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Stress-dependent hole effective masses and piezoresistive properties of p-type monocrystalline and polycrystalline silicon

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Piezoresistive effects of p-type polycrystalline silicon underline that longitudinal and transversal piezoresistive properties in monocrystalline silicon do not have the same physical origin, which is not accounted for in current models. This difference is highlighted by the study of the mechanical stress effect on the valence band, which shows that piezoresistive properties of p-type monocrystalline silicon can be explained in terms of both hole transfer between heavy- and light-hole valence bands and stress-dependent hole effective masses. The quantification of these phenomena points out that longitudinal piezoresistive properties are mainly due to the hole transfer, whereas transversal ones are mainly attributed to the effective mass change effects. This enables one to model p-type polycrystalline silicon piezoresistivity, in particular the sign change of the transversal gauge factor at high doping level. [S0163-1829(98)01615-4]

I. INTRODUCTION

Since piezoresistive properties of silicon were discovered by Smith[1] forty years ago, monocrystalline and polycrystalline silicon have been widely used in the framework of mechanical sensors. However, whereas the piezoresistivity in n-type silicon has been well explained in terms of a many-valley model,[2] piezoresistivity in p-type silicon still has not been fully clarified due to the complexity of the valence-band structure.[3] The more recent model explains the piezoresistivity of p-type silicon by a stress-induced decoupling of the degenerate valence band and concludes that both longitudinal and transversal piezoresistive properties have the same physical origin.[3] On the other hand, the piezoresistivity of polycrystalline silicon shows different behavior between longitudinal and transversal effects. This last point can be noticed in Fig. 1, in which we have reported experimental longitudinal and transversal gauge factors (K_l and K_t, respectively) as a function of doping concentration for both boron-doped monocrystalline and polycrystalline silicon.[4,5] Indeed, from this figure it is interesting to point out the experimental sign change of the polysilicon transversal gauge factor, even when the longitudinal gauge factor does not show the same behavior. Moreover, since K_t in monocrystalline silicon is negative whatever the doping concentration, existing models do not enable one to explain the sign change of the polysilicon transversal gauge factor with doping concentration.[4]

In this paper we suggest an explanation of these experimental results, first by showing differences between longitudinal and transversal piezoresistive properties in the case of monocrystalline silicon. This point requires one to take an interest in the physical origin of p-type silicon piezoresistivity, which can be explained by studying the stress effect on the valence-band structure. In a second part, we will apply this study to the case of polycrystalline silicon piezoresistivity. Since the pioneering works of Seto[6] and Obermeier,[7] it is well known that electrical and piezoresistive properties of polysilicon differ from those of silicon due to grain boundaries. In p-type polysilicon, the main effect of grain boundaries is to induce potential barriers that carriers have to get over. This will enable us to explain the piezoresistivity of polysilicon, taking into account a piezoresistive effect of the potential barrier as suggested by French and Evans.[8] This last effect will be deduced in a similar manner as the monocrystalline silicon piezoresistivity using the expression of the conductivity in the potential barrier.

First of all, let us recall that by neglecting the geometrical effect the piezoresistivity can be quantified by the gauge factor K as well as by the piezoresistance coefficient π, as follows:[9]

$$K=\frac{1}{\varepsilon}\frac{\Delta\rho}{\rho}=-\frac{1}{\varepsilon}\frac{\Delta\sigma}{\sigma},\quad \pi=\frac{1}{\chi}\frac{\Delta\rho}{\rho}=-\frac{1}{\chi}\frac{\Delta\sigma}{\sigma} \tag{1}$$

depending on whether the relative variation of resistivity $\Delta\rho/\rho$ (or conductivity $\Delta\sigma/\sigma$) is ascribed to the strain ε or to the stress χ, respectively.

