Paper

Grain boundary effect on the anisotropy piezoresistance of laser-recrystallized polysilicon layers in SOI-structures

Yury Pankov and Anatoly Druzhinin

Abstract — A physical model of grain boundary influence on the piezoresistive effect of p-type conductivity of polysilicon layers in SOI-structures is developed. Software calculating piezoresistive properties of boron-doped p-type polysilicon layers has been developed. These properties may be calculated over wide concentration and temperature ranges with anisotropy taken into account and with the average grain size as a parameter. The potential barrier regions around the grain boundaries influence the deformation changes of anisotropy resistance in the fine-grained non-recrystallized SOI-structures doped with boron up to $3 \cdot 10^{19}\mathrm{cm}^{-3}$ only.

Keywords — SOI, polysilicon layers, MLR.

1. Introduction

The increasing requirements imposed on polycrystalline silicon films, which are suitable for fabrication of low-cost MEMS-sensors, stimulate studies aimed to improve the properties of polysilicon. A possible way to obtain high-quality poly-Si layers is the microzone laser recrystallization (MLR), a process used in the fabrication of SOI-structures. MLR changes the microstructure of poly-Si layers modifying their piezoresistive properties. Thus microzone laser recrystallization of poly-Si layers is a prospective way to obtain high-quality SOI-structures. This method allows poly-Si films with predetermined orientation to be melted locally. Moreover, crystallite growth and defect formation may be controlled. Finally, the method affects the structure and other parameters of the semiconductor.

The appearance of anisotropy in electrical conductivity is the primary effect of anisotropy strain action and scalar component of resistance remains nearly constant. This is the result of Smith's classical investigations of single-crystal bulk silicon [1]. Previous well-known investigations of piezoresistance in both n- and p-type polycrystalline polysilicon consider longitudinal and transverse gauge factors under uniaxial stress [1, 2]. But these parameters do not describe the behavior of microelectronics sensors adequately. Scalar isotropy resistance changes, which are averaged in all directions, are given by

$$\Delta r = 1/3\,\mathrm{Sp}\boldsymbol{r} = 1/3 \sum_{i,k=1}^{3} \Delta r_{ik}\,. \tag{1}$$

The fully symmetrical current bridge circuit compensates the total isotropy resistance. This compensation is a result of the temperature change of resistance compensation without stress (an additive temperature error). It has been shown that in conditions of optimum tenzoresistors location the output signal of piezoresistive microelectronic sensor is proportional to the maximum anisotropy resistivity

$$U_{out} \sim i_p \max\left(r_{ik} - 1/3 \sum_{i,k=1}^{3} r_{ik}\right), \tag{2}$$

where i_p is the current bridge power supply.
Therefore, the resistance anisotropy

$$\mathrm{Dev}\boldsymbol{r} = r - 1/3\mathrm{Sp}\boldsymbol{r} = r_{ik} - 1/3 \sum_{i,k=1}^{3} r_{ik} \tag{3}$$

is the fundamental parameter in MEMS-sensors. This conclusion opens the possibility to reduce negative influence of grain boundaries on sensor characteristics by means of laser recrystallization of the SOI-structures.

2. Theory

The aim of our studies was to investigate the electrical conductivity anisotropy, changes of carrier mobility and hole effective mass under general strain of boron-doped polysilicon-on-insulator patterns both before and after the laser recrystallization. This model considers the contribution to both anisotropy and isotropy piezoresistance from the grain and the isotropy Schottky-type barrier regions around the grain boundaries.

Polysilicon consists of small single-crystalline (grains), which have point symmetry of the cubic group O_h. Single crystals are separated by non-crystalline regions with isotropy symmetry SO(3). Broken bonds on the grain boundaries form the so-called traps, which capture charge carriers. As a result of trapping, boundary areas depleted of carriers are created on both sides of the grain boundaries. Thus, the crystalline structure of a polycrystalline semiconductor is characterized by the isotropy and the energy structure is characterized by the presence of potential barriers at the grain boundaries.

The theoretical analysis of piezoresistive characterization of poly-Si layers is based on the consideration of the resistivity tensor of both the bulk silicon and the barrier regions. The carrier transport through the potential barrier is supposed to be due to the thermionic emission combined with diffusion.

