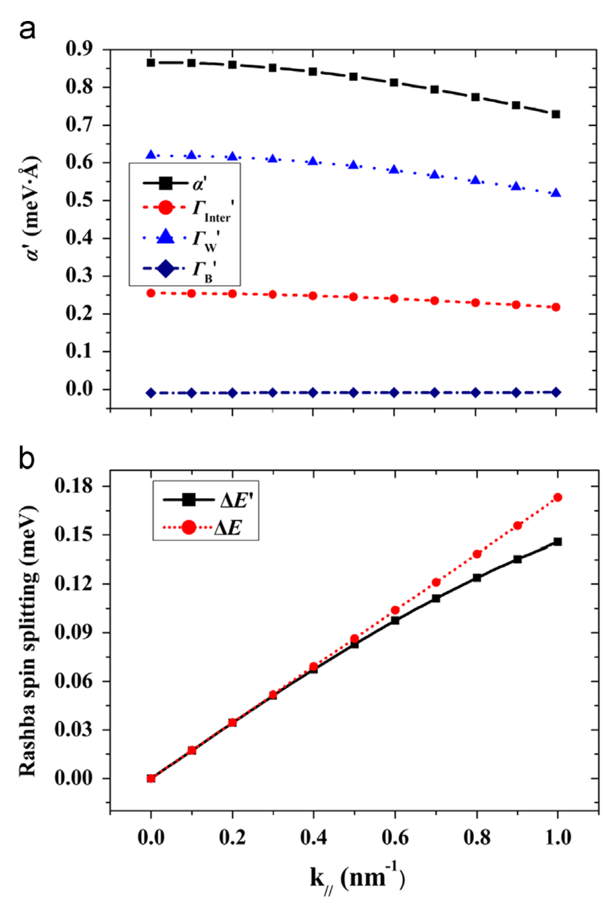

Fig. 1. (a) The corrected Rashba coefficient (α') for the first subband of the $Al_{0.5}Ga_{0.5}N/GaN$ QW, and the contributions from the interface (Γ'_{Inter}), the well (Γ'_W), and the barrier (Γ'_B); (b) The original and the corrected Rashba spin splitting (ΔE and $\Delta E'$).