The study of mechanical stress in NEMS heterostructures

X. Xu, B. Bercu, F. Lime and L. Montès

IMEP-LAHC laboratory, Minatec, UMR 5130 Grenoble Institute of technology
BP257, MINATEC, 3 PARVIS LOUIS NEEL, Grenoble, France, 38016
xux@minatec.inpg.fr, bercu@minatec.inpg.fr, montes@minatec.inpg.fr

ABSTRACT

Mechanical stress is increasingly applied in microelectronics. For instance, strained silicon technology is widely used to improve carrier mobility and driver current for advanced MOS transistors. For micro electromechanical systems, piezoresistive effects are widely used in pressure sensors. In this paper we present an original method for studying mechanical stress in nanodevices placed on ultra-thin membranes, which has several advantages compared with the conventional four-point-bending method. Using this architecture, we use FEM simulations of an innovative NEMS pressure sensor to investigate its static and dynamic modes. We study the optimal orientation and position of a nanowire on the membrane We show that a large improvement in pressure measurement sensitivity can be obtained by adopting tunnel junction technology. We also investigate the dynamic multi-bends of the nanostructure in its dynamic deformation modes and introduce the transport matrix method to calculate the tunnel current. Finally, our work helps to understand the electrical and mechanical properties of the nanostructure under the influence of large mechanical stress and to design innovative NEMS pressure sensors.

Keywords: Mechanical stress/strain, pressure sensor, ultra-thin membrane, NEMS, hetero junction nanowire

1 INTRODUCTION

Mechanical stress plays an increasingly important role in microelectronics. For instance, by using strained silicon technology for advanced MOS transistors, carrier mobility and therefore the drive current are significantly improved[1]. On the other hand, in the domain of MEMS piezoresistive effects are used in pressure sensors.

To investigate the impact of the mechanical stress on the properties of microelectronic devices and nanostructure, it is necessary to introduce new method. Compared with the conventional four-point-bending method [2], our ultra-thin membrane technique shows several advantages. These include the ability to induce heavier mechanical stresses. It is also a unique way to obtain dynamic deformations with frequencies up to several MHz.

In this paper, we present an innovative NEMS pressure sensor based on a (i) tunnel junction, (ii) nanowire and (iii) heterostructure on a membrane. The finite element method (FEM) simulation shows a large variation of tunneling current with applied pressure in static mode. In the dynamic mode, the nanowire can be multi-bended. The character of the tunnel junction thickness variation of the nanowire is investigated under different frequency excitations. To evaluate the tunnel current, we have also used the transport matrix method. This method is very suited to calculate electron transport probability in the case of hetero structures and thereby to estimate the tunneling current value both for the case of the multi quantum wells or the multi quantum barriers.

Finally, for our NEMS pressure sensor based on hetero nanostructure, we conclude by demonstrating the large improvement in measurement sensitivity.

2 ULTRA THIN MEMBRANE TECHNIQUE

To obtain a highly accurate area and thickness, the ultra-thin membranes are fabricated by deep reactive ion etching (DRIE) on silicon on insulator (SOI) wafer [3]. We can vary the membrane area from square micrometers up to square millimeters and the membrane thickness is of the order of a few hundred nanometers up to a few micrometers. In this study, the area of the membrane is 150 μm×150 μm. This membrane is made of three layers: one silicon layer of 300 nm sandwiched between two silicon dioxide layers of 400 nm. There are two main kinds of membrane actuation: static and dynamic. Using a vacuum chamber placed under the membrane, a static deformation is induced on the membrane corresponding to the differential pressure (up to 3 atm). As far as dynamic actuation is concerned, we choose a piezoelectric device as the oscillation source. By placing a membrane cover on this piezoelectric device which is driven by an AC voltage, the membrane vibrates. In this way, the frequency of oscillation can be up to several MHz. When the oscillation frequency approaches the membrane natural frequency, the maximum amplitude is observed with little damping.

3 OPTIMAL ORIENTATION AND POSITIONING STUDY OF THE NANOSTRUCTURE ON THE MEMBRANE

At nano scale, instead of using the piezoresistive effect for design the traditional MEMS pressure sensor, we can find a new way to improve poor pressure measurement sensitivity of conventional nanowires ($\Delta R/R < 1\%$). Consequently, we propose to use tunnel current as an extremely sensitive gauge. In our case, the diameter of the heavy n-type doping silicon heterostructure nanowire is 800 nm, the length is 10 μm, and the tunnel junction is made of silicon dioxide. Its thickness is 2 nm, thus the direct tunneling phenomenon dominates [4]. To calculate the direct tunneling current value, we used the Register [4] and the Lee models [5] which are appropriate for different tunnel junction thicknesses. In the other hand, for increasing the interface area between the nanowire and the membrane, we employ a hexahedral model instead of a cylinder model.