Let's extend the well-known model of the polysilicon piezoresistance for the total case of arbitrary strains and total resistance changes. In the limit of small voltages, the barrier can be modelled by anisotropy linear resistors. Thus, the total anisotropy resistivity ρ can be written in terms of an anisotropy grain and approximate isotropy barrier resistivity ρ_g and ρ_b by

$$\rho_{ik}(\varepsilon, T) = \rho_{g,ik}\left[1 - \frac{2W+\delta}{L}\right] + \rho_b \frac{2W+\delta}{L}\,\delta_{ik}\,, \qquad (4)$$

where W is width of the carrier-depleted zones formed on both sides of the grain boundary, δ is the grain boundary thickness, L is the grain size and δ_{ik} is the Kronecker delta. This equation can be concluded by the consideration of total resistivity tensor in major axes.

For the thermionic emission-diffusion theory the total isotropy conductivity from both heavy and light holes in p-type material is given by [2]

$$\sigma_b \sim \sum_{l=1}^{2} B_l \exp\left(-E_f/kT\right)\exp\left(-qV_b/kT\right)\,, \qquad (5)$$

where E_f is the Fermi energy, and

$$V_b = V_{bo}\left(1+\zeta T\right),\;\; \zeta \approx 1.5\cdot 10^{-3} K^{-1} \qquad (6)$$

is the temperature-depending height of the potential barrier at the grain boundary and factor B_l is defined by the effective mass of holes in l-th sub-zone m_l and the relaxation time τ_l:

$$B_l(\varepsilon, T) = m_l \,/\, \left[1 + \left(2m_l kT \,/\, \pi q^2 \xi^2 \tau_l\right)^{1/2}\right]\,, \qquad (7)$$

where ξ is the dielectric permitivity.

3. Results and discussion

Details of the complicated valence band structure of silicon were taken into consideration. A special method was developed for piezoresistance calculations in the grain volume that allowed both the main effect due to the carriers redistribution between the sub-bands and a significant effect on the magnitude because of change in warpage of the constant energy surfaces in strained silicon to be estimated. In the case of p-type semiconductors the anisotropy strain splits initially degenerate parabolic valence band, but essential non-parabolic effects appear in their energy spectrum under this kind of the strain. Therefore, effective masses of holes essentially depend on the energy and anisotropy strain. Details of the complicated valence band structure in strained silicon were taken into consideration [4]. Carrier concentration in semiconductor with arbitrary energy spectrum is given by

$$n = \frac{1}{4\pi^3}\int f(E)\,dk^3 = \int_{S_E} f(E)\,g(E)\,dE\,. \qquad (8)$$

From this expression it follows that the density of states in the strained semiconductor with any given energy spectrum is given by the following total definition: Lebesgue measure, originating from the energy surface averaging of volume element dk^3:

$$dE = <\left(dk^3\right)> = \frac{dE}{4\pi^3}\int_{S_E} \mathrm{Det}\left(\mathbf{J}_l^{-1}\right) dS_E\,, \qquad (9)$$

where $\mathbf{J}_l$ is the Jacobi matrix of transformation to arbitrary coordinates $(E, \zeta_1, \zeta_2) \to (k_1, k_2, k_3)$, which are associated with constant energy surfaces $S_E : dS_E = d\zeta_1\, d\zeta_2$.

In the semiconductor with isotropic and parabolic zone states density is defined by

$$g(E) = (2m)^{3/2} E^{1/2} / \left(2\pi^2 \hbar^3\right)\,. \qquad (10)$$

From this relation it follows that the effective masses in strained p-type semiconductor may be given as [4]:

$$m_{dl}\left(E, \varepsilon\right) = \frac{\pi^{2/3}\hbar^2}{2^{5/3}E^{1/3}}\int_{S_E} \mathrm{Det}\left(\mathbf{J}_l^{-1}\right) dS_E\,. \qquad (11)$$

In our calculation the modified energy Bir spectrum of valence zone was used [4, 5]. Calculated effective masses of holes are shown in Fig. 1 for uniaxial stressed p-type Si.

