Modeling of Directional Dependence in Nanowire Flow Sensor

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Abstract: Three dimensional finite element analysis model has been constructed for testing the directional dependence in a novel form of nanowire array gas flow sensor. Single nanowire (p-type single crystal Silicon) model is developed using fluid structure interaction and piezoresistivity components in COMSOL MEMS module. Change in resistivity tensor due to induced stress in the nanowire base will result in generating output voltage proportional to the gas flow in the channel. It is found that the two main components of stress tensor σ_{xz} and σ_{yz} are proportional to the induced electrical field within the nanowire base. Current results show that the anisotropic properties of the material can be successfully used in the gas flow sensor to differentiate flow components in different directions.

Keywords: Gas flow sensor**,** Piezoresistivity, Nanowire, Anisotropic Property

1. Introduction

Microelectromechanical devices have been widely used these days concurrently with the decades' fast development in the micro- and nano-electromechanical system (MEMS/NEMS) technology. Availability of a reliable and robust micro-scale gas flow sensor has proven to be an important requirement in these MEMS devices. Current study is focused on modeling a novel form of multi-directional gas flow sensor which is designed by utilizing a Si nanowire array and its piezoresistive properties to change conductivity upon flow pressure on the sensor material. Finite element analysis (FEA) model constructed using COMSOL Multiphysics® software has been used for modeling piezoresistive phenomena in the nanowire array. Figure 1 displays the configured model of a nanowire array sensor with gas flowing through the channel.

The piezoresistance properties of Silicon (Si) and Germanium (Ge) were first discovered by Smith in 1953 [1], since then numerous studies have been conducted on Si and various other materials attempting to enhance the piezoresistive properties and develop new applications [2, 3]. Si has become a prominent candidate for piezoresistive devices due to multiple reasons, such as its high piezoresistant coefficients, high operating temperature, low cost, etc..

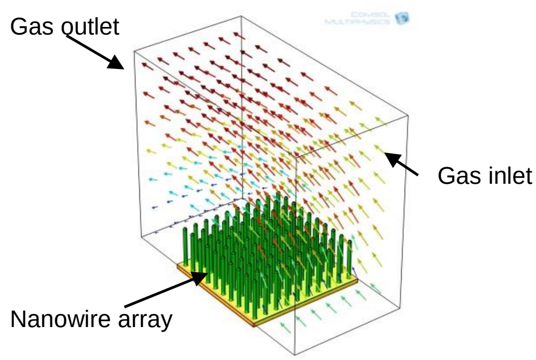

Figure 1 - Nanowire array gas flow sensor

In addition, nanoscale Si structures have electrical properties distinct from those in bulk form owing to a significant change in their electronic structures and therefore behaviors. Particularly low dimensional structures such as nanosheets and nanowires have radically different electronic structures. Numerous experiments conducted on p-doped Si nanowires in the past decade have revealed its giant longitudinal piezoresistant coefficient [4, 5] as supported by multiple theoretical studies using first principle calculations [6, 7].

2. Theory

In this section we will develop the theoretical framework and derive the governing formulae for the Si nanowire based piezoresistive sensor.

Mechanism of the nanowire flow sensor is based on the voltage induced in the nanowire base upon applied stress and current density as schemed in Figure 2. The electrical field within the material can be written as a function of its current density and resistivity.

$$\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \begin{bmatrix} \rho_{xx} & \rho_{xy} & \rho_{xz} \\ \rho_{yx} & \rho_{yy} & \rho_{yz} \\ \rho_{zx} & \rho_{zy} & \rho_{zz} \end{bmatrix} \times \begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix}$$

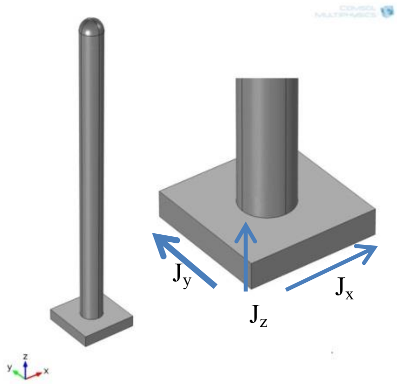

Figure 2 - Current density of nanowire base

When there is no stress applied on the system resistivity tensor takes a diagonal form,

$$\rho_{xx} = \rho_{yy} = \rho_{zz} = \rho_0 = 8 \times 10^{-5} \Omega\, m$$

Applying external stress on the nanowire will change the resistivity tensor and non-diagonal elements will gain non-zero values depending on the external stress and piezoresistive tensor of the material. New resistivity tensor of the material under stress can be written as the sum of initial resistivity tensor and change in resistivity tensor.