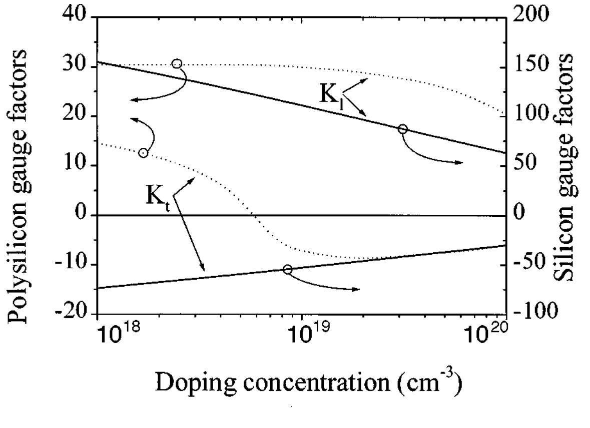

FIG. 1. Longitudinal K_1 and transversal K_t gauge factors for p-doped silicon (Ref. 5) (solid lines) and polysilicon (Ref. 4) (dotted lines) as a function of the doping concentration at room temperature.

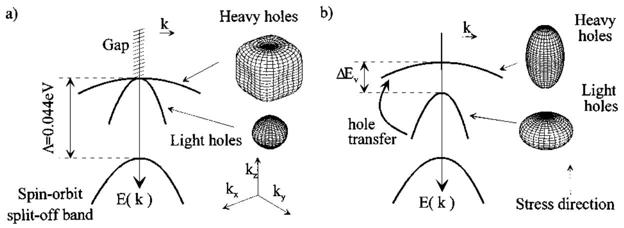

FIG. 2. Valence-band and energy surfaces in k space (for both heavy- and light-hole bands) in the case of (a) unstressed silicon. The energy surfaces are warped due to the degeneracy, (b) highly tensile stressed silicon. The energy surfaces are elongated and oblate ellipsoids, both having axial symmetry along the stress direction.

II. MECHANICAL STRESS EFFECT ON THE VALENCE-BAND STRUCTURE AND CONSEQUENCES ON THE HOLE TRANSPORT PROPERTIES

It is well known that the valence-band structure of silicon is comprised of three bands, usually designated as the heavy-hole, light-hole, and spin-orbit split-off bands [Fig. 2(a)]. The first two bands are degenerated at $k=0$ and the coupling between them is responsible for the warp of the energy surfaces.[10] On the other hand, the spin-orbit split-off band is shifted downward by 0.044 eV and consequently is widely depopulated as compared to those of heavy and light holes.[11] Thus, the hole conductivity in silicon is given by

$$\sigma=q^2\tau\left(\frac{p_1}{m_1}+\frac{p_2}{m_2}\right), \tag{2}$$

where q, p, τ, and m are the electron charge, the hole concentration, the relaxation time, and the hole effective mass, respectively, and where the subscripts 1 and 2 refer to the heavy and light holes, respectively. It must be noted that the relaxation time τ is assumed to be the same for both heavy and light holes, isotropic, and stress independent[3] and that effective masses are given in units of free-electron mass.

When a uniaxial stress is applied, the degeneracy between heavy- and light-hole valence bands is lifted [Fig. 2(b)],[10] leading to a resistivity change (piezoresistive effect) that can be explained in terms of hole transfer and mass change phenomena.

A. Hole transfer phenomenon

The hole transfer is due to the fact that holes fill lower energy levels. This well-known effect can be easily quantified knowing the band splitting ΔE_v as a function of the applied stress χ and assuming that the total number of conduction holes does not change (all acceptor levels are exhausted with and without stress).[12] In the following, for the sake of simplicity, we will study only the case of a uniaxial tensile stress χ applied in the [111] crystallographic direction. In that case the heavy-hole band moves up while the light one goes down and the band splitting ΔE_v is given by

$$\Delta E_V=\frac{2}{3}\,D'_u\,\frac{1}{C_{44}}\,\chi, \tag{3}$$

where $D'_u=4.4$ eV and $C_{44}=0.795\times10^{11}$ N m^{-2} are the deformation potential and the elastic stiffness constant relevant to a stress applied in the [111] direction, respectively.[3] Thus, according to the physics of semiconductors, in the case of nondegenerated silicon and weak stress ($\Delta E_v \ll 2kT$) the hole concentration relative change for each band can be easily expressed as

