Giant piezoresistance effect in p-type Silicon

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***Abstract* — This article presents a study of the giant piezoresistance effect in p-type silicon using full-band Monte Carlo simulation. This effect has been demonstrated experimentally in Si nanowires by He and Yang [1]. By introducing a law of variation of the surface potential according to the applied mechanical stress, we can reproduce this effect. The modulation of the width of the depletion region associated with the variation of surface potential induces a strong modulation of the total amount of carriers available for the conduction, which increases drastically this piezoresistive effect. This is probably the main origin of this effect, which may be used to achieve high performance MEMS sensors.**

I. INTRODUCTION

The piezoresistance is defined as the change in electrical resistance under the effect of mechanical stress [2]. Indeed, depending on its orientation with respect to the crystallographic direction, strain can induce major changes in the band structure of semiconductors and therefore in the carrier mobility [3-6]. This effect has been reported for the first time in the 50s by the group of Smith [2].

Recently, He and Yang have reported measurements of giant piezoresistance in p-type silicon nanowires, for diameters ranging from 50 to 350 nm. High piezoelectric coefficients (up to about 3500×10^{-11} Pa^{-1}) were obtained for structures of high resistivity (i.e. lightly doped) and small diameter [1]. It opens the way to the design and implementation of very small piezoresistive sensors, 5 to 10 times smaller than current MEMS components, with performance at least equal or even superior to those of the state of art. For this purpose, the theoretical understanding of this phenomenon by means of accurate simulation is of practical importance.

Some studies have attempted to explain the origin of this giant piezoresistance effect [7-8] which, at the microscopic level is not fully understood yet. In the study presented here, we investigate the effect of piezoresistance in thin silicon layers using the particle Monte Carlo (MC) method to solve the Boltzmann transport equation within a "full-band" description of the band structure [9]. The model proposed by Rowe is used to model the effect of stress on the surface potential [10].

II. MODEL AND SIMULATED STRUCTURES

The Monte Carlo method of solving the Boltzmann equation provides an accurate description of transport mechanisms including collisions experienced by the charge carriers (interaction with phonons, ionized impurities, rough interfaces...). For p-type material, we consider scattering mechanisms related to elastic acoustic phonons, inelastic optical phonons and ionized impurities. In the case of hole transport in Si, the strong anisotropy of the valence band requires an accurate description of the energy bands. In this work, we use a full-band model based on the **k.p** method, including up to 30 bands and taking strain into account through the Bir-Bikus anisotropic model [10-13]. The simulator is self-consistently coupled to a Poisson equation solver.

A nanowire is essentially a three-dimensional object. However, in a first approach to the problem of giant piezoresistance, to reduce the computation time, we restricted ourselves to the consideration of silicon nano-layers of infinite width described in 2D real space. The effect of stress on the surface potential is applied on both sides of the nano-layer, as illustrated in Figure 1 that schematizes the simulated structures.

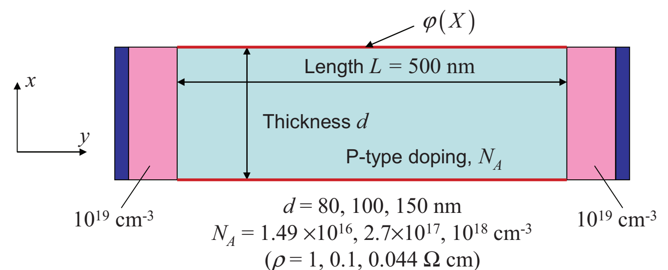

Figure 1. Schematic cross-section of simulated structures.

In nanostructures, the size quantization effects may be very important. Several works on silicon nanowires have shown that these effects may influence substantially their electrical and mechanical properties. In particular, for diameter smaller than 20 nm, many physical quantities such as the Young's modulus, the Poisson ratio, the electron and hole effective mass, the band gap and the mobility are strongly affected with respect to bulk data. [3][14-16]. However, in this study, to compare with available experimental data, we simulated structures with minimum

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thicknesses of 80 nm which is much larger than the critical size mentioned above. Quantization effects are thus safely neglected here.

All simulated structures have an effective length of 500 nm. The thickness is 80 nm, 100 nm or 150 nm. The p-type Si layer is doped to 10^{18} cm^{-3}, 2.7×10^{17} cm^{-3} or 1.49×10^{16} cm^{-3}, which corresponds to a bulk resistivity of 0.044 Ω.cm, 0.1 Ω.cm and 1 Ω.cm, respectively. At both ends, the Si layer is overdoped to 10^{19} cm^{-3} and contacted by an Ohmic contact which injects / detects the flux of particles flowing through the structure. The uniaxial stress is uniformly applied along the [110] transport direction *y*.

