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k·p Hamiltonian and band structure fitting strategies applied to III-V semiconductors to determine interband momentum elements and spin-orbit interaction elements

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III-V type semiconductors are very important in technological applications, with GaAs as an example, second only to Si as the most used semiconductor. The physical properties of semiconductor materials can be studied through their band structures, which can be described using effective Hamiltonians. (1-2) Spin effects, such as increased degeneracy in the conduction band, occur due to bulk inversion asymmetry (BIA) and are essential in spintronic designs and g-factor anisotropy effects in multilayer materials. (3) Constructed using the k·p method, effective Hamiltonians have been used for several decades for a realistic description of band structures and have lower computational costs compared to first-principles methods. (1-2) Associated with Löwdin partitioning, these Hamiltonians use various numerical methods developed by the IFSC Computational Physics Laboratory at IFSC (LFC) to extract effective mass parameters by fitting previously calculated band structures. (1) This research makes use of group theory, with double group representations, using the symmetry properties of the crystalline group to be studied, associated with Löwdin partitioning and effective mass terms that go beyond zero order in the process of constructing the k·p Hamiltonian. The whole process aims to extract interband momentum parameters, P_1, P_2 and Q_0, by means of realistic fittings that describe the spin-splittings and that can result in realistic g-factor calculations. In addition to excellent fittings in regions far from the Γ point, up to 40% of the Brillouin zone, the method produced g-factor values very close to the experimental ones for AlAs, GaAs and InAs in zinc-blende crystaline structures. The versatility of band selection and weighting in the calculation processes allowed for better fitting, and consequently parameter values that avoid spurious solutions with control of the parabolicity of the bands, with steps that indicate that the method is suitable for use in high-throughput computing.

Palavras-chave: III-V semiconductor; k·p Hamiltonian; g-factor.

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