

A tunneling piezoresistive model for polysilicon*

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Abstract: Based on the trap model, the band structure and the conductive mechanism of polysilicon were analyzed, and then an equivalent circuit used to interpret the tunneling piezoresistive effect was proposed. Synthesizing the piezoresistive effect of the grain boundary region and grain neutral zone, a new piezoresistive model—a tunneling piezoresistive model is established. The results show that when the doping concentration is above 10^{20} cm^{-3} , the piezoresistive coefficient of the grain boundary is higher than that of the neutral zone, and it increases with an increase in doping concentration. This reveals the intrinsic mechanism of an important experimental phenomena that the gauge factor of heavily doped polysilicon nano-films increases with an increase in doping concentration.

Key words: polysilicon nanofilm; tunnelling piezoresistive effect; Gauge factor; piezoresistive properties

DOI: 10.1088/1674-4926/33/9/092003

PACC: 7220F; 7360F; 7340G

1. Introduction

Since the 1970s, concern has increased regarding the piezoresistive properties of polysilicon films (PSFs), which are used for the development of mechanical sensors^[1,2]. Since this period, theoretical studies on polysilicon piezoresistive films have been systematically performed^[3], however research into the piezoresistive properties of the grain boundary (GB) and both sides of the GB barrier is not comprehensive enough. In 1984, French and Evans described the piezoresistive mechanism of the polysilicon GB region^[4,5]. They considered that both the grain neutral zone and the barrier region contribute to polysilicon piezoresistive characteristics, and the piezoresistive effect of the barrier zone is mainly due to the variation of the thermionic emission current with strain, as the gauge factor (GF) is about half of the grain neutral zone^[6]. Obviously, the smaller the grain size is, the larger the scale which the potential barrier occupies. Typically, the size of the grain decreases as the film thickness decreases; therefore according to French and Evans's theory, the GF of PSF should also decrease with decreasing film thickness.

However, for polysilicon nano-films (PSNFs), $\leq 100 \text{ nm}$ in thickness, the above conclusions are different from the experimental results^[7]. GFs of heavily doped PSNFs are larger, up to 30 or more, which is obviously higher than the predicted values of the theoretical model given by French and Evans. The reason for this is that besides the thermionic emission current, the tunneling current should be also considered. When the doping concentration exceeds 10^{19} cm^{-3} , the tunneling current usually exceeds the thermionic emission current, and thus plays a major role in the barrier current. The variation of the tunneling current with stress is more obvious when compared to the thermionic emission current, which brings a more significant tunneling piezoresistive effect^[7], and therefore heavily

doped PSNFs have a higher GF. A calculation method for the GF of the GB is proposed based on PSNF experimental results by analyzing the dependences of the tunneling current and stress^[7]. At present, several researchers have successfully developed pressure sensors utilizing PSNFs^[8,9], and proved that this kind of piezoresistive material has advantages, such as improving the stability of high temperature piezoresistive devices and enhancing the sensitivity. In order to give a comprehensive explanation for the piezoresistive properties of PSNFs and to develop a piezoresistive sensor utilizing the advantages of PSNFs more conveniently, in this paper, the intrinsic factor of the polysilicon piezoresistive effect and the role of the tunneling piezoresistive effect were analyzed, which began from the band structure of polysilicon and the current formation mechanism. On this basis, synthesizing the piezoresistive characteristics of the GB region and the grain neutral zone, a new piezoresistive model—a tunneling piezoresistive model was established. The model was verified by a comparison of different experimental results.

2. Polysilicon energy band structure and piezoresistive mechanism

Polysilicon is composed of grains and GBs, and the grains that are separated by GBs have different scale and orientation. The grain neutral zone is a monocrystalline structure with the piezoresistive properties of monocrystal. However, GBs with an amorphous structure conduct multiply, of which the piezoresistive properties are far more complex than the monocrystal's. Its electrical properties can be usually described by the carrier trap model. The trap model was originally proposed by Kamins^[10] and Rai-Choudhury and Hower *et al.*^[11], which has been widely accepted and successfully explains lots of experimental phenomena about polysilicon conductivity.

* Project supported by the National Natural Science Foundation of China (No. 60776049), the Science and Technology Foundation of Liaoning Province (No. 20072036), and the Fund of Liaoning Province Education Department (No. 2007T130).

