Strain Induced $k$-Linear Spin Splitting in III-V semiconductors

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We present first-principles studies of the zero field spin splitting of energy bands in typical III-V semiconductors. Our calculations reveal that the strain induces linear-$k$ spin splitting in the conduction and valence bands in the neighborhood of $\Gamma$ point. The effective Hamiltonian for description of the linear-$k$ spin splitting in the conduction band contains two terms (i) first corresponding to the reduction of the cubic symmetry to the tetragonal one, (ii) the second contribution that is responsible for the reduction of the cubic symmetry to the uniaxial one. These two terms in the effective Hamiltonian are proportional to the linear combinations of the strain tensor components that guarantee required symmetry and to one material constant each. We determine the two material constants in the effective Hamiltonian by comparing of the spin splitting obtained from the ab initio calculations with the analytic solutions of the effective Hamiltonian. We consider tetragonal, orthorhombic, and trigonal strains. In the case of cubic crystal subject to the orthorhombic and trigonal deformation, the position of the atoms in the unit cell is not determined by the symmetry. Therefore, we perform full optimization of unit cell geometry within the ab initio scheme and determine the so-called internal strain. We include this strain into the effective Hamiltonian. We are not aware of previous studies that take effects of the internal strain on spin splitting into account.

In our studies, we have employed the local density functional method (LDA) that we have implemented with fully relativistic pseudopotentials. This method reproduces the experimentally known zone-center split-off energies $\Delta_0$ in the valence band of bulk semiconductors very accurately.

Knowing the magnitudes of the material constants, one can design the suitable deformation of the crystal that would lead to the situation where the linear-$k$ spin splitting disappears. The most significant consequence of this configuration is that the spin lifetimes would be extended for any spin direction. We discuss such possibilities.

Along the same lines we discuss strain induced linear-$k$ spin splitting in valence bands. However, for the valence bands, the stress induced $k$-linear spin splitting is generally larger than in the conduction bands. Ab initio calculation of the spin splitting allows the determination of the higher order in $k$ terms in the effective Hamiltonian. We discuss here the third order terms just employing the effective Hamiltonian obtained through group analysis [1].