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# First principles study of spin-electronics: Zero-field spin-splitting in superlattices

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**Abstract** We present first-principles calculations of the fundamental coupling mechanisms that give rise to spin-splittings of the electronic energy bands in semiconductors at zero magnetic field. We show that these effects are induced by asymmetric chemical bonds in heterostructure interface layers but are neither caused nor influenced by macroscopic electric fields such as charge depletion or piezoelectric fields, in contrast to widely accepted notions. The k-linear Rashba coupling is found to be negligible for GaAs/AlAs heterostructures and superlattices.

## 1 Introduction

Zero-field spin-splittings of electronic band edge states near III-V heterostructure interfaces are an important ingredient for the realization of spin-transistors [1,2] and have been observed mostly near interfaces [3,4]. It is well established by now (see [5] for an excellent review) that there are two mechanisms that give rise to splittings of band edge Kramer pair states that are linear in the Bloch wave vector, namely the Dresselhaus effect or bulk inversion asymmetry (BIA) [6] and the Rashba effect [7,8] or structure inversion asymmetry (SIA) [5,6,8,9]. However, the physical origin of the latter, i.e. its magnitude and the relevance and role of macroscopic electric fields and strain has remained controversial [5]. No quantitative calculations of BIA plus SIA effects beyond semi-empirical k·p-theories have been published so far.

## 2 Results and discussion

We have studied the spin splitting of conduction and valence bands by performing first-principles local density functional calculations of pseudomorphic AlAs/s-GaAs and InP/s-AlSb superlattices with [001] and [111] growth orientation. The latter orientation gives rise to large built-in piezoelectric fields. These allow us to study the effect of macroscopic fields on the spin-splittings. Within the first-principles total-energy pseudopotential method [10], we have generated fully relativistic, separable pseudopotentials [11] and determined the ground state energy by minimizing the electronic and ionic degrees of freedom simultaneously. The band structure of superlattices has been calculated with a preconditioned conjugate gradient algorithm that allowed us to include up to 25000 plane waves.

### *2.1 Effective Hamiltonian*

The zero-field spin splitting of a nondegenerate (Kramers doublet) band edge state can be characterized by an effective spin Hamiltonian $H = \boldsymbol{\sigma}\cdot\mathbf{B}_{eff}(\mathbf{k}_{\|})$ [6] where $\boldsymbol{\sigma}$ is the Pauli matrix vector and $\mathbf{k}_{\|}$ is the lateral wave vector. The magnitude and the direction of the effective field $\mathbf{B}_{eff}$ is determined by symmetry and depends on $\mathbf{k}_{\|}$ and the considered band state but we omit the latter label for brevity. The spin splitting of a Kramers pair near $\Gamma$ is then given by $\Delta E_{spin}(\mathbf{k}_{\|}) = 2|\mathbf{B}_{eff}(\mathbf{k}_{\|})|$ and contains a term linearly proportional to $\mathbf{k}_{\|}$. Generally, the effective magnetic field term can be written as $\mathbf{B}_{eff} = \mathbf{B}_R + \mathbf{B}_B$, where the Rashba or SIA term equals $\mathbf{B}_R = \alpha_R\, \mathbf{k} \times \mathbf{n}$ ($\mathbf{n}$ is the unit vector along the growth direction) and the bulk Dresselhaus or BIA term (see e.g. [5,6]) equals $\mathbf{B}_B = \alpha_B(-k_x, k_y, 0)$ and $\mathbf{B}_B = \alpha_B(k_y - k_z, k_z - k_x, k_x - k_y)$ for the [001] and [111] growth directions, respectively. For the [111] growth direction, $\mathbf{B}_B$ and $\mathbf{B}_R$ are parallel to each other and one obtains $\Delta E_{spin}(\mathbf{k}_{\|}) = 2\,|\mathbf{k}_{\|}\,(\alpha_R + \alpha_B)|$ independently of the direction of $\mathbf{k}_{\|}$. Thus, $\alpha_R$ and $\alpha_B$ cannot be determined separately in an ab-initio calculation., For the [001] growth direction, on the other hand, the spin splitting is $\Delta E_{spin} = 2\,|\mathbf{k}_{\|}|\,[\alpha_B^2 + \alpha_R^2 - 2\alpha_B\alpha_R\sin(2\theta)]^{1/2}$ and depends on the angle $\theta$ between $\mathbf{k}_{\|}$ and [100] which allows a separate determination of $\alpha_R$ and $\alpha_B$.

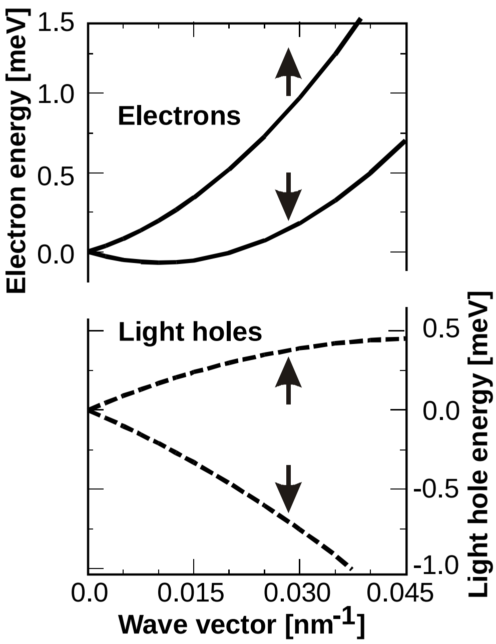


**Fig. 1** Calculated dispersion relations for lowest conduction and light hole bands near the $\Gamma$ point for a [111] $(AlAs)_3(GaAs)_3$ superlattice as a function of the lateral wave vector.