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Received 18 February 2012, revised manuscript received 19 March 2012

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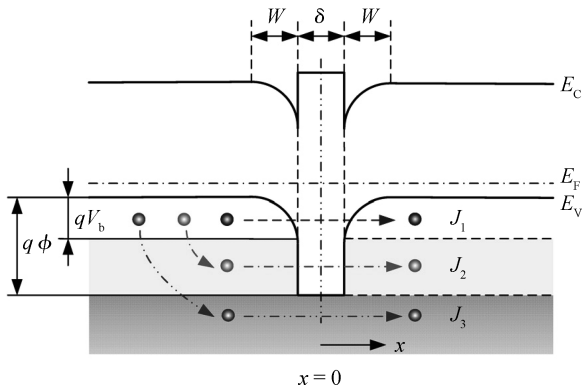


Fig. 1. Energy band diagrams near a grain boundary under thermal equilibrium.

According to the basic assumption of the trap model, there are a large number of carrier traps in the GB with impurities being uniformly distributed in the polysilicon. For boron-doped p-type polysilicon, the traps form positive charged centers after capturing holes, which uniformly distribute on the grain boundaries. Due to requirements of electric neutrality, hole depletion layers must exist on both sides of the GB, resulting in the barrier zone forming on both sides of the GB. In the case of moderate doping, the barrier width, W , is often much higher than the natural GB thickness, δ . Thus, during the analysis of the electrical properties, the natural GB can be ignored and only the depletion barrier effect is taken into account.

As the piezoresistive device is fabricated from PSNFs, a doping concentration^[12] more than 10^{20} cm^{-3} is generally chosen. In this heavily doped case, the depletion layer is narrow and the potential barrier is low, and the GB has more remarkable effects on the carrier transport processes than the depletion region, which cannot be ignored. So, the physical properties of the GB are further complemented and it is assumed:

(1) The GB is a kind of disordered amorphous material, of which the band gap is much greater than that of monocrystal. Generally, the amorphous silicon band gap is about 1.5–1.6 eV, and the Fermi level is clamped in the middle of the forbidden gap^[13].

(2) The structure of PSF can be seen as a large number of small size monocrystal grains with thin intervals. The thin interval (about a few atomic layers) is a kind of amorphous material. Heterojunctions form between each grain and the amorphous material of its surrounding GB. Then a position barrier appears between the grain and the GB in the energy band structure diagram.

Based on the above assumptions, the energy band structure of polysilicon is shown in Fig. 1, Where the position barrier height equals the difference between the top of monocrystal valence band to the mobility edge of the amorphous valence band, as denoted by $q\phi$. For convenience, a polysilicon model with a one-dimensional array is analyzed as an example, which assumes the grain is a uniform cube with a side length of L . When E_x , the kinetic energy along the x direction, is less than qV_b (the potential barrier height of the depletion layer), the holes can pass the depletion layer within the crystal grain and the GB barrier only in tunnel mode, forming a field emission current, and the current density is denoted by J_1 .

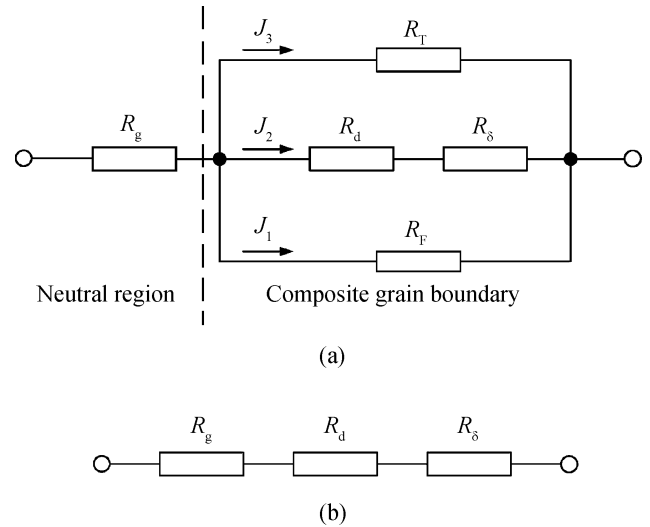


Fig. 2. Equivalent circuit of tunnel piezoresistive model. (a) The general form. (b) The simplified form at moderate temperature.