We thus can study the optimal positioning of this heterostructure nanowire on the membrane in order to optimize the measurement sensitivity.

Two possibilities were investigated here, transversal (see figure 1 inset) and longitudinal orientation (figure 1). Firstly, we consider the transversal orientation. The variable ζ is defined as the distance between the edge of the membrane and the tunnel junction in nanowire, as shown in figure 1. For different values of ζ, we find that the tunnel junction thickness remains almost invariant. The result of this simulation shows the relative rate does not exceed 0.1%. This relative rate is the variation of tunnel thickness compared to the initial thickness. If nanowires are mounted longitudinally, substantial tunnel junction thickness variation can be observed. Thereby, we conclude that a longitudinal orientation will result in larger measurement sensitivity than a transversal orientation.

To model the optimal position of the nanostructure on the membrane, we should find the relationship between the membrane dimension and this optimal position. Depending on the Timoshenko model [6], the membrane deflection (w) under the pressure can be calculated by the equation (1)

$$\omega(\zeta) = \omega_0(\zeta) + 2\omega_1(\zeta) \tag{1}$$

Here the ω_1 and ω_2 are presented by equation (2) and (3) respectively.

$$\omega_1(\zeta) = \frac{4PL^4}{\pi^5 D_R} \sum_{m=1,3,5,\cdots}^{\infty} \frac{(-1)^{\frac{m-1}{2}}}{m^5} \cos(\frac{m\pi\zeta}{L})$$
$$(1 - \frac{\alpha_m(1-\tanh(\alpha_m)+2)\cosh(\frac{m\pi\zeta}{L})}{2\cosh(\alpha_m)} + \frac{\frac{m\pi y}{L}\sinh(\frac{m\pi y}{L})}{2\cosh\alpha_m}) \tag{2}$$

$$\omega_1(\zeta) = \frac{-L^2}{2\pi^2 D_R} \sum_{m=1,3,5,\cdots}^{\infty} \frac{E_m \cos(\frac{m\pi\zeta}{L})(-1)^{\frac{m-1}{2}}}{m^2\cosh(\alpha_m)} \tag{3}$$
$$(\frac{m\pi y}{L}\sinh(\frac{m\pi\zeta}{L}) - \alpha_m \tanh(\alpha_m)\cosh(\frac{m\pi\zeta}{L}))$$

And L is the membrane side length of the membrane, P is the pressure, the D_R is the flexural rigidity, E_m can be described by the equation (4)

$$E_m = C_m \frac{4PL^2}{\pi^3}_{m=1,3,5,\cdots} \tag{4}$$

Where, the $C_m (m = 1, 3, 5, \cdots)$ are the constants depending on the boundary condition of membrane.

Firstly, the t_{ox} is made up of 3 deflection components $xt_{ox}, yt_{ox}, zt_{ox}$ that can be described by the equation:

$$t_{ox} = \sqrt{(xt_{ox} + t_{ox0})^2 + (yt_{ox})^2 + (zt_{ox})^2} \tag{5}$$

Compared with the zt_{ox} component, the components xt_{ox} and yt_{ox} are negligible. The maximum zt_{ox} induces the maximum t_{ox}, here zt_{ox} can be calculated by:

$$zt_{ox} = \frac{d\omega(\zeta)}{d\zeta} t_{ox0} \tag{6}$$

thereby, t_{ox} can be calculated by the following equation

$$t_{ox} \approx (t_{ox0})\sqrt{1 + [\frac{d\omega(\zeta)}{d\zeta}]^2} \tag{7}$$

We found the maximum first derivation of $\omega(\zeta)$, this value produces the maximum tunnel junction thickness variation. Thereby, the point of inflection which satisfies the condition of

$$\frac{d^2\omega(\zeta)}{d\zeta^2}_{\zeta=optimalposition} = 0 \tag{8}$$

In addition, there is a range where t_{ox} is very close to its maximum and at least 99.9% of this value. In this range, all the values of ζ can satisfy the condition as follow:

$$\mid \frac{d\omega(\zeta)}{d\zeta} \mid \geq \sqrt{(\frac{t_\varepsilon}{t_{ox0}})^2 - 1} \tag{9}$$