The surface potential φ is defined as the difference in the top of valence band between the surface and the volume of the material where neutrality is assumed to be recovered. The effect of stress is modeled along the line proposed by Rowe who investigated the giant piezoresistance effect in Si nanowires using a very simple approach of transport [9]. For a uniaxial stress X, the surface potential φ varies according to the law

$$\frac{d\varphi}{dX} = 0.5 \text{ meV/MPa} \tag{1}$$

considering that for unstrained Si, φ_0 = 0.54 eV. The nano-layers are simulated under a bias voltage of 0.5 V for stresses ranging from 0 to ± 100 MPa applied along the <110> crystallographic direction (the sign "+" for a tensile stress, the "-" for a compressive stress).

III. SIMULATION RESULTS

According to Eq. (1), the surface potential is reduced under tensile strain while it is enhanced under compressive strain. Figure 2a shows the typical potential profile in the middle of the device along the transverse direction x for three values of stress and a small resistivity ρ = 0.044 Ω.cm. The stress essentially modulates the depth of the surface depleted region, while the potential in the center of the structure remains unchanged and equal to its equilibrium position. Accordingly, the maximum hole density remains equal to the impurity concentration in the central region. The stress controls only the width of this neutral region, i.e. the conductive area, as shown in Figure 2b.

The situation is different for a higher resistivity ρ = 0.1 Ω.cm, as shown in Figure 3. Due to lower doping concentration, the depleted region extends more deeply in the structure and the potential does not fully recover its equilibrium position (Figure 3a). Accordingly there is no longer any neutral region in the device and the stress not only controls the width of the conductive area but also the height of the potential barrier for holes and the maximum hole density (Figure 3b).

These results are in qualitative agreement with experimental C-V measurements on nanowires [17].

Figure 4 shows the current as a function of stress in the nano-layers for a thickness of 100 nm and various resistivity values. In the low-resistivity structure (ρ = 0.044 Ω.cm) structure, the current is controlled by the width of the conductive area and is linearly dependent on stress.

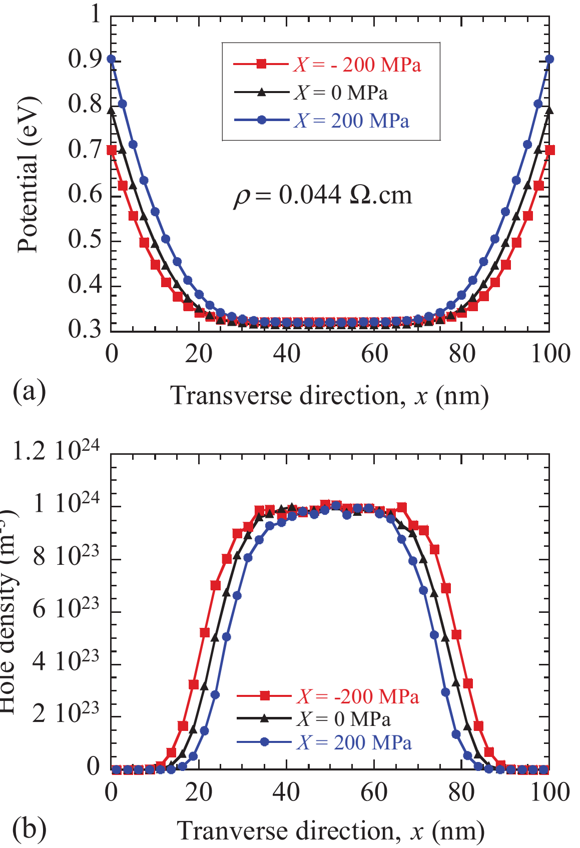

Figure 2. (a) Potential and (b) hole density profiles in an 100 nm-thick Si layer of resistivity 0.044 Ω.cm for three stress conditions X.