While $qV_b < E_x < q\phi$, the holes pass the depletion layer by thermionic emission, and then tunnel through the GB barrier, the current density formed in this way is expressed as J_2 . While $E_x > q\phi$, the holes completely pass through the depletion region and the GB barrier by thermionic emission, forming a thermionic emission current whose density is expressed as J_3 .

For the p-type material, whether it is monocrystal silicon or polysilicon, the piezoresistive effects are due to the split of the degeneracy band near the top of the valence band by stress, which leads to some changes in the effective mass of holes. However, for polysilicon, the change of effective mass not only varies the grain resistivity in the neutral zone, which generates a piezoresistive effect the same as the mechanism of monocrystal silicon, but also directly varies the current flowing through the GB, which brought the GB piezoresistive effect. Therefore, the piezoresistive effect of the grain neutral zone and the GB region together determine the piezoresistive properties of polysilicon.

J_2 is a kind of mixed current where the holes tunnel through the GB after passing the depletion region through thermal emission. In order to analyze the piezoresistive characteristics of compound GB (GB and both sides of its barriers), the mixed current path will be seen as two equivalent series resistances. One is the equivalent emission resistance of the depletion region determined by thermal emission, as denoted by R_d , the other is the equivalent tunneling resistance of GB determined by tunneling which is denoted as R_δ . Therefore, the model of the tunneling piezoresistive equivalent circuit is given. As shown in Fig. 2(a), R_g is the resistance of the grain neutral zone, R_T is the resistance determined by the thermal emission current J_3 , R_F is the resistance determined by the field emission current J_1 .

Although the three types of current co-exist, in general, only J_2 is dominant. Therefore, the equivalent circuit of the piezoresistive model can be simplified as the form shown in Fig. 2(b). Therefore, the GF of polysilicon can be expressed as:

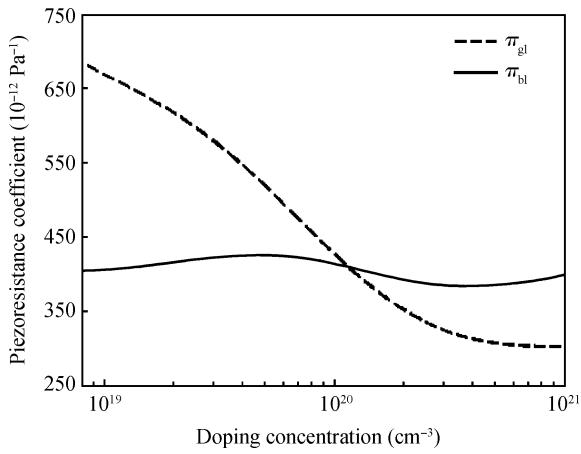


Fig. 3. Dependences of piezoresistance coefficients π_{gl} and π_{bl} on doping concentration.

$$G_p = \frac{R_g}{R_g + R_b} G_g + \frac{R_b}{R_g + R_b} G_b, \quad (1)$$

where R_b is a compound GB resistance, which satisfies $R_b = R_d + R_g$; G_g and G_b are the GFs of R_g and R_b , respectively. G_g and G_b are determined respectively by π_g , the piezoresistive coefficient (PRC) of monocrystal silicon and π_b , the PRC of compound GB and the elasticity of the monocrystal silicon substrate.

3. Calculations of the GFs of PSNFs

Using Eq. (1), the GF of PSNF can be expressed as:

$$\begin{aligned} G_p &= \frac{R_g}{R_p} G_g + \left(1 - \frac{R_g}{R_p}\right) G_b \\ &= \frac{2W + \delta \frac{\rho_g}{\rho_p}}{L} G_g + \left(1 - \frac{2W + \delta \frac{\rho_g}{\rho_p}}{L}\right) G_b, \end{aligned} \quad (2)$$

where $R_p = R_g + R_b$, ρ_g and ρ_p are the grain neutral zone resistivity and the polysilicon resistivity, respectively. If the polysilicon grain orientation is uniform, for example, in the orientation of $\langle 111 \rangle$, G_g and G_b can be obtained from the corresponding π_g and π_b .