If we define the function θ that is

$$\theta = \sqrt{(\frac{t_\varepsilon}{t_{ox0}})^2 - 1} \tag{10}$$

Finally, we can deduced the optimal position region width equation as follow:

$$\omega^{-1}(\int \theta d\zeta) < \zeta < \omega^{-1}(-\int \theta d\zeta) \Longrightarrow \Delta\zeta \qquad (11)$$

Here, ω^{-1} is the inverse function of ω. This equation describes the optimal position range width of the nanowire on the membrane. For example, in our case, under the 2 atm. pressure, this optimal position range width could be as large as 7.5 μm (in figure 2). The optimal position region (D) can be described as follow:

$$D = \zeta_{optimal} \pm \frac{1}{2}\Delta\zeta \qquad (12)$$

More importantly, this optimal position region allows for large photolithographic misalignment and easy positioning.

4 ELECTRICAL TRANSPORT IN NANOSTRUCTURE ON MEMBRANE

Having placed the nanostructure in an optimal orientation and position, we now investigate the tunneling current as a function of the applied pressure. We have checked that the von Mises stress value in the nanowire is still within the range permitted by its tensile and compressive strength. Moreover, we must also take into account the effect of the mechanical stress on the energy band structure. The deformation matrix $[\varepsilon]$, transformation matrix $[s]$ [7] and the mechanical stress matrix $[\sigma]$ can be written as [8]:

$$[\varepsilon] = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} = [s] \cdot [\sigma]$$

$$[\Delta E_c] = \begin{bmatrix} \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} & \varepsilon_{xx} \\ \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} & \varepsilon_{yy} \\ \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} & \varepsilon_{zz} \end{bmatrix} \cdot \begin{bmatrix} \Xi_d \\ \Xi_u \end{bmatrix}$$

Where, $[\Delta E_c]$ is the conduction band variation matrix corresponding to the 3 degenerate valleys of silicon and Ξ_d, Ξ_u are the independent constants. For stress values and heavy n-type doping nanowire considered in this paper, the calculation result of matrix $[\Delta E_c]$ shows that that the conduction band structure variation is not negligible. We know that this stress value is quiet enough to alter the conduction band structure and to reduce the barrier height.

According to the direct tunneling current model Register [4] and Lee [5], we calculated the direct tunneling current density as a function of the applied pressure from 0 atm to 2 atm. Both models give very similar results in this pressure range. Figure 4 shows the result of the Register model on a log-scale. The current density (***J***) in the nanowire as a function of the t_{ox} shown by this plot can be fitted by an exponential law in the range of 1 atm to 2 atm:

$$J = J_0 \cdot e^{-A \cdot t_{ox}} \qquad (13)$$

where, J_0 is the initial current density value, ***A*** is a constant corresponding to the nanowire material. The direct tunneling current is an exponentially decreasing function of the thickness of tunnel junction. Because the pressure is pseudo-linearly proportional with the tunnel junction thickness variation, we can describe the relationship between the current density and the pressure by:

$$J = J_0 \cdot e^{-B \cdot \delta(P)} \qquad (14)$$

where, ***B*** is a constant corresponding to the nanowire material. P is the pressure. $\delta(P)$ is the function can be presented by the equation

$$\delta(P) = (t_{ox0})\sqrt{1 + [C_P \cdot P]^2} \qquad (15)$$

Here, C_P is the constant depending on the membrane dimension and material. Figure 3 shows the result of the Register model on a log-scale. This exponential relationship between the tunneling current and the pressure is truly remarkable for improving the pressure measurement sensitivity.

The dynamic simulation of the nanostructure takes into account the impact of damping. The damping factor was evaluated by the half-power bandwidth method [9]. Very high frequency excitations (frequency > 6 MHz) produce very weak deformations. Whereas, the deformation amplitude was produced by the low frequency excitation, its value is nearly same as static deformation. Furthermore, near the natural frequency, the deformation of the membrane can be extremely large. For higher forcing frequencies, more oscillatory deformations emerge on the surface of membrane (inset of figure 4). This will induce frequency-dependent multi-bends in the nanostructure as shown in figure 4. These oscillatory deformations and the nanostructure multi-bending can lead to an interesting new way to study the impact of mechanical stress in nanostructures.

5 CONCLUSION

In this paper, we studied the mechanical stress in a $Si/SiO_2/Si$ nanostructure placed on an ultra-thin membrane which is used as the experimental inter-media element. We demonstrated that the optimal measurement sensitivity can be obtained by mounting the nanostructure on the membrane with a longitudinal orientation and have a wide optimal position zone allowing for large photolithographic misalignment and easy positioning. We simulated the electrical transport behavior of this heterostructure nanowire by using two direct tunneling current models. An exponential relationship between the direct tunneling current and the pressure is obtained and demonstrates that the interest of this kind of NEMS device to design ultra sensitive pressure sensor. This nanostructure is very attractive as it can also be used to realize dynamic deformation in the nanowires for high forcing frequencies, the oscillatory deformation causes multi-bending in the nanostructure. This innovative approach can thus be used to investigate the impact of mechanical stresses on nanostructures and NEMS.