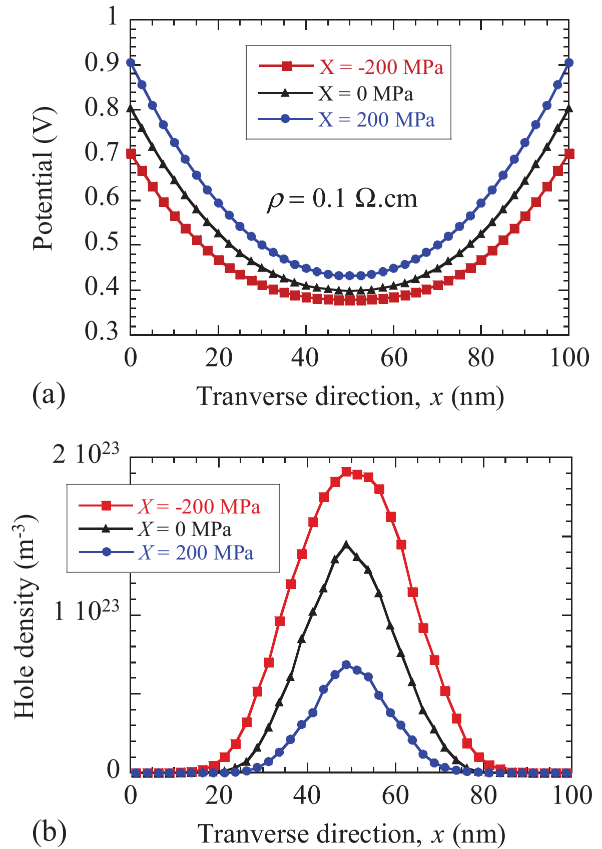

Figure 3. (a) Potential and (b) hole density profiles in an 100 nm-thick Si layer of resistivity 0.1 Ω.cm for three stress conditions X.

For higher resistivities ($\rho = 0.1$ Ω.cm and 1 Ω.cm), the current is much smaller and controlled by the height of the potential barrier in the center of the structure, which leads to a quasi-exponential dependence of the current as a function of stress.

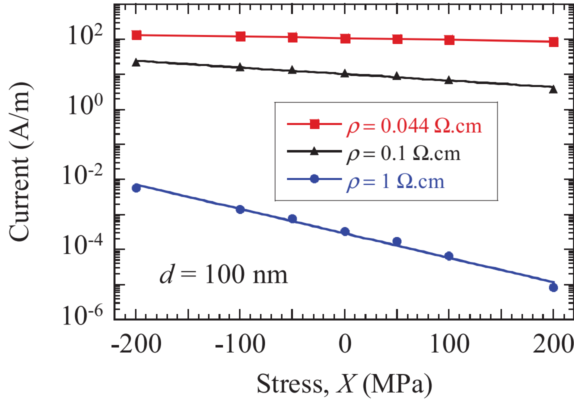

Figure 4. Currents versus stress in nano-layers of 100 nm-thickness for different resistivities. For the two highest resistivities, the solid lines are exponential fitting curves.

To quantify the piezoresistive phenomenon, the most relevant factors of merit are the relative variation of conductivity $\Delta\sigma/\sigma_0$ and the longitudinal piezoresistive coefficient π_l^{σ}. Some results of relative change in conductivity $\Delta\sigma/\sigma_0$ as a function of stress are shown in Figures 5 and 6 for three thicknesses of 80, 100 and 150 nm and three resistivities of 0.044, 0.1 and 1 Ω.cm.

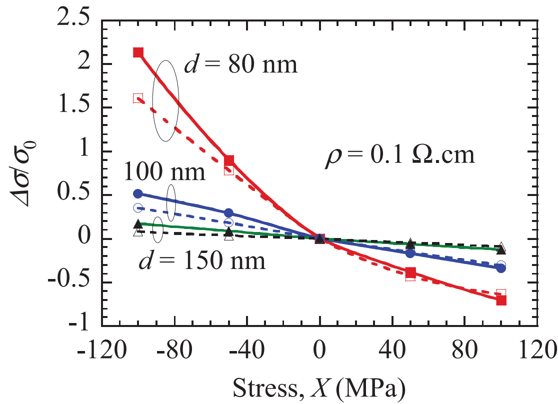

Figure 5. Relative variation of conductivity $\Delta\sigma/\sigma_0$ as a function of stress with (solid lines) and without (dashed lines) change in band-structure for the resistivity of 0.1 Ω.cm.

To separate the contributions of stress-induced changes in the valence band structure and in the surface potential, we first considered the only effect of surface potential modulation while keeping the band structure of unstrained Si. The effect of stress on the band structure was considered in a second stage. The comparison of the solid and dashed lines in Figure 5 shows that both contributions of the potential surface variation and of the change in bands must be taken into account, though the latter smaller, especially in the case of thin layers. The change in conductivity is not always linear and depends strongly on both the doping level and the thickness (that is to say, the diameter in the case of a nanowire). At a given resistivity, the variation $\Delta\sigma/\sigma_0$ as a function of stress is higher and more nonlinear when reducing the layer thickness. The amplitude of variation of conductivity obviously increases when increasing the resistivity (see Figure 6).