The compound boundary PRC, π_b , can be obtained from the PRCs of R_d and R_g . For the $\langle 111 \rangle$ orientation, π_{bl} the longitudinal PRC of the compound GB can be expressed as^[7]:

$$\pi_{bl} = 0.525 \left(1 - \frac{V_{gb}}{V_0}\right) \pi_{gl} + 1.406 \frac{V_{gb}}{V_0} \pi_{gl}, \quad (3)$$

where π_{gl} is the longitudinal PRC of $\langle 111 \rangle$ orientation of monocrystal silicon, V_0 is the bias voltage of the compound GB, V_{gb} is the bias voltage of GB. Equation (3) reflects the dependence between π_{bl} and π_{gl} . At room temperature, using the relationship between π_{bl} and π_{gl} and the doping concentration, the dependence between the PRC of compound GB and doping concentration N_A can be obtained from Eq. (3), as shown in Fig. 3^[7].

Our experiment results prove that the grain-orientation of PSNF is random^[12]. Tanikawa's results also proved this^[14]. Therefore, for analysis of the piezoresistive properties of PSNFs, $\langle G_{gl} \rangle$ the average longitudinal GF of grain neutral zones with various orientation and $\langle G_{bl} \rangle$ the average longitudinal GF of corresponding compound GBs should be used to replace G_{gl} , the longitudinal GF of grain neutral zone, and G_{bl} , the longitudinal GF of compound GB respectively. For the PSFs with a random grain orientation, until now, almost all research has averaged the GFs of monocrystal silicon in all possible grain orientations to calculate the GF of the grain neutral zone^[2], and this method is widely accepted. In this work, we adopt Schubert's method^[15] to calculate the average GF of the grain neutral zone. The ratio between the average longitudinal GF of the grain neutral zone of the PSF with random grain orientation and $\langle 111 \rangle$ monocrystal silicon longitudinal GF was calculated to be 0.537, then

$$\langle G_{gl} \rangle = 0.537 (1 + 2\nu + Y\pi_{gl}) f, \quad (4)$$

$$\langle G_{bl} \rangle = 0.537 (1 + 2\nu + Y\pi_{bl}) f, \quad (5)$$

where $Y = 1.87 \times 10^{11}$ Pa, $\nu = 0.25$, are Young's modulus of $\langle 111 \rangle$ orientation and Poisson's ratio, respectively. f is the adjustment factor. The purpose of the introduction of adjustment factors is to compensate for errors, which are caused by the following three main factors. The first one is the error of Young's modulus values. Here, we used the value of monocrystal silicon. Generally, Young's modulus of polysilicon is slightly smaller, sometimes less than 70% of the monocrystal silicon Young's modulus^[16, 17]. Secondly, the errors are caused by the dispersion of grain size. The last one is due to the uncertainty of the grain orientation, which also brings some errors. For the samples of p-type PSNFs with a thickness of 80 nm and an average grain size of 32 nm^[7], f equals 0.86, which was obtained from the comparison between the theoretical calculation G_p-N_A curves and experimental results.

In order to describe the dependences between polysilicon GF and doping concentration using Eq. (2), the resistivity ratio of the grain neutral zone to polysilicon should be determined. Usually, during the calculation of polysilicon GF, the resistance of the grain neutral zone is calculated by utilizing the resistivity of monocrystal silicon^[2, 15]. The resistivity of polysilicon can be obtained from the test results. For the above discussed PSNF with a thickness of 80 nm, according to the fitting curve of actual test results at room temperature, the dependences between resistivity and doping concentration can be given as:

$$\rho_p = 15.651e^{-1.73 \times 10^{-19} N_A} + 0.014 (\Omega \cdot \text{cm}). \quad (6)$$

According to semiconductor physics, at room temperature, the resistivity of p-type monocrystal silicon is:

$$\rho_g = \frac{m_p^* (P_s + P_i)}{qN_A}, \quad (7)$$

where m_p^* is effective mass of hole; P_s is the scattering probability caused by acoustic waves, which is considered as a constant that is independent to the doping concentration at room temperature; P_i is the scattering probability due to ionized impurities, which is in proportion to the doping concentration.