$$\begin{bmatrix} \rho_{xx} & \rho_{xy} & \rho_{xz} \\ \rho_{yx} & \rho_{yy} & \rho_{yz} \\ \rho_{zx} & \rho_{zy} & \rho_{zz} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rho_0 + \begin{bmatrix} \Delta\rho_{xx} & \Delta\rho_{xy} & \Delta\rho_{xz} \\ \Delta\rho_{yx} & \Delta\rho_{yy} & \Delta\rho_{yz} \\ \Delta\rho_{zx} & \Delta\rho_{zy} & \Delta\rho_{zz} \end{bmatrix} \rho_0$$

Change in resistivity can be written as a function of external stress and piezoresistivity tensor.

$$\begin{bmatrix} \Delta\rho_{xx} \\ \Delta\rho_{yy} \\ \Delta\rho_{zz} \\ \Delta\rho_{yz} \\ \Delta\rho_{xz} \\ \Delta\rho_{xy} \end{bmatrix} = \begin{bmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} & \Pi_{14} & \Pi_{15} & \Pi_{16} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} & \Pi_{24} & \Pi_{25} & \Pi_{26} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} & \Pi_{34} & \Pi_{35} & \Pi_{36} \\ \Pi_{41} & \Pi_{42} & \Pi_{43} & \Pi_{44} & \Pi_{45} & \Pi_{46} \\ \Pi_{51} & \Pi_{52} & \Pi_{53} & \Pi_{54} & \Pi_{55} & \Pi_{56} \\ \Pi_{61} & \Pi_{62} & \Pi_{63} & \Pi_{64} & \Pi_{65} & \Pi_{66} \end{bmatrix} \times \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix}$$

Considering the crystal symmetry (m3m) of Si, [8] the above formula reduces to:

$$\begin{bmatrix} \Delta\rho_{xx} \\ \Delta\rho_{yy} \\ \Delta\rho_{zz} \\ \Delta\rho_{yz} \\ \Delta\rho_{xz} \\ \Delta\rho_{xy} \end{bmatrix} = \begin{bmatrix} 6.6 & -1.1 & -1.1 & 0 & 0 & 0 \\ -1.1 & 6.6 & -1.1 & 0 & 0 & 0 \\ -1.1 & -1.1 & 6.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 138.1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 138.1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 138.1 \end{bmatrix} * 10^{-11} \times \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix}$$

It can be seen that the non-diagonal elements in $\Delta\rho$ tensor have following relationships with the stress components.

$$\Delta\rho_{yz} = 138.1 \times 10^{-11} \times \sigma_{yz}$$
$$\Delta\rho_{xz} = 138.1 \times 10^{-11} \times \sigma_{xz}$$
$$\Delta\rho_{xy} = 138.1 \times 10^{-11} \times \sigma_{xy}$$

Considering the applied voltage (input) in z-direction,

$$J_x \approx 0$$
$$J_y \approx 0$$
$$J_z \neq 0$$

the induced electrical fields can be written as:

$$E_x = \Delta\rho_{xz} \times J_z$$
$$E_y = \Delta\rho_{yz} \times J_z$$
$$E_z = (1 + \Delta\rho_{zz}) \times J_z$$

$$V_x = E_x \times X = \Delta\rho_{xz} \times J_z \times X$$
$$V_y = E_y \times Y = \Delta\rho_{yz} \times J_z \times Y$$
$$V_z = E_z \times Z = (1 + \Delta\rho_{zz}) \times J_z \times Z$$

$$V_x = 138.1 \times 10^{-11} \times \sigma_{xz} \times J_z \times X$$
$$V_y = 138.1 \times 10^{-11} \times \sigma_{yz} \times J_z \times Y$$
$$V_z = (1 + (-1.1 \cdot \sigma_{xx} - 1.1 \cdot \sigma_{yy} + 6.6 \cdot \sigma_{zz}) \times 10^{-11}) \times J_z \times Z$$

As seen in the Figure 2 and above formulae, electrical field induced in the x and y direction will depend on their respective stress components, piezoresistive value and current density in z direction.

3. COMSOL Model and Governing Equations

Considering the higher computational cost of modeling the entire nanowire array sensor, which consists of thousands of nanowires, current study has been conducted on a reduced single nanowire model. Since the main focus of the study is to test the directional dependence of the gas flow sensor single nanowire model will be sufficient for the task in hand. Figure 3 shows the configured single wire model used in this study.

