Valley Splitting and Spin Lifetime Enhancement in Strained Silicon Heterostructures

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Semiconductor spintronics is promising because it potentially allows creating data storages and processing elements that are smaller and consume less energy than present charge-based microelectronic devices. Silicon is an ideal material for spintronic applications due to the long spin lifetime in the bulk material. However, large spin relaxation was experimentally observed in gated silicon structures [1].

We investigate the spin relaxation in (001) silicon structures by taking into account surface roughness and phonon scattering. The surface roughness scattering matrix elements are assumed to be uncorrelated at different interfaces. They are proportional to the product of the corresponding subband wave functions derivatives at each interface [2]. Electron-phonon scattering is taken into consideration in the deformation potential approximation. To find the wave functions and matrix elements for spin relaxation we use the effective $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian written at the *X*-point for the two relevant valleys along the *OZ*-axis with the spin degree of freedom included [3]. We generalize the deformation potential theory to include the shear deformation potential and the deformation potential due to spin-orbit interaction responsible for spin relaxation in confined systems [4].

Including the valley coupling through the *Γ*-point [5] results in a subband splitting in relaxed structures [6]. The values of the valley splitting obtained from a 30-band $\mathbf{k}\cdot\mathbf{p}$ model [7] and tight-binding models [6,8] are summarized in Fig.1a. Although looking irregular, the data follow a certain law. By using the analytical expression for the valley splitting $\Delta E_C = \frac{2\pi^2 \Delta_\Gamma}{(k_0 t)^3} |\sin(k_0 t)|$ [3], where $2\Delta_\Gamma$=4eV is the splitting at *Γ* point, $k_0 = 0.85\frac{2\pi}{a}$, a is the lattice constant, and t is the film thickness, the 30-level $\mathbf{k}\cdot\mathbf{p}$ model data are well reproduced (Fig.1b). A comparison of the tight-binding model with the analytical expression (Δ_Γ=5.5eV) is shown in Fig.2a. Fig.2b shows the dependence of the spin relaxation matrix elements and the valley splitting as a function of shear strain ε_{xy}. The matrix elements display a strong increase at the strain values where the subband splitting is minimal. These points are the hot spots characterized by strong spin relaxation. For higher shear strain values the hot spots are pushed to higher energies (Fig.3a) from the subband minima. A strong increase of the spin lifetime with strain is demonstrated in Fig.3b. Thus, shear strain used to enhance mobility can also be used to increase spin lifetime.

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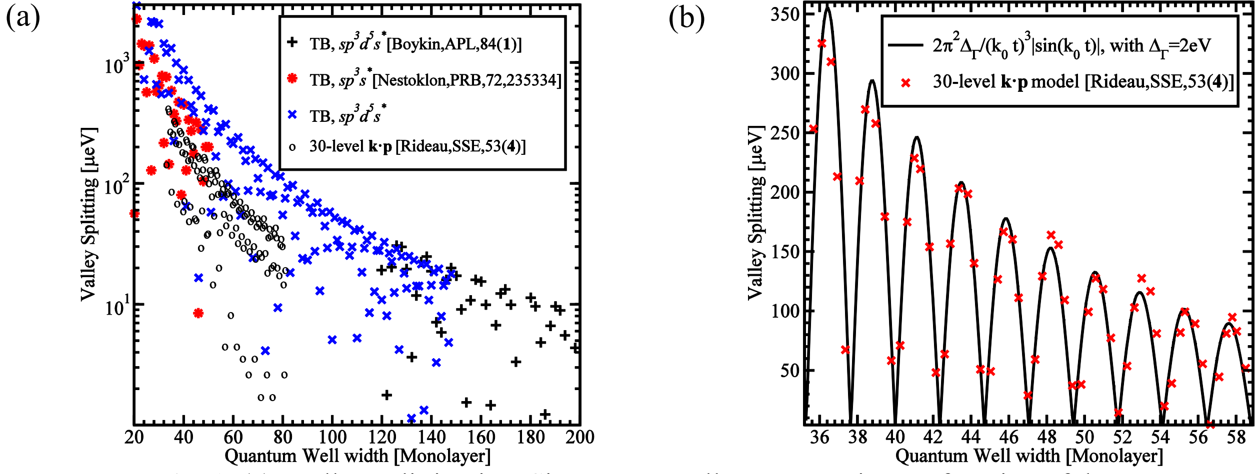

Fig. 1: (a): Valley splitting in a Si quantum well at zero strain as a function of the quantum well width including results from literature [6,7,8]; (b): Valley splitting for 30-band **k·p** [7] and analytical expression with Δ_Γ=2eV versus well width.