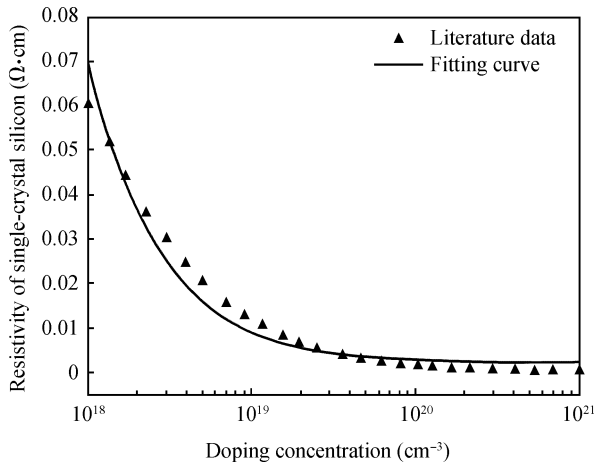


Fig. 4. Dependence of monocrystal silicon resistivity and the boron-doped concentration.

Therefore, at room temperature, Equation (7) can be rewritten as:

$$\rho_g = a_s N_A^{-1} + a_i, \quad (8)$$

where a_s and a_i are constants determined by P_s and P_i , respectively. Then, according to the curve^[18] of dependence between the p-type silicon resistivity and the doping concentration, doping concentration data are selected in a range of $5 \times 10^{18} - 10^{21} \text{ cm}^{-3}$. Using the data, the functional relationship between resistivity and doping concentration is fitted according to Eq. (8), and the fitting result is shown in Fig. 4. Thereafter, at room temperature, the dependence between the resistivity of monocrystal silicon and the doping concentration is proposed, which is expressed as:

$$\rho_g = 6.8741 \times 10^{20} N_A^{-1} + 2 \times 10^{-5} \text{ (}\Omega \cdot \text{m)}. \quad (9)$$

The smaller the grain size is, the higher the defect density is. For the polysilicon grain neutral zone, due to a higher defect density, the resistivity can not be calculated simply by Eq. (9), the lattice defect scattering must be also considered. If it was assumed that the defect density is not related to the doping concentration, then a correction factor a_d could be introduced which is determined by defect density, thereby, during the calculation of the resistivity of the neutral zone, Equation (9) can be modified as:

$$\rho_g = (6.8741 \times 10^{20} + a_d) N_A^{-1} + 2 \times 10^{-5} \text{ (}\Omega \cdot \text{m)}. \quad (10)$$

For PSNFs, by comparing the theoretical calculation $G_p - N_A$ with the experimental results, the value of a_d is determined to be $1.2 \times 10^{22} \text{ }\Omega/\text{m}^2$. The role of the defect scattering is equivalent to ionized impurity scattering with an impurity concentration of $6 \times 10^{20} \text{ cm}^{-3}$, which is well understood for polysilicon nano-film with a thickness of 80 nm and a grain size of 32 nm. If the grain surface dangling bonds are considered as defects, the magnitude of the defect density is 10^{21} cm^{-3} .

For the samples of p-type PSNFs, by synthesizing Eqs. (2), (4), (5), (6) and Eq. (10), combining with the dependences between PRCs and doping concentration shown in Fig. 3, the theoretical curve between GF of PSNF and doping concentration can be obtained, as shown in Fig. 5.

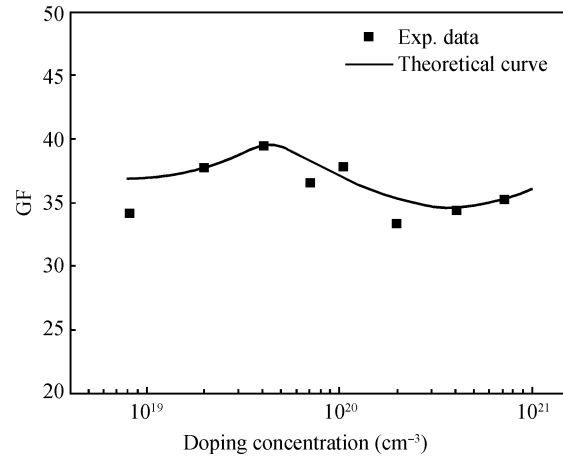


Fig. 5. The theoretical and experimental $G_p - N_A$ relationship of PSNF.