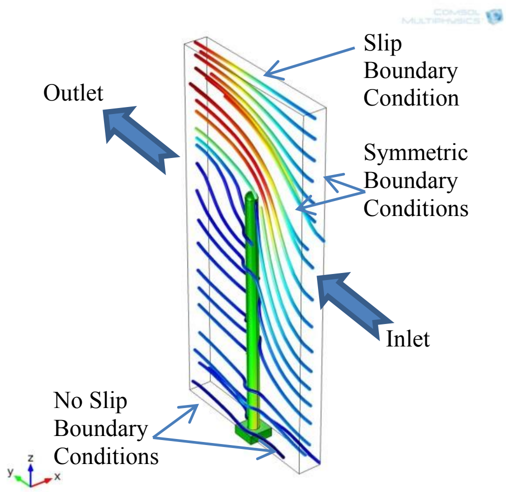

Figure 3 - COMSOL model, Single wire gas flow

Constructed model consists of three types of physics coupled together, fluid flow and structural mechanics (Fluid Structure interaction) and piezoresistivity (MEMS module). 3D FEA model of p-type single crystal Si nanowire has been constructed and tested for multiple variables such as induced stress tensor, induced voltage and electrical field with varying gas flow direction in the channel. Parametric study has been used to analyze the flow direction dependence of the induced stress/voltage of the sensor by rotating the gas channel around the nanowire from 0^o to 360^o (full circle) in increments of 45^0.

3.1 Dimensions, parameters and boundary conditions used in the model

The model consists of a single wire with a length of 8um and a radius of 200nm. Nanowire base has dimensions of 800nm in x and y directions and 300nm in z direction (thickness). Gas channel used in the model is 30µm in height (z direction), 11.2µm in depth (y direction) and 800nm in width (x direction). P-type single crystal Si has been assigned to both nanowire and its base and the gas channel is filled with air selected from the built-in material selection database. Nanowire base is defined as the piezoresistive material with a dopant concentration of 1.32 x 10^{19} cm^{-3}.

Figure 4 shows the nanowire base with its voltage input and output boundaries. For the single nanowire model 1µV has been used as the input voltage. Gas flow induced stress and input voltage will generate an electrical field within the nanowire base, which will create a voltage difference between vertical boundaries that can be measured as the output voltage of the device.

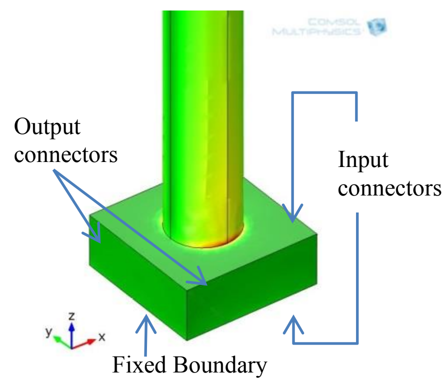

Figure 4 - Nanowire base with input / output

Gas velocity at the inlet is set to be 0.05m/s and the outlet pressure is defined as atmospheric pressure. None-slip boundary conditions are enforced at the bottom surfaces of the gas channel to get a rough surface effect while slip boundary conditions are enforced at the top surface to simulate the gas flow above the top surface. Periodic structure in the x direction is supported by the symmetric boundary conditions defined at the side walls of the gas channel.

3.2 Governing equations of the COMSOL model.

The fluid flow in the channel is described by the incompressible Navier-Stokes equations for the velocity field, u; and the pressure, p

$$\rho\frac{\partial u}{\partial t} - \nabla\cdot[-pI + \eta(\nabla u + (\nabla u)^T)] + \rho\big((u-u_m)\cdot\nabla\big)u = F$$

$$-\nabla\cdot u = 0$$

The nanowire is fixed to the piezoresistive base and all the other surfaces of the nanowire experience a load from the gas flow which is given by, (n is the normal vector to the boundary)

$$F_T = -n\cdot(-pI + \eta(\nabla u + (\nabla u)^T))$$

The relation between the electrical field, E, and the current, J, within a piezoresistor is given by the following formula:

$$E = \rho\cdot J + \Delta\rho\cdot J$$

Where ρ is the resistivity and Δρ is the induced change in the resistivity which is related to the stress, σ and piezoresistive tensor Π by the constitutive relationship:

