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Spin-orbit interaction and spin relaxation of conduction band electrons in Si and Ge¹

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Group IV element semiconductors, silicon and germanium, are promising material candidates in spintronics due to their intrinsic long electron spin lifetimes. To describe the spin properties of conduction electrons in these indirect band-gap multivalley semiconductors, the method of invariants is employed to build 8×8 (for Si) and 10×10 (for Ge) spin-dependent Hamiltonians that capture the symmetries of the zone edge states (X-point of Si [1] and L-point of Ge) and their spin dependent parameters. Concise expressions of the energy bands, and more importantly, of the spin mixed states are derived and verified by numerical results of an empirical pseudopotential method. These analytical state expressions are powerful tools to study the behavior of electron spins similar to the way that the Kane model is being used in direct band-gap semiconductors. Mechanisms of spin relaxation by electron-phonon scattering are studied based on this model. We reveal fundamental differences between spin and momentum relaxation mechanisms. In the case of silicon, intravalley spin flipping is governed by scattering with transverse acoustic (TA) phonons via the interband deformation potential that couples the upper and lower conduction bands (this deformation potential would also break the degeneracy of the conduction band at the X point if off-diagonal stress is applied). The intervalley g-process spin flipping couples the lowest conduction bands of different irreducible representations in opposite valleys via acoustic phonons; the intervalley f-process spin flipping, which is the dominant contribution of spin relaxation in a wide temperature range, couples the conduction and valence band components of the states by scattering with Σ_1 and Σ_3 phonons. In the case of germanium, intervalley spin-flip scattering, which is also the main contribution of spin relaxation, couples the lowest and upper conduction bands of different valleys by X-phonons. The intravalley spin flip scattering, which is about two orders of magnitude smaller, couples the conduction and valence bands mostly via TA phonons.

[1] Pengke Li and Hanan Dery, Phys. Rev. Lett. 107, 107203 (2011)

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