$$\frac{\Delta p_1}{p_1}=\frac{1}{kT}\,\frac{\Delta E_V}{1+(m_1^*/m_2^*)^{3/2}}\;\frac{\Delta p_2}{p_2}=-\frac{1}{kT}\,\frac{\Delta E_V}{1+(m_2^*/m_1^*)^{3/2}}, \tag{4}$$

where m^* are the density-of-states effective masses. Thus, a tensile stress ($\chi>0$) causes a hole transfer from the light-hole band to the heavy-hole band.

B. Mass change phenomenon

The mass change phenomenon has two origins: The first one is due to the mixing between the light hole and the spin-orbit split-off bands, leading to a mass shift for light holes[10] [afterwards we will designate it as the band mixing (BM) mass change effect]. This effect has been quantified by Hasegawa by expressing the inverse effective mass variations as linear functions of the stress χ:[13]

$$\Delta\left(\frac{1}{m_{2\parallel}}\right)=\alpha_\parallel\chi \quad\text{and}\quad \Delta\left(\frac{1}{m_{2\perp}}\right)=\alpha_\perp\chi, \tag{5}$$

where $\alpha_\parallel=-5.2\times10^{-9}$ m^2 N$^-$ and $\alpha_\perp=2.7\times10^{-9}$ m^2 N^{-1} relevant to a stress applied in the [111] direction. The second mass change effect is caused by the decrease of the interaction between the heavy- and light-hole bands, following the lifting of the degeneracy [afterwards we will designate it as the degeneracy lifting (DL) mass change effect]. The DL mass change effect has an influence on both types of holes and occurs as long as the applied stress is insufficient to completely remove the coupling between the heavy- and light-hole bands.

For highly stressed silicon, when the degeneracy is completely removed, the energy surfaces become elongated and oblate ellipsoids for heavy and light holes, respectively [Fig. 2(b)].[10] The piezoresistivity of silicon has been explained by Susuky starting from this particular case and then without taking into account the DL mass change effect.[3,12] However, according to the works of Hensel, the case of highly stressed silicon is reached only if the band splitting ΔE_v is markedly higher than $2kT$, which is absolutely not the case at room temperature for common stress conditions.[10] Indeed, starting from Eq. (3), at room temperature and for a stress $\chi=2\times10^8$ N m^{-2}, calculations lead to $\Delta E_v=7\times10^{-3}$ eV while $2kT=52\times10^{-3}$ eV. Thus, it is necessary to consider the case of weakly stressed silicon and consequently to take into account the DL mass change effect. This effect is unfortunately hardly quantifiable.[13,14] However, working at the temperature of 1.26 K, Hensel has determined effective masses by cyclotron resonance experiments in the case of highly stressed silicon. Indeed, at this temperature the $2kT$ term is weak and a common stress is sufficient to completely remove the coupling between the heavy- and light-hole bands. We have reported in Table I the hole effective masses for unstressed silicon and highly stressed silicon taken from the

TABLE I. Hole effective masses in silicon relevant to the [111] direction (in units of the free-electron mass) for two cases: unstressed silicon and highly stressed silicon in the [111] direction.

	Heavy holes	Light holes
Unstressed	$m_{1\|\|}=0.870$	$m_{2\|\|}=0.135$
silicon	$m_{1\perp}=0.647$	$m_{2\perp}=0.143$
	$m_1{}^*=0.490$	$m_2{}^*=0.160$
Highly	$m_{1\|\|}=0.870$	$m_{2\|\|}=0.135$
stressed	$m_{1\perp}=0.170$	$m_{2\perp}=0.369$
silicon	$m_1{}^*=0.293$	$m_2{}^*=0.264$

literature.[10,11] The study of the piezoresistive effect requires the knowledge of three effective masses for both heavy and light holes. The longitudinal one $m_{\parallel}$, is the hole effective mass in the direction of the applied stress. The transversal one $m_{\perp}$, is the hole effective mass perpendicular to the applied stress and the density of states effective mass m^*. Starting from this table, it is possible to estimate the magnitude of the DL mass change effect. In Fig. 3 one can notice the important variation of transversal effective masses (attributed to the DL effect), which has to play a significant role in the explanation of transversal piezoresistive properties.