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*2.2 AlAs/GaAs superlattices*

We first consider strained layer short-period AlAs/s-GaAs superlattices and depict in Fig.1 the 2 lowest conduction and top light hole bands very close to the Γ-point . The two lowest conduction bands in both [001] and [111] superlattices have predominantly Γ-character with some mixing of X and L states, respectively. In contrast to the [001] superlattice, the lower symmetry in the biaxially strained [111] superlattice induces a macroscopic field that we find to be equal to 0.5 MV/cm (see Fig. 2).

In the [001] $(AlAs)_3(GaAs)_3$ superlattice, our analysis of the linear-k spin splittings yields $\alpha_B$ = 0.034 eVÅ and $\alpha_R$ = -0.002 eVÅ for the lowest conduction band. These values change only weakly for longer superlattice periods; we find $\alpha_B$ = 0.029 eVÅ and $\alpha_R$ = -0.001 eVÅ in an $(AlAs)_6(GaAs)_6$ superlattice. This extremely small Rashba term originates in the interface-induced microscopic structural asymmetry.

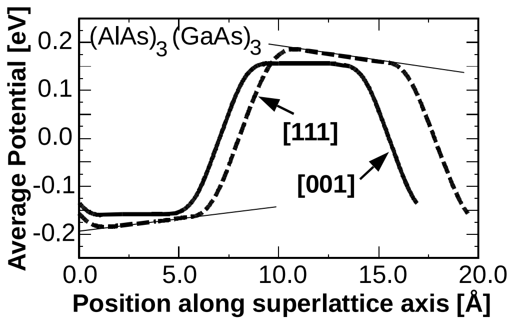


**Fig. 2** The macroscopic average of the electrostatic potential in $(AlAs)_3(GaAs)_3$ [001] and [111] superlattices along the superlattice axis. The thin lines guide the eye to show the macroscopic electric field. The potential change across the interface corresponds to the dipole contribution to the valence band offset. Note that the atomic distances differ for [111] and [001].

In the [111] $(AlAs)_3(GaAs)_3$ superlattice, on the other hand, the sum $\alpha_R+\alpha_B$ = 0.13 eVÅ is much larger for the lowest conduction band. This large difference is caused by pronounced band folding effects in the short-period [111] superlattice and originates in the mixed Γ and Λ character of the lowest conduction band. Indeed, in bulk GaAs, we find $\alpha_R+\alpha_B$ = 0.20, 0.15, and 0.135 eV Å for **k** = 1/3L, 2/3L, and the L-point, respectively. The values in AlAs are slightly smaller. The macroscopic electric field can be altered by varying the lateral lattice constant and has only a small effect on this result, consistent with the detailed results given below. In the absence of band folding - such as in a single GaAs/AlAs heterostructure - we thus find the Rashba-coupling to be negligible, irrespective of the presence or absence of any macroscopic electric field.

*2.3 InP/AlSb superlattices*

To further investigate the role of the interface asymmetry versus macroscopic field, we have performed calculations for lattice matched [001] and [111] InP/s-AlSb superlattices. Contrary to the AlAs/GaAs system, the bulk constituents share no common elements in this case which, by symmetry, leads to a macroscopic electric field even in the [001] case. Quantitatively, this macroscopic field is about 2 MV/cm for the unrelaxed $(InP)_3(AlSb)_3$ superlattice but becomes nearly zero once the atoms are allowed to relax so as to minimize the total crystal energy. For the lowest conduction band (which has dominantly InP-type Γ-character), we find $\alpha_B$ = 0.11 and $\alpha_R$ = 0.015 eVÅ for the unrelaxed case with the high electric field. In the relaxed case, where the field is almost zero, $\alpha_R$ = 0.10 eVÅ becomes larger whereas $\alpha_B$ remains unchanged. This result clearly shows that the microscopic arrangement of atoms at the interface, rather than the macroscopic field, determines the magnitude of Rashba effect.

In the [111] $(InP)_3(AlSb)_3$ superlattice, the piezoelectricity of the strained AlSb leads to a strong macroscopic electric field also in the relaxed superlattice. Nevertheless, we find $\alpha_B + \alpha_R$ = 0.10 eVÅ for the lowest conduction band which implies a smaller value for the linear-k spin splittings than for the [001] superlattice.

*2.4 Rashba effect in strained bulk*

Finally, we have calculated the strain dependence of the Rashba coupling in bulk AlSb in order to analyze the strain and interface induced linear-k splitting separately. For the first conduction band in tetragonally strained bulk AlSb, we find a very small $\alpha_R^{001} = (1/2)C_4' \mid e_{xx} - e_{zz} \mid$ with the constant $C_4'$ = 0.077 eVÅ. In [111]-strained AlSb, we predict a value of $\alpha_R = C_3 e_{xy}/2$, with $C_3$=6.3 eVÅ. This result depends sensitively on the (self-consistently calculated) internal strain parameter. In fact, $C_3$ decreases by 30% if the internal strain parameter is set to zero. This additionally confirms the Rashba effect to be controlled by microscopic bonding asymmetries rather than by macroscopic fields.

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