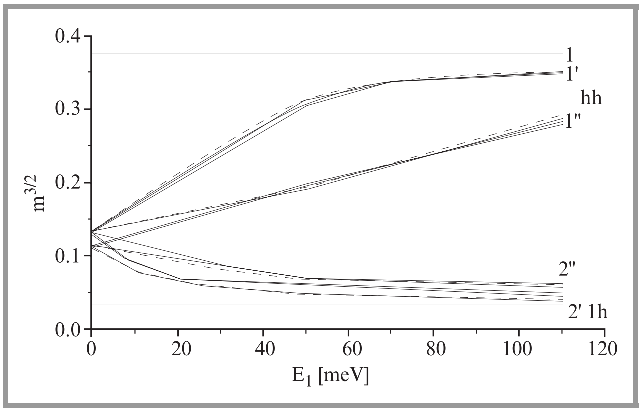

Fig. 1. Hole effective masses of uniaxial stressed Si: 1, 1', 1" – heavy holes, 2,2',2" – light holes; under the strain: $1,2 - \varepsilon = 0, 1', 2' - \varepsilon = 0.4\%, 1'', 2'' - \varepsilon = 1.2\%$. Dashed lines represent compression and solid ones tension.

Fermi energy and relaxation time changes, which belong to Eq. (7), were computed through solving the electroneutrality equation for the real strain energy spectrum [4]. The strain dependence of the relaxation time is revealed through the strain dependence of effective masses. Changes of Fermi energy versus uniaxial strain are shown in Fig. 2.

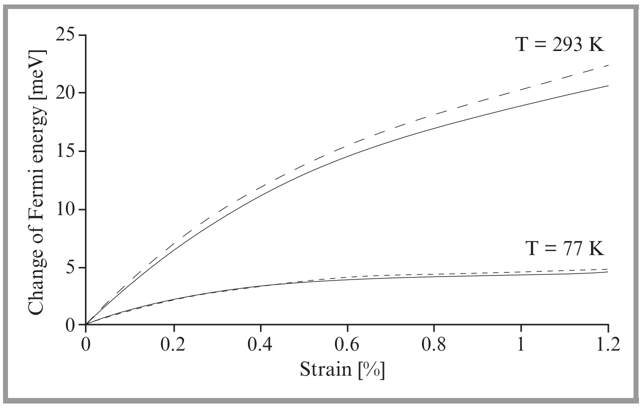

Fig. 2. Changes of Fermi energy versus uniaxial strain. Dashed lines represent compression and solid ones tension.