REFERENCES

[1] S. Chattopadhyay, L.D. Driscoll, K.S.K. Kwa, S.H. Olsen, and A.G. O'Neill. Strained si mosfets on relaxed sige platforms. *Solid-State Electronics*, 48:1407–1416, 2004.

[2] C. Gallon, G. Reimbold, G. Ghibaudo, R.A. Bianchi, and R. Gwoziecki. Electrical analysis of external mechanical stress effects in short channel mosfets on (001) silicon. *Solid-State electronics*, 48:561–566, 2004.

[3] B. Bercu, L. Montès, and P. Morfouli. Fea calculations for ultra thin piezoresistive pressure sensor on soi for heatspreader integration. *Proceedings of IEEE EuroSimE 2006*, 2006.

[4] L.F. Register, E. Rosenbaum, and K. Yang. Analytic model for direct tunneling current in polycrystalline silicon-gate metal-oxide-semiconductor devices. *Applied physics letters*, 74:457–459, 1999.

[5] W.C. Lee and C.M. Hu. Modeling gate and substrate currents due to conduction- and valence-band electron and hole tunneling. *VLSI Technology, 2000. Digest of Technical Papers. 2000 Symposium*, pages 198–199, 2000.

[6] S. Timoshenko S.Woinowsky-Krieger. Theory of plates and shells. *McGraw-Hill College, second edition*, pages 197–202, 1970.

[7] J.S. Wortman and R.A. Evans. Young modulus, shear modulus and poisson's ratio in silicon and germanium. *Applied physics*, 36:153–156, 1965.

[8] C. Herring and E. Vogt. Transport and deformation potential theory for many-valley semiconductors with anisotropic scattering. *Physical review*, 101:944–961, 1956.

[9] R.W. Clough and J. Penzien. Dynamics of structures. *Mcgraw-Hill College, Second edition*, pages 54–56, 1993.

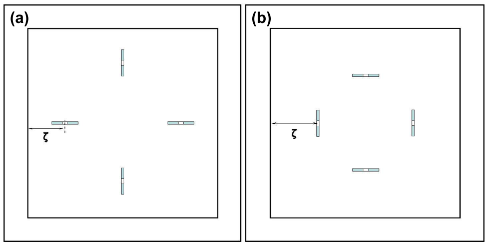

Figure 1: the longitudinal orientation (a) and the transversal orientation (b) of nanowire on membrane.

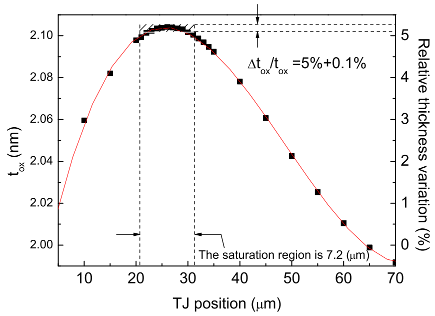

Figure 2: Tunnel junction thickness variation as a function of the tunnel junction position ***d*** for 150μm×150μm×1.1μm membrane

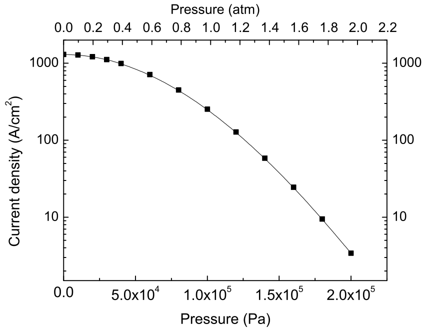

Figure 3: Tunneling current density variation as a function of pressure.

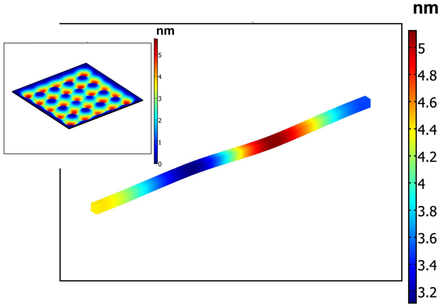

Figure 4: Multi-bend dynamic deformation of the nanowire on the dynamic deformation membrane (20Hz, see the inset of this figure)