According to the works of Hensel, from room temperature, the silicon is always weakly stressed for common stress conditions and thus the piezoresistive properties have to be explained starting from the effective masses of unstressed silicon. This enables consistency with the density-of-states effective mass values used for carrier transport modeling in p-type silicon ($m_1{}^*=0.49$ and $m_2{}^*=0.16$) (Refs. 11 and 15) and leads to the well-known result that the heavy-hole concentration is five times larger than that of light holes. Indeed,

$$p_1=\frac{m_1^{*3/2}}{m_1^{*3/2}+m_2^{*3/2}}\,p \quad \text{and} \quad p_2=\frac{m_2^{*3/2}}{m_1^{*3/2}+m_2^{*3/2}}\,p, \tag{6}$$

where p is the total number of conduction holes, which can be calculated starting from the doping concentration.[15] It has to be noted that the case of highly stressed silicon leads to a markedly different case since the density-of-states effective mass values for both heavy and light holes are comparable ($m_1{}^*=0.293$ and $m_2{}^*=0.264$).

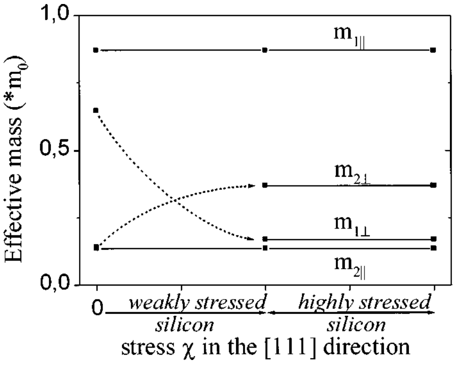

FIG. 3. Mass shift due to incomplete decoupling between the heavy-and light-hole bands (DL mass change effect) without taking into account the MB mass change (according to Table I).

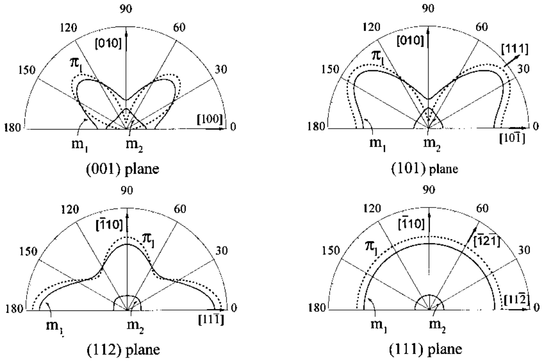

FIG. 4. Heavy- and light-hole effective masses (Ref. 11) and longitudinal piezoresistance coefficient π_1 (Ref. 16) in different planes. For each curve the full scale corresponds to 10^{-10} m^2 N^{-1} for piezoresistance coefficient and to one unit of free electron mass for m_1 and m_2.

III. LONGITUDINAL PIEZORESISTIVE PROPERTIES INTERPRETATION IN MONOCRYSTALLINE SILICON

Figure 3 shows that the DL mass change does not have any influence on longitudinal effective masses. Therefore longitudinal piezoresistive properties of silicon can be explained only in terms of hole transfer and BM mass change. The first one induces an increase of the resistivity for tensile stress according to the fact that the total number of heavy holes increases, leading to an average effective mass growth (since $m_{1\parallel}$ is higher than $m_{2\parallel}$). The BM mass change also induces an increase of the resistivity which is due to the increase of $m_{2\parallel}$ with the stress ($\alpha_{\parallel}<0$). These two points enable us to understand the positive sign of the longitudinal piezoresistance coefficient $\pi_{1[111]}$ which is given by