The experimental data shown in Fig. 5 are from the actual test results^[7]. A comparison of the curve shown in Fig. 5 and the experimental results show that the tunnel piezoresistive model is in good agreement with the experimental data; proving the validity of the tunnel piezoresistive model.

4. Discussions

Figure 3 shows that the variation of the PRC of compound GB with the doping concentration is more complex compared to that of monocrystal silicon, but the variation magnitude is much smaller, and the PRC is greater than for monocrystal silicon in the heavily doped case. This is the intrinsic reason that the PRC of heavily doped PSNF is larger. As the doping concentration increases further, the ratio of equivalent tunneling resistance and the equivalent emission resistance becomes larger, and the GF of heavily doped PSNF increases with increasing doping concentration, as shown in Fig. 5.

The thickness of conventional PSF used for piezoresistive sensors is typically a few hundred nanometers, or even up to several microns, and the grain size is generally more than 80 nm. As the grain size is larger, in the heavily doped case, the piezoresistive effect in the grain neutral zone dominates, and ignoring the tunneling piezoresistive effect will incur much error. When the doping concentration is low, the influence of the depletion layer barrier is much more than the effect of the GB barrier, so the tunneling piezoresistive effect can also be ignored. Thus, although the tunneling piezoresistive effect was not considered in previous model, there is still a good explanation for general piezoresistive characteristics of conventional PSFs. Obviously, the characteristics of conventional PSFs also can be explained by the tunneling piezoresistive model. To prove this, the new model has been used to simulate the $G_p - N_A$ relationship of the PSFs made by Schubert *et al.*^[15]

Schubert *et al.* deposited 400 nm-thickness PSFs on a $\langle 100 \rangle$ silicon substrate at 625 °C. The grain orientation of the PSFs was mainly $\langle 110 \rangle$, and the average grain size L was 120 nm. They measured resistivity at different doping concentrations, and used a simple beam structure to test piezoresistive characteristics. In theoretical calculations, they ignored the piezoresistive effect of compound GB, and only considered the piezoresistive effect of the grain neutral zone, and then calcu-

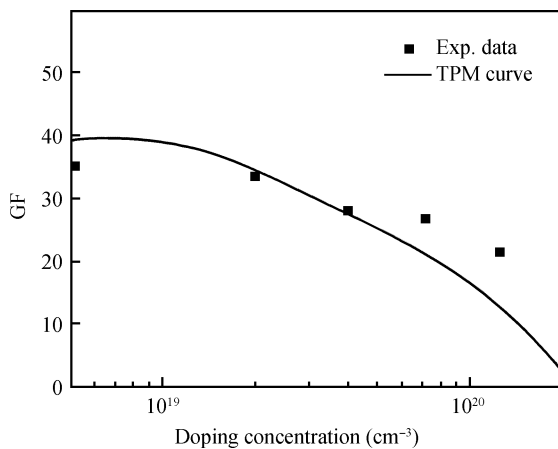


Fig. 6. G_p-N_A relationship simulation of PSF and experimental results.

lated the theoretical curve of the G_p-N_A relationship utilizing the dependences given by Kanda^[19] between the p-type silicon PRCs and the doping concentration. For the GB trap density, they took data of $1.9 \times 10^{12} \text{ cm}^{-2}$ presented by Lu *et al.*^[20]. The resistivity ratio of monocrystal silicon to polysilicon was amended so that the ratio is 0.58 at a doping concentration of $2.5 \times 10^{19} \text{ cm}^{-3}$.

Based on the experimental results of Schubert *et al.*, the G_p-N_A relationship was simulated using the tunneling piezoresistive model, as shown in Fig. 6. During the simulation, we fully adopted the parameters used by Schubert *et al.*, and took a GB thickness of 1 nm.

In Fig. 6, it shows that the simulation result of tunneling piezoresistive model is broadly consistent with the experimental results. There is an error at the high doping concentrations, just the same as the theoretical results by Schubert, due to using the dependencies given by Kanda between the p-type silicon PRCs and the doping concentration. In the heavily doped case, there is a large deviation from the dependences given by Kanda and the experimental results^[21].

5. Conclusions

Through analyzing the polysilicon band structure and the conductive mechanism, the tunneling piezoresistive model is established. The results showed that: in heavily doped (usually more than 10^{20} cm^{-3}) concentrations, the PRC of the compound GB of a PSNF is not only greater than that of the grain neutral zone, but also increases with increasing doping concentration. The piezoresistive model reveals the intrinsic mechanism of important experimental phenomena that the GF of a PSNF increases as the doping concentration increases in a heavily doped case.

