Piezoresistance and the Drift-Diffusion Model in Strained Silicon

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Abstract

We have computed the strain-dependent tensorial mobility values for p-type Si based on a rigorous analysis of the valence band structure taking into account spin-orbit coupling effects. The mobilities, computed for not too large strain levels, are in agreement with the well known measured piezoresistance coefficients. Thus we now have a very convenient form of description for the drift-diffusion current density which can be incorporated in any device simulator.

1. Introduction

Mechanical strain can noticeably alter the carrier transport properties of silicon. Whilst on the one hand this can be usefully exploited for the realization of MEMS-based devices, it can have adverse effects on material characterization and on the operation of other microsensors as well as VLSI bipolar and MOS devices. For example, in Hall-based material characterization experiments, because of the strain-induced material anisotropy (resistivity, Hall coefficient) in the device, the values retrieved for the Hall mobility may not be meaningful. In magnetic sensors, the encapsulation-induced mechanical stresses and intrinsic stresses in the overlying conducting and dielectric thin films can affect the accuracy and long-term stability of the output response [1,2]. In trench-isolated VLSI technologies, there are regions of high stresses (see [3]) that can have undesirable effects on device characteristics and on device matching. Thus it has become imperative to account for the dependence of the various transport coefficients on strain for reliable prediction of device behavior.

2. Effects of strain on band structure in silicon

In general, the presence of mechanical strain alters the conduction and valence band structures by either shifting it in energy, distorting it, removing degeneracy effects, or any combination of the three. With n-type silicon, the

interpretation of the effects of strain are less involved since the conduction band to first order, only shifts in energy. Since the shape of the ellipsoids remain unaltered, the effective mass of each conduction band remains unaltered but the concentration of electrons in each band can be altered due to energy shifts. The resulting change in resistivity can be reduced to an effective mobility change [4].

The effects of strain on the valence band of silicon, however, are quite different due to its strongly degenerate nature. The shape of the valence band is altered resulting in change of the effective masses and mobility. In addition, the symmetry is reduced and the bands are shifted in energy. In view of the multitude of different effects, the piezoresistance in p-silicon is more dominant than in n-type silicon. Using **k.p** perturbation theory coupled with deformation potential theory, we have extended the analysis of [5] to include spin-orbit coupling effects in computation of the valence band structure [6]. The computed band structure is shown in Figs. 1 and 2. Figure 1 illustrates the energy spectra (E-k) in the [100] and [111] directions for the heavy hole (HH) band at zero stress, uniaxial stress (10^9 dynes/cm^2), and shear stress (10^9 dynes/cm^2). As expected, the stress introduces significant asymmetry and the bands become nondegenerate at $\mathbf{k} = 0$; the HH band moves upward and the light hole band (LH), although not shown, moves downwards. The energy shift associated with the light hole band is less pronounced in comparison to the HH band implying a larger proportion of the hole concentration in the HH band. The constant energy surfaces (taken at −15 meV from the top of the corresponding band) at zero stress and shear stress of 10^9 dynes/cm^2, are shown in Fig. 2. The band distortion with shear stress is the largest leading to the largest change in mobility, yielding also the largest piezoresistance coefficient (π_{44}).

3. Relation of strained mobility with piezoresistance

The dependence of mobility on stress can be computed using the expression

$$\mu_{ij} = [(q/h^2) \int d^3k\, \tau(E)\, (\partial E/\partial k_i)\, (\partial E/\partial k_j)\, (\partial f/\partial E)] \,/\, [\int d^3k\, f(E,E_f,T)] \qquad (1)$$

derived from the Boltzmann transport equation at low fields. Here, f is the distribution function, E is the distorted energy spectrum of the valence band, and τ is the relaxation time due to scattering events which are a function of the wavevector, k. Since the valence band is made up of predominantly the HH and LH bands, the computed mobility is a weighted sum of the individual mobilities in the corresponding bands. The mobility becomes highly directional-dependent and its variation with applied stress can be easily related to the well known piezoresistance coefficients that have been measured by Smith [7]. Here, the normalized change in resistivity ($\Delta\rho$) per unit stress was measured, and assuming a first order change in the resistivity with stress, the piezoresistance coefficients were retrieved. Since, the sample

was uniformly stressed, the global change in hole concentration can be assumed unaltered ($\Delta p = 0$) and the change in mobility can thus be expressed in terms of the piezoresistance coefficients, *viz.*,

$$\Delta\mu_{pij} / \mu_{po} = - \Delta\rho_{ij} / \rho_o = - \Sigma_{k,l} \pi_{ijkl} T_{kl} \tag{2}$$

where $\Delta\mu_{pij} / \mu_{po}$ is the normalized change in the mobility, π_{ijkl} is the tensor of piezoresistance coefficients, and T_{kl} are the components of the stress tensor. In view of cubic symmetry of silicon, there are only three distinct piezoresistance coefficients. Table 1 illustrates a comparison of the calculated (using eqns. (1) and (2)) and measured piezoresistance coefficients [7].

coefficient	calculated	measured
π_{11}	8	6.6
π_{12}	− 2	− 1.1
π_{44}	140	138.1

Table 1 Values shown are in units of 10^{-12} cm^2/dyne.

