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ADVANCEMENTS IN MODELING THE SPACE CHARGE INDUCED FLEXOELECTRIC EFFECT

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ABSTRACT

Flexoelectricity offers an energy harvesting alternative to piezoelectric materials. Although flexoelectricity is generally weak in most materials, recent findings show that bending a semiconductor with insulating barrier layers could induce a significantly enhanced flexoelectric response. We call this effect the Space Charge Induced Flexoelectric (SCIF) effect. This study explores the induced polarization resulting from free charge redistribution in a doped silicon beam. To understand the underlying physics, a 3D numerical model combining flexoelectric principles and the drift-diffusion theory of semiconduction was developed. The effective flexoelectric coefficient was computed by comparing the differential charge accumulation at the top and bottom of the beam and compared that with the experimental observations.

KEYWORDS

Flexoelectricity, Semiconducting materials, Finite element analysis, Transducers.

INTRODUCTION

Flexoelectricity refers to the coupling between strain gradient and electric polarization that exists, in principle, in all dielectric materials and would allow for an energy harvesting alternative to piezoelectric materials. In recent years, significant efforts have been directed toward discovering an eco-friendly substitute for lead zirconate titanate (PZT), a commonly utilized material in piezoelectric energy harvesting transducers. Although flexoelectricity provides a potential alternative, the flexoelectric effect is weak in most materials. However, recently it has been shown that bending a semiconductor with insulating barrier layers could induce a significantly enhanced flexoelectric response [1]. The presence of significantly enhanced flexoelectricity in the semiconducting materials is promising as it opens the path for replacing current piezoelectric-based transducers.

According to the linear continuum theory of flexoelectricity, the electric polarization P in a linear dielectric is

$$P_i = \chi_{ij} E_j + \mu_{klij} \nabla_j \varepsilon_{kl} \qquad (1)$$

where E_j is the electric field component, ε is the mechanical strain tensor, χ is the second-order dielectric susceptibility tensor, and μ is the fourth-order tensor of flexoelectric coefficients. The above equation indicates that the flexoelectric induced polarization is function of the flexoelectric coefficient and the strain gradient. The flexoelectric coefficient is itself a function of permittivity [2], [3]. Space charge structures, in which charge carriers can traverse a substantial distance before encountering an insulating boundary, can exhibit a notably elevated effective dielectric permittivity [4], thus increasing the effective flexoelectric coefficient. Achieving a high strain gradient is the second ingredient of a large flexoelectrically induced polarization. Bending structures exhibit strain gradients, but to achieve very high gradients, sub-micron scale structures are necessary [5]. An alternative means of achieving a heightened strain gradient with larger structures involves compressing truncated pyramids [6]. Thus, truncated pyramidal structures made of semiconducting materials with dielectric barrier layers could exhibit a large polarization and potentially be used as a replacement for piezoelectric transducers.

The space charge induced effect in semiconductors can be significant. For barium strontium titanate (BST) with mobile charges, the very high value of nearly $1000\ \mu Cm^{-1}$ has been reported [1]. In order to enhance the effect and achieve a higher effective flexoelectric coefficient in other semiconducting materials, it is necessary to study the interaction between mechanical fields and mobile charges in flexoelectric semiconducting materials. The research on the induced redistribution of free carriers in flexoelectric semiconductors is scattered and limited to 1D beam models [7], [8], and semiconductive nanowire [9], [10], and there are no existing computational tools accessible to facilitate the investigation of the physics involved in these materials for more sophisticated models.

This paper will report on the experimental and numerical investigation of SCIF semiconductors as a potential replacement for piezoelectric transducers. For this purpose, a 3D model developed earlier that is capable of simulating flexoelectricity in solids is utilized [11]. However, this model did not explicitly solve for the enhancement due to the mobile space charge in a semiconductor. Here, that work is extended to develop a 3D numerical model consisting of the theory of flexoelectricity and the drift-diffusion theory of semiconduction. More specifically, the model solves the coupling between Newton's law, the charge equation of electrostatics, and the conservation of charge for holes and electrons.

FLEXOELECTRIC SEMICONDUCTORS

In order to obtain the set of three-dimensional coupled equations describing the electromechanical behavior of flexoelectric semiconductors, in this study, the theory of flexoelectricity and the drift-diffusion theory of semiconduction are used which gives the following set of governing equations.

$$\sigma_{ij,j} - \tau_{ijk,jk} + f_i = \rho\ddot{u}_i$$
$$D_{i,i} = q(p - n + N_D^+ - N_A^-) \quad (2)$$
$$J_{i,i}^{hole} = q\dot{p}$$
$$J_{i,i}^{electron} = q\dot{n}$$

where σ is the usual stress tensor, τ is a higher-order stress that involves the effect of micro-structural inhomogeneities [12], ρ is the mass density, f is the force, u is the mechanical displacement vector, D is the electric displacement vector, q is the elementary charge, p and n are the concentrations of holes and electrons, N_D^+ and N_A^- are the concentrations of ionized donors and accepters, and J^{hole} and $J^{electron}$ are the hole and electron current densities. It is assumed that 1. all donors and acceptors are ionized, 2. The doping level (p_0) is uniform, and 3. the small perturbation (Δp) of carrier concentration allows use of a linearization method [7]. These assumptions lead to the following constitutive relations.

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$
$$\tau_{ijk} = h_{ijklmn}\eta_{lmn} - \mu_{lijk}E_l$$
$$D_i = \kappa_{ij}E_j + \mu_{ijkl}\eta_{jkl} \quad (3)$$
$$J_i^{hole} \cong qp_0\mu_{ij}^{hole}E_j - qD_{ij}^{hole}(\Delta p)_{,j}$$
$$J_i^{electron} \cong qp_0\mu_{ij}^{electron}E_j + qD_{ij}^{electron}(\Delta n)_{,j}$$

where $\eta_{lmn} = \varepsilon_{lm,n}$ is the strain gradient, E_l is the electric field vector, c_{ijkl} are the elastic stiffness, h_{ijklmn} are higher-order material constants, μ_{ijkl} are the flexoelectric constants, κ_{ij} are the dielectric constants, μ_{ij}^{hole} and $\mu_{ij}^{electron}$ are the carrier mobilities, and D_{ij}^{hole} and $D_{ij}^{electron}$ are the carrier diffusion constants. According to Equation (2), under a mechanical load, the carriers move due to the electric field produced through flexoelectric coupling (see Figure 1).

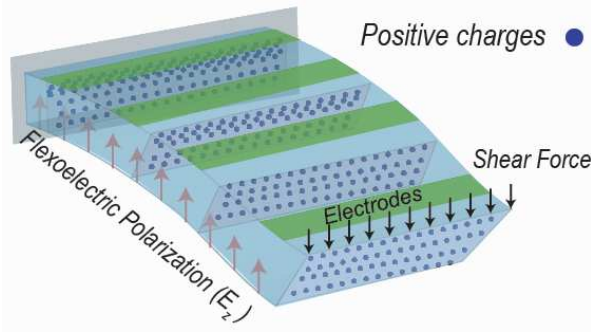

Figure 1. Schematic illustrating the redistribution of free charge carriers in a deformed flexoelectric semiconductor beam.

EXPERMENTAL RESULTS

The experimental setup shown in Figure 2 was used to measure the induced polarization due to free charge redistribution in a doped silicon beam (1 cm long, 5 cm wide, and 520 μm thick) with an insulating HfO_2 layer of