$$\pi_{1[111]}=-\frac{1}{\chi}\,\frac{\sigma_{\chi[111]}-\sigma_{[111]}}{\sigma_{[111]}}, \tag{7}$$

where $\sigma_{[111]}$ and $\sigma_{\chi[111]}$ are the hole conductivity in the [111] direction without stress and under stress χ, respectively. At room temperature and for nondegenerated silicon, calculation of $\pi_{1[111]}$ using Eqs. (2)–(7) leads to $\pi_{1[111]}=890\times10^{-12}$ m^2 N^{-1} ($K_1=167$), which is in good agreement with the experimental value $\pi_{1[111]}=935\times10^{-12}$ m^2 N^{-1} ($K_1=175$).[4] Longitudinal piezoresistive properties of silicon are mainly due to the hole transfer and thus proportional to the difference between the heavy- and light-hole masses. This fact is valid in any direction, as shown in Fig. 4, where we have reported the heavy and light hole masses and the longitudinal piezoresistance coefficient π_1 for different crystallographic planes.

Let us recall that calculations have been made in the case of nondegenerated silicon and at room temperature. The general case requires one to study hole transfer and mass change effects as a function of doping concentration and temperature. This has been made by Kanda, taking into account the hole transfer effect.[16]

IV. TRANSVERSAL PIEZORESISTIVE PROPERTIES INTERPRETATION IN MONOCRYSTALLINE SILICON

Figure 3 clearly shows that transversal effective masses $m_{1\perp}$ and $m_{2\perp}$ are strongly stress dependent. Therefore, the explanation of transversal piezoresistive properties requires in addition to take into account the DL mass change effect. In the transversal case, the hole transfer tends to induce an increase of resistivity for tensile stress (positive gauge factor) in the same way as for the longitudinal piezoresistive effect. Let us note that this last point is in contradiction with current models where piezoresistivity is explained starting from effective masses in highly stressed silicon.[3] Actually, in this latter case $m_{1\perp} < m_{2\perp}$ and consequently the hole transfer induces a decrease of resistivity. This enables one to explain the experimental negative sign observed for the transversal piezoresistance coefficient $\pi_{1[111]}$ (Fig. 1).

However, in the weakly stressed silicon case, although the hole transfer tends to induce an increase of resistivity the negative sign for the transversal piezoresistance coefficient is explained by the DL mass change. Indeed this latter effect induces a large decrease of the resistivity owing to the large decrease of $m_{1\perp}$. It has to be noted that the increase of $m_{2\perp}$, which should produce the opposite, has a limited effect in silicon because the light hole concentration is five times smaller that the heavy one [Eq. (6)]. In order to evaluate $\pi_{t[111]}$ it is necessary to quantify the DL mass change effect. For this purpose, we introduce two constants β_1 and β_2 in the same way as for the BM mass change [Eq. (5)]. Taking into account both the BM and DL mass change effects, inverse effective mass variations can be expressed as a function of the applied stress χ, as follows:

$$\Delta\left(\frac{1}{m_{1\perp}}\right)=\beta_1\chi \quad \text{and} \quad \Delta\left(\frac{1}{m_{2\perp}}\right)=\beta_2\chi+\alpha_\perp\chi. \tag{8}$$

Starting from this equation, the experimental value[12] $\pi_{t[111]} = -445\times10^{-12}\ \mathrm{m^2\,N^{-1}}$ is fitted taking $\beta_1=-\beta_2=2.4\times10^{-9}\ \mathrm{m^2\,N^{-1}}$, which is in good agreement with the transversal mass variations reported by Hensel. Indeed, starting from values in Table I and assuming a linear variation of inverse effective masses between unstressed silicon and highly stressed silicon, we find $\beta_1=-\beta_2=3.1\times10^{-9}\ \mathrm{m^2\,N^{-1}}$ at room temperature. However, this last point has to be taken carefully because the transversal effective mass variations as a function of stress are badly known. It simply enables us to estimate the importance of the DL mass change effect in the explanation of transversal piezoresistive properties. Contrary to the longitudinal piezoresistivity, the transversal one is mainly attributed to the mass change effect. At this level, it is interesting to point out that the transversal piezoresistivity is the sum of two opposite phenomena. The hole transfer, which is in the minority, tends to induce an increase of resistivity under positive stress. The mass change effect, which is in the majority, tends to induce a decrease of resistivity under positive stress. This will enable us to explain the experimental sign change of transversal piezoresistive properties of polysilicon, showing that for low doping concentration hole transfer can become the major phenomenon.