$$\Delta\rho = \Pi\cdot\sigma$$

3.3 Parametric study

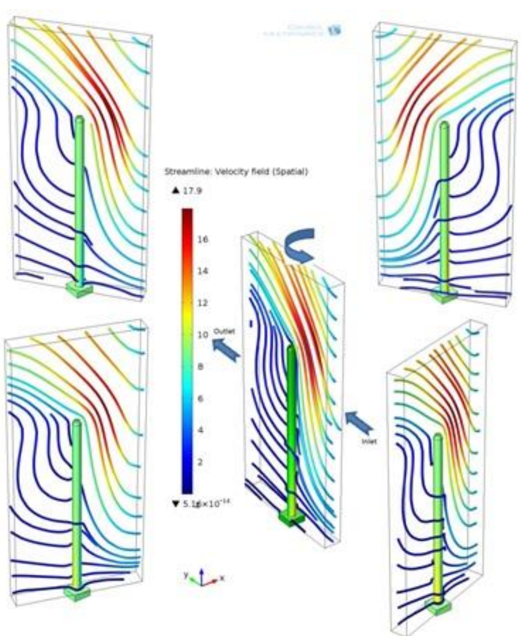

Figure 5 - Directional dependence of single nanowire model

Induced stress in the nanowire base has been calculated for changing flow direction by rotating the gas channel around the nanowire axis using a parametric study as shown in Figure 5.

4. Results

Average induced stress in the piezoresistor has been calculated for changing gas flow direction. Stress components σ_{xz} and σ_{yz} Vs flow direction is plotted in Figure 6.

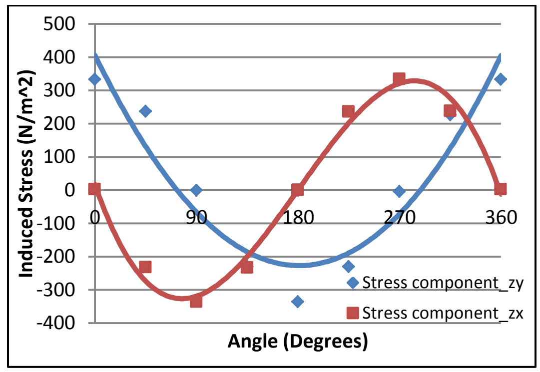

Figure 6 – σ_{xz} and σ_{xz} vs. flow direction

Gas flow induced stress will change the resistivity tensor of the piezoresistive base, $\Delta\rho_{zy}$ and $\Delta\rho_{zx}$ vs. flow direction is plotted in Figure 7.

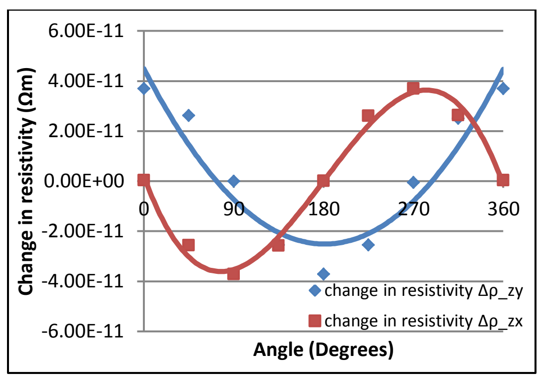

Figure 7 - Resistivity change vs. flow direction

From Figure 8 it shows the change in induced electrical field in the nanowire base with the varying flow direction in the channel.

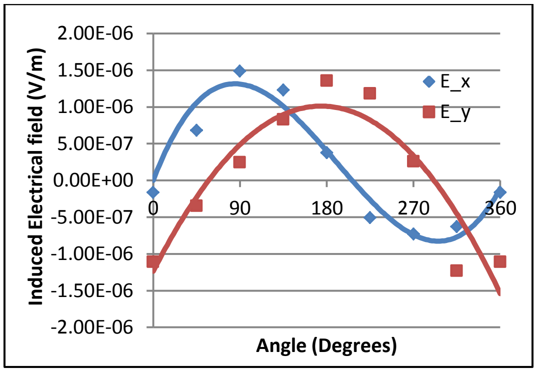

Figure 8 - Induced electrical field in the nanowire base vs. flow direction

Nanowire array flow sensor can be used in determining the flow direction by analyzing the two voltage outputs, V_x, due to induced E_x and V_y, due to the induced E_y from the sensor.

Flow in +y direction :-

$$E_x \approx 0\ ,\ E_y \approx negative\ maximum$$

Flow in - y direction :-

$$E_x \approx 0\ ,\ E_y \approx positive\ maximum$$

Flow in +x direction :-

$$E_y \approx 0\ ,\ E_x \approx negative\ maximum$$

Flow in - x direction :-

$$E_y \approx 0\ ,\ E_x \approx positive\ maximum$$

5. Conclusion

In summary, a 3D model has been developed to test the directional dependence of nanowire gas flow sensor. Output of the nanowire flow sensor is directly proportional to the induced stress in the nanowire base. Average values of the stress components σ_{xz} and σ_{yz} vary with flow direction allowing the sensor to detect the gas flow direction inside the channel. Current results suggest that the anisotropic properties of the material can be successfully used in the nanowire array gas flow sensor to differentiate flow components in different directions.

6. References

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7. Acknowledgements

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