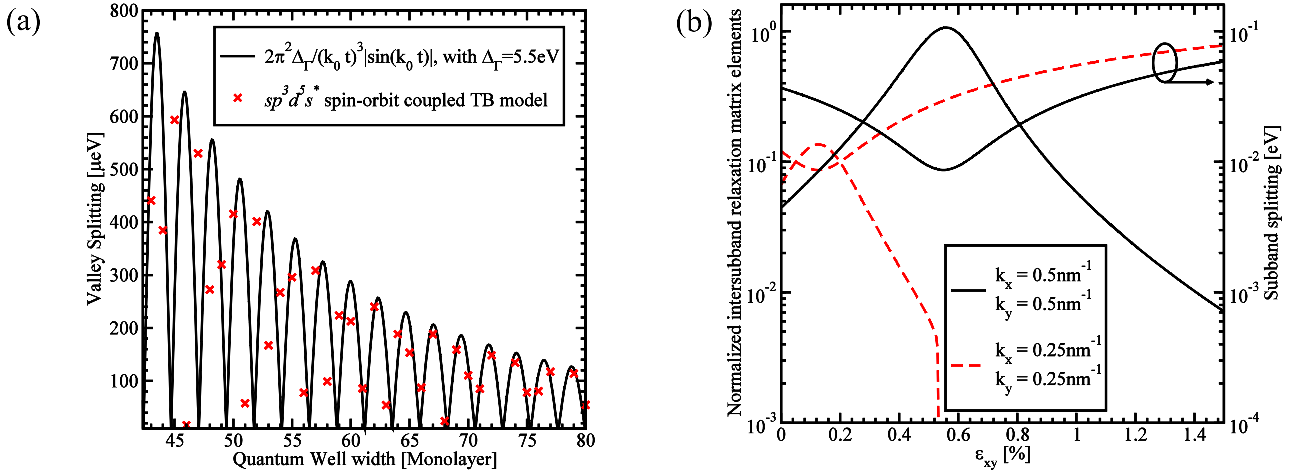

Fig. 2: (a): Dependence of the valley splitting on the quantum well width from the tight binding (TB) model and the analytical expression with Δ_Γ=5.5eV;
(b): Dependence of the intersubband spin relaxation matrix elements normalized on the intrasubband scattering matrix elements at zero strain and the lowest subband splitting on shear strain calculated with taking into account the zero-strain splitting.

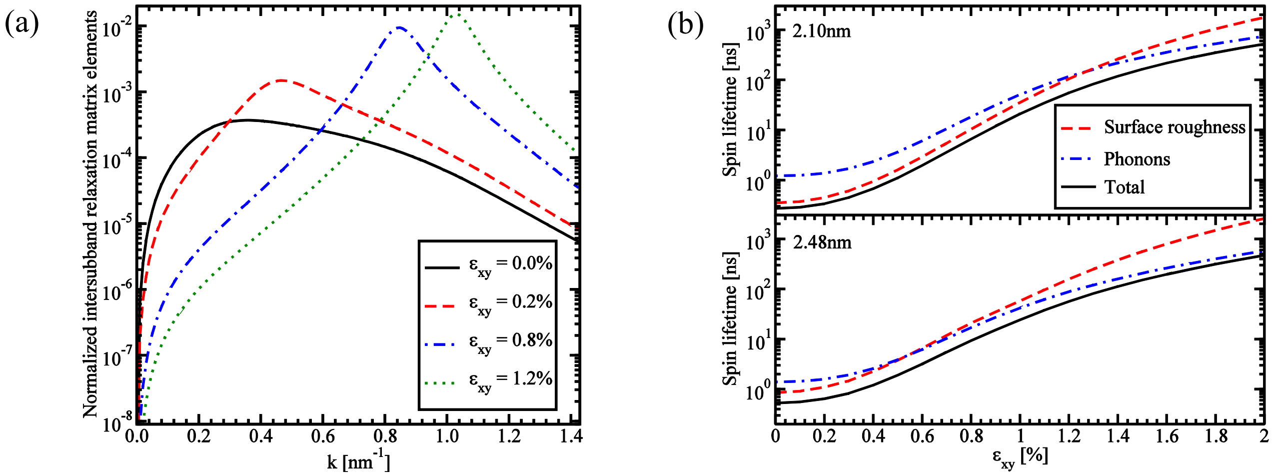

Fig. 3: (a): Normalized intersubband spin relaxation matrix elements as a function of the wave vector in [110] direction; (b): Dependence of total, phonon-, and surface roughness-limited spin lifetime on shear strain for two thickness values, T=300K, and electron concentration $2.59\cdot10^{12}$cm^{-2}.