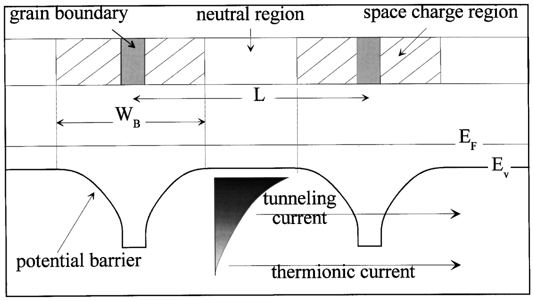

FIG. 5. Structure of polysilicon and representation of one valence band.

V. PIEZORESISTIVITY OF POLYCRYSTALLINE SILICON

In order to study effects of hole transfer and mass change phenomena in the case of polycrystalline silicon, first it is necessary to take an interest in carrier transport properties. It is well known that these properties differ from those of silicon due to grain boundaries, which has been extensively studied the past decade.[17] In the case of p-type polysilicon, the common basis is to model the electrical behavior of grain boundaries by a potential barrier, which limits the carrier transport (Fig. 5). On the one hand, this potential barrier is due to the trapping of free carriers by grain boundaries, which creates a space-charge region inside the grain.[6] On the other hand, the potential barrier at the grain boundary level expresses that the grain boundary behaves as an intrinsic wide-band-gap semiconductor, the gap of which is different from that of silicon.[18]

Thus, polysilicon resistivity ρ_{poly} can be expressed by a neutral region and a potential barrier contribution, as follows:

$$\rho_{\mathrm{poly}}=\rho_{\mathrm{mono}}\left(1-\frac{W_B}{L}\right)+\rho_b\,\frac{W_B}{L}, \tag{9}$$

where L is the average grain size, W_B the width of the potential barrier, ρ_{mono} and ρ_b are the monocrystalline silicon and potential barrier resistivities, respectively. Starting from this expression, the polysilicon piezoresistive study consists in establishing a mechanical stress effect on terms ρ_{mono} and ρ_b. In a first approximation, the stress effect on the neutral region resistivity ρ_{mono} can be considered to be the same as for silicon resistivity. However, as the piezoresistivity in silicon is anisotropic, it is necessary to average the neutral region piezoresistivity in order to take into account all possible orientations of crystallites.[20] This hypothesis is used by many authors.

Concerning the ρ_b term, most authors consider that it is stress independent.[19] However, this hypothesis does not enable to one model either the polysilicon piezoresistivity at low doping level[8] or the thermal drifts.[21] The potential barrier piezoresistivity has been first shown by French and Evans[8] and can be studied starting from the ρ_b resistivity expression. In the more general case, this resistivity is calculated taking into account thermionic emission and tunneling effect through the potential barrier.[18] Let us note that in the same way as for monocrystalline silicon we have to consider heavy-hole and light-hole valence bands. Calculations require using a numerical model.[22] However, in the case of nondegenerated polysilicon, for each band the potential barrier conductivity can be expressed, as follows:

$$\sigma_{b_{1,2}}=\frac{4\pi q^2 W_B}{h^3}\, m_{1,2}\, \exp\left(-\frac{\xi_{1,2}}{kT}\right)\times\int_0^\infty \exp\left(-\frac{E}{kT}\right)\tau_{1,2}(E)dE, \qquad (10)$$