The calculated values shown in Table 1 are consistently larger in magnitude and this can be attributed to numerical errors arising from evaluation of the integrals over the entire (whole) energy surface that are required to compute the difference in mobility, $\Delta\mu_p$; at zero stress, the computations are simplified resulting in evaluation of integrals over just 1/8 of the total energy surface.

4. The strained drift-diffusion model

The diffusion coefficient, in the presence of stress, becomes a tensor and using Einstein's relation, $D_{pij} = (kT/q)\mu_{pij}$, we can express the standard isothermal drift-diffusion relation for the hole current density as

$$\mathbf{J_p} = - q \mathbf{D_p} [\text{grad } p + p \text{ grad } (q\psi/kT)] \tag{3}$$

which becomes modified, in the presence of a magnetic field, to read

$$\mathbf{J_p} - q p \mu_p [(\mathbf{R_H B}) \times \mathbf{J_p}] = - q \mathbf{D_p} [\text{grad } p + p \text{ grad } (q\psi/kT)]. \tag{4}$$

In eqns. (3) and (4), the transport coefficients $\mathbf{D_p}$, μ_p, and $\mathbf{R_H}$ are tensors, and $\mathbf{B}$ denotes the magnetic field vector. Equations (3) and (4) are valid only within the cubic cell coordinate system. They can be transformed to the Cartesian system of arbitrary orientation using a transformation matrix expressed in terms of the Euler's angles. In the absence of stress, the mobility, diffusion coefficient, and the Hall coefficient in eqn. (4) become scalars, and we recover the usual form of the galvanomagnetic transport equation in terms of the Hall mobility, μ_{Hp} (= $|qp\mu_p R_H|$). A relation for the electron current density can be obtained along similar lines.

References

[1] A. Nathan and T. Manku, Appl. Phys. Letts., vol. 62 (1993) 2947.
[2] H.P. Baltes and R.S. Popovic, Proc. IEEE, vol. 74 (1986) 1107.
[3] J.L. Egley and D. Chidambarrao, Sol.-St. Electron., vol. 36 (1993) 1653.
[4] C. Herring and Vogt, Phys. Rev., vol. 78 (1950) 173.
[5] G.E. Pikus and G.L. Bir, Soviet Physics-Technical Physics, (1958) 2194.
[6] T. Manku and A. Nathan, J. Appl. Phys., vol. 73 (1993) 1205.
[7] C.S. Smith, Phys. Rev., vol. 94 (1954) 42.

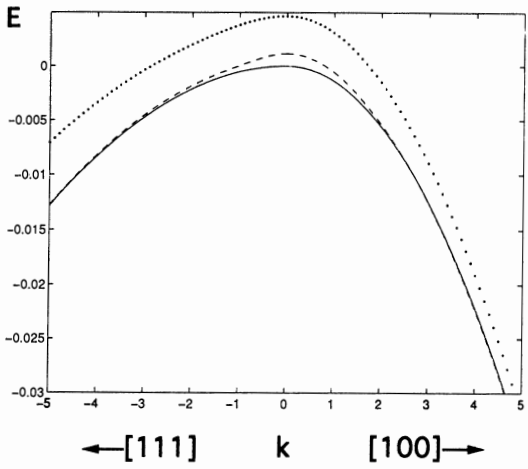

Fig. 1 Energy spectra for the heavy-hole (HH) band at zero stress (solid line), uniaxial stress (dashed line) and shear stress (dotted line).
The energy (E) is in eV and the wave-vector (k) in 10^8/m.

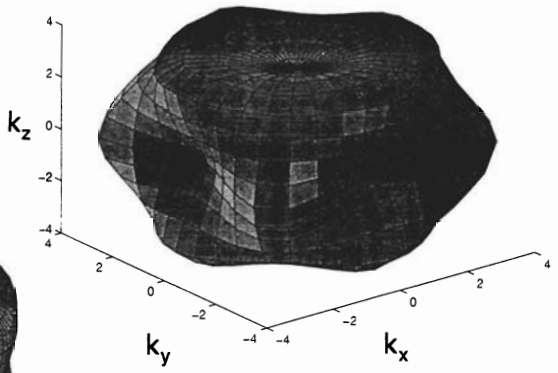

Fig.2a Constant energy surface of HH band at zero stress. Units of k are in 10^8/m.

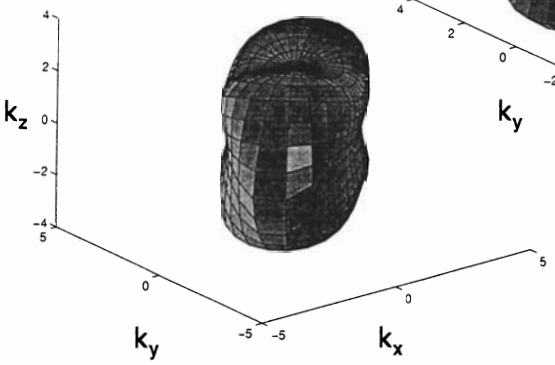

Fig.2b Constant energy surface of HH band under shear stress. Units of k are in 10^8/m.