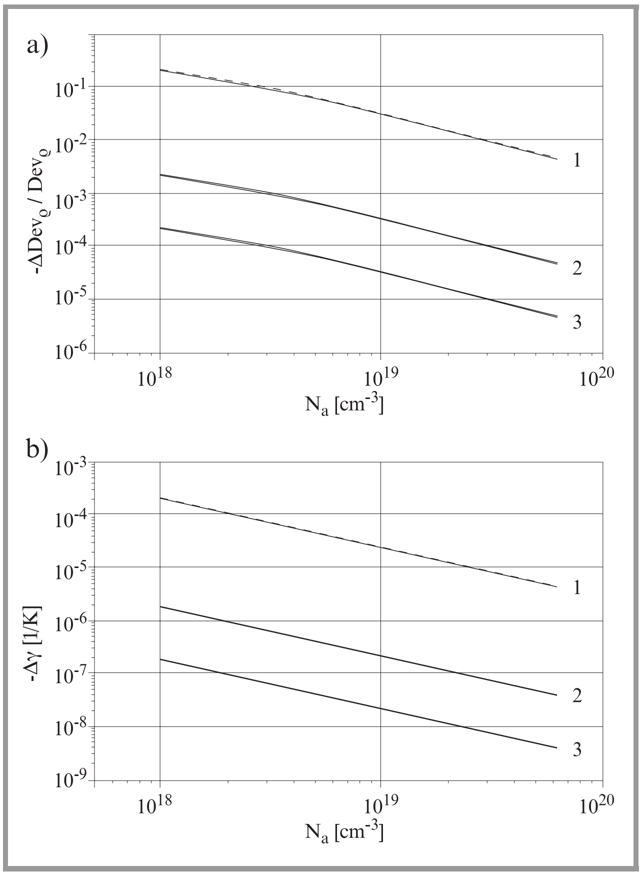

Fig. 3. Relative changes of strain anisotropy resistivity versus the doping concentration after taking into account the grain boundary effects (a) and changes of its temperature coefficient for average grain size: $1 - L = 0.1\,\mu$m, $2 - L = 10\,\mu$m, $3 - L = 100\,\mu$m (b). Dashed lines correspond to situation before whereas solid ones – after laser recrystallization.

According to selection rules of strain effect tensors in cubic semiconductor [6], the total conductivity/resistivity tensor cannot have a linear term relative to anisotropy strain. As a result the strain dependence of effective masses could only increase nonlinearity of SOI-sensor output characteristics. Numerical calculations of the anisotropy resistivity tensor (as a function of boron doping concentration) were made for different types of practically interesting patterns: initial ones with the average grain size $L \sim 0.1\,\mu$m; after laser recrystallization with a chevron-like structure and $L \sim 10\,\mu$m; and after laser recrystallization with lateral seed region ($L \sim 100\,\mu$m). The carrier energy $E \approx E_T = = 3/2kT$ was estimated through calculations. In Fig. 3a the corresponding results are presented for the calculated changes of maximum strain anisotropy resistivity after taking into account potential barrier at the grain boundary and in Fig. 3b – changes of its temperature coefficient are shown.

The results of calculations demonstrate that potential barrier regions around the grain boundaries influence the deformation changes of anisotropy resistance in the fine-grained non-recrystallized boron-doped SOI-structures with boron concentration less than $3 \cdot 10^{19}$ cm^{-3}. This is in good agreement with the results of measurements of all the components of elastoresistance tensor in laser-recrystallized polysilicon layers. A set of theoretical and experimental investigations was curried out to reveal the possibilities of SOI-structures in microelectronic piezoresistive mechanical sensors [7].

4. Conclusion

After laser recrystallization the grain bulk dominates in the specific strain resistance of polycrystalline material. Thus this recrystallization enables negative influence of grain boundaries on piezoresistive sensor characteristics of the SOI-structures to be reduced.

References

[1] C. Smith, „Piezoresistance effect in germanium and silicon”, *Phys. Rev.*, vol. 94, no. 1, pp. 42–49, 1954.

[2] P. French and A. Evans, „Piezoresistance in and its applications to strain gauge”, *Solid State Electron.*, vol. 32, pp. 1–10, 1989.

[3] E. Lavitskaya *et al.*, „Structure influence on piezoresistance of thin polysilicon films”, *Funct. Mat.*, vol. 3, no. 1, pp. 58–61, 1996.

[4] Y. Tchoric, I. Maryamova, and Y. Pankov, „Computation of strain gauge non-linearity”, *Phys. Electron.*, no. 39, pp. 33–39, 1989.

[5] G. Bir and G. Pikus, *Symmetry and Strain Effects in Semiconductors*. Moscow: Nauka, 1972.

[6] A. Druzhinin, I. Maryamova, E. Lavitska, and Y. Pankov, „Physical aspects of multifunctional sensors based on piezothermomagnetic effects in semiconductors”, *Sensors and Actuators: A. Phys.*, vol. 68, no. 1–3, pp. 229–233, 1998.

[7] Y. Pankov, A. Druzhinin, and I. Maryamova, „Piezoresistance sensor”, 1998, Ukraine patent 23103A, G01L9/06, H01L21/28, pp. 1–4, 1995.

Yury Pankov was born in Ukraine in 1950. He graduated from Lviv Polytechnica University in 1971, and obtained his Ph.D. degree in 2000. He works as senior researcher on theory and experiment of piezoresistive effects semiconductors and sensors development on their basis.

Lviv Polytechnical University
Kotlarevsky st 1
Lviv 79013 Ukraine

Anatoly Druzhinin – for biography, see this issue, p. 44.