where h is the Planck's constant, ξ the energy difference between the valence-band energy E_v and the Fermi level energy E_F, and $\tau(E)$ the transmission probability of a carrier with energy E through the potential barrier. This probability is dependent on potential barrier dimensions and effective masses. It is calculated using the one-dimensional time-independent WKB approximation.[23] As crystallites are more or less randomly oriented in polysilicon, m_1 and m_2 are average effective masses. In that way we can assume that

$$m_1=m_1^*=0.49 \quad \text{and} \quad m_2=m_2^*=0.16. \qquad (11)$$

Expressing ξ_1 and ξ_2 as a function of heavy- and light-hole concentrations p_1 and p_2, respectively, the total potential barrier conductivity σ_b can be expressed as follows:

$$\sigma_b=\frac{q^2 W_B}{\sqrt{2\pi}(kT)^{3/2}}\left(\frac{p_1}{\sqrt{m_1}}\Gamma_1+\frac{p_2}{\sqrt{m_2}}\Gamma_2\right), \qquad (12)$$

with $\Gamma_{1,2}=\int_0^\infty \exp(-E/kT)\tau_{1,2}(E)dE$.

Compared to expression (2) this expression enables one to clearly show the potential barrier piezoresistivity since hole concentrations and effective masses are stress dependent. However, hole transfer and mass change phenomena do not intervene in the same way as for silicon piezoresistivity. Furthermore, expression (12) shows that this piezoresistivity is dependent on the potential barrier shape (through Γ terms). Thus it is not possible to study the potential barrier piezoresistivity properties of one and the same problem, since potential barrier dimensions depend, among others, on the polysilicon texture. However, limiting the study to the model of Seto[6] (only the thermionic current is taken into account) it is possible to qualitatively explain the piezoresistivity of polysilicon. Indeed, in this case expression (12) leads to

$$\sigma_b=\frac{q^2 W_B}{\sqrt{2\pi}(kT)^{3/2}}\exp\left(-\frac{qV_B}{kT}\right)\left(\frac{p_1}{\sqrt{m_1}}+\frac{p_2}{\sqrt{m_2}}\right), \qquad (13)$$

where V_B is the height of the potential barrier. In that case, only carriers that have enough energy to get over the potential barrier take place in electrical conduction. Now, Chao shows that the mass change effect mainly concerns carriers that have weak energy.[14] Thus, for low doping concentration, as the potential barrier is high, both longitudinal and transversal potential barrier piezoresistivity can be interpreted only in terms of hole transfer. This enables one to explain the positive sign of K_t, in the same way as K_1. At room temperature, using expressions (3), (4), (6), (11), and (13), calculation leads to $\pi_b=130\times10^{-12}\ \mathrm{m^2\,N^{-1}}$ $(K_b=21)$. This value is valid for both longitudinal or transversal effects as well as. This is in relatively good agreement with the values reported on Fig. 1, knowing that the tunneling effect has been neglected. When the doping concentration increases, the potential barrier height decreases[6] and more carriers take place in electrical conduction, notably those having weak energy. Thus the mass change phenomenon is gaining ground and K_t becomes negative as in silicon.

However in the same way as for p-type monocrystalline silicon piezoresistivity it is not possible to well quantify the variation of the potential barrier piezoresistivity with doping concentration and temperature, due to little knowledge of the effective mass change effect, all the more because of the tunneling current through the barrier, which is very sensitive to effective mass variations.

VI. CONCLUSION

The particular behavior of the p-type polysilicon transversal gauge factor with doping concentration enables one to underline that the physical origin of longitudinal and transversal piezoresistive properties are different for both p-type monocrystalline and polycrystalline silicon. By studying the mechanical stress effect on the silicon valence-band structure we have shown that the longitudinal piezoresistive effect is mainly attributed to the hole transfer phenomenon whereas the transversal one is mainly due to the mass change effect. Applying this to the case of polysilicon, we have shown that it is possible to explain the experimental sign change of the transversal gauge factor. However, quantification of both silicon and polysilicon piezoresistivity as a function of doping concentration and temperature would require a better understanding of the stress-dependent hole effective mass effect in silicon.

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