For PSNFs and conventional PSFs, the dependence between GF and doping concentration has been simulated respectively using the tunneling piezoresistive model. The results of the two simulations are in good agreement with the corresponding experimental test results. This indicates that the tunneling

piezoresistive model can not only be used for analyzing the piezoresistive characteristics of PSNFs, but also for the conventional PSFs.

References

- [1] Jaffe J M. Monolithic polycrystalline-silicon pressure transducer. *Electron Lett*, 1974, 10(20): 420
- [2] Mosser V, Suski J, Obermeier E. Piezoresistive pressure sensors based on polycrystalline silicon. *Sensors and Actuators*, 1991, A28: 113
- [3] Obermeier E, Kopystynski P. Polysilicon as a material for microsensor applications. *Sensors and Actuators*, 1992, A30(1/2): 149
- [4] French P J, Evens A G R. Piezoresistance in polysilicon. *Electron Lett*, 1984, 20: 999
- [5] French P J, Evens A G R. Polycrystalline silicon strain sensors. *Sensors and Actuators*, 1985, 7: 135
- [6] Liu Xiaowei, Huo Mingxue, Chen Weiping, et al. Theoretical research on piezoresistive coefficients of polysilicon films. *Chinese Journal of Semiconductors*, 2004, 25(3): 292
- [7] Chuai Rongyan, Liu Bin, Liu Xiaowei, et al. Tunneling piezoresistive effect of grain boundary in polysilicon nano-films. *Journal of Semiconductors*, 2010, 31(3): 032002
- [8] Liu Xiaowei, Lu Xuebin, Chuai Rongyan, et al. Polysilicon nanofilm pressure sensor. *Sensors and Actuators*, 2009, A154: 42
- [9] Zhao Xiaofeng, Wen Dianzhong. Fabrication and characteristics of a nano-polysilicon thin film pressure sensor. *Journal of Semiconductors*, 2008, 29(10): 2038
- [10] Kamins T I. Hall mobility in chemically deposited polycrystalline silicon. *Appl Phys*, 1971, 42: 4357
- [11] Rai-Choudhury P, Hower P L. Growth and characterization of polycrystalline silicon. *Electrochem Soc*, 1973, 120: 1761
- [12] Chuai Rongyan, Liu Xiaowei, Huo Mingxue, et al. Influence of doping level on the gauge factor of polysilicon nanofilm. *Chinese Journal of Semiconductors*, 2006, 27(7): 1230
- [13] Spear W E, le Comber P G. Electronic properties of substitutionally doped amorphous Si and Ge. *Phil Mag*, 1976, 33: 935
- [14] Tanikawa A, Taisumi T. (100) oriented poly-Si film grown by ultrahigh vacuum chemical vapor deposition. *J Electrochem Soc*, 1994, 141(10): 2848
- [15] Schubert D, Jenschke W, Uhlig T, et al. Piezoresistive properties of polycrystalline and crystalline silicon films. *Sensors and Actuators*, 1987, 11: 145
- [16] Ding Jianning, Meng Yonggang, Wen Shizhu. Young's modulus of polysilicon microcantilever beams by deflection using nanoindentation. *Chinese Journal of Scientific Instrument*, 2001, 22(2): 186
- [17] Yi T, Kim C J. Measurement of mechanical properties for MEMS materials. *Meas Sci Technol*, 1999, 10: 706
- [18] Warner R M, Grung B L. *Semiconductor-device electronics*. Beijing: Publishing House of Electronics Industry, 2002: 160
- [19] Canda Y. A graphical representation of the piezoresistance coefficients in silicon. *IEEE Trans Electron Devices*, 1982, 29: 64
- [20] Lu N C C, Gerzberg L, Lu C Y, et al. Modeling and optimization of monolithic polycrystalline silicon resistors. *IEEE Trans Electron Devices*, 1981, 28: 818
- [21] Harley J A, Kenny T W. 1/F noise considerations for the design and process optimization of piezoresistive cantilevers. *J Microelectromech Syst*, 2000, 9: 226