For a high resistivity of 1 Ω.cm, the relative change of conductivity as a function of stress seems to be nearly independent of the layer thickness, as shown in Figure 7. This is probably associated with the fact that the current in a quasi-fully-depleted region is exponentially controlled by the potential barrier whatever the thickness, which makes the stress-dependent change of relative conductivity weakly dependent of thickness.

Overall, these results are in agreement with trends observed experimentally by He and Yang's for nanowires [1].

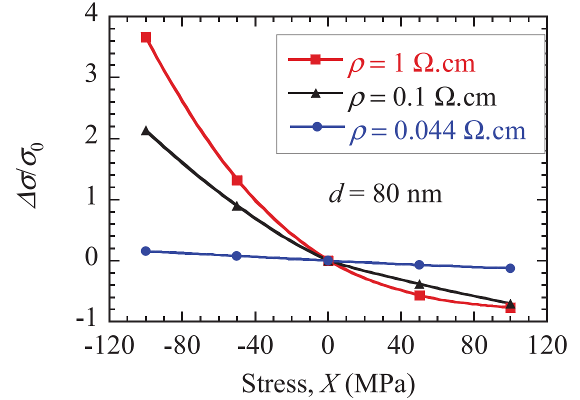

Figure 6. $\Delta\sigma/\sigma_0$ as a function of stress including stress-effects on bands for the thickness of 80 nm and for different resistivities.

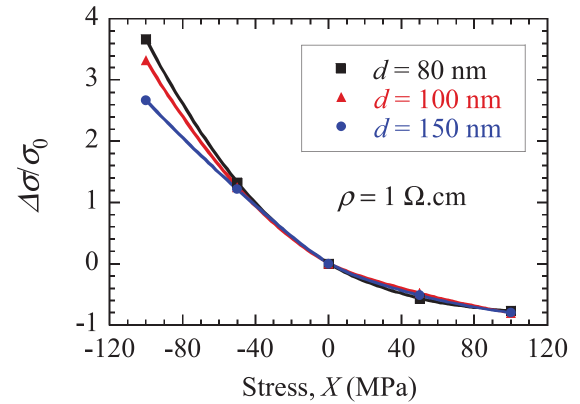

Figure 7. $\Delta\sigma/\sigma_0$ as a function of stress for the resistivity of 1 Ω.cm and for diffrent thicknesses.

The corresponding piezoresistive coefficients were calculated around $X = 0$ using the following expression

$$\pi_l^{\sigma} = \frac{1}{\sigma_0}\frac{d\sigma}{dX} \tag{2}$$

where σ_0 is the conductivity under zero stress. The resulting piezoresistive coefficients are summarized in Table 1. As expected, they are strongly dependent on the nano-layer thickness and resistivity. A large piezoresistive coefficient of 1750×10^{-11} Pa^{-1} is obtained for a 80 nm thick layer with resistivity of 1 Ω.cm.

The results obtained are quite consistent with experimental results of He and Yang. For instance, they

obtained a first order piezoresistive coefficient of 660×10^{-11} Pa^{-1} for a 75 nm thick <110> oriented nanowire with resistivity of 0.3 Ω.cm. The highest piezoresistive coefficient measured was 3100×10^{-11} Pa^{-1} for a nanowire with resistivity of 10^2 Ω.cm. Accurate MC calculation in such a high resistivity layer is very difficult because of very small current level.

TABLE I. PIEZORESISTIVE COEFFICIENT IN P-TYPE <110> -ORIENTED SI NANO-LAYERS FOR DIFFERENT THICKNESSES AND RESISTIVITIES (VALUES GIVEN IN 10^{-11} PA^{-1})

Thickness *d* (nm)	Piezoresistive coefficient (x $10^{-11}Pa^{-1}$)		
	ρ= 0.044 Ω.cm	*ρ =0.1 Ω.cm*	*ρ = 1 Ω.cm*
80	141	842	1750
100	111	420	1589
150	80	149	1564
200	60	105	1505

IV. CONCLUSION

Using the 2D Monte Carlo simulation, we are able to modulate the depletion zone *via* the surface potential in silicon nano-layers with thickness of 80 – 150 nm which are are assumed to behave as nanowires. The effective conduction area, wide in the case of compression, becomes much narrower in the case of tensile strain. Taking into account the effects of stress on both the surface potential and the valence band, the relative variation of conductivity depends on both the thickness and the resistivity. Through this modulation, p-type nano-layers have shown the effect of giant piezoresistance and the results are in satisfying agreement with experimental data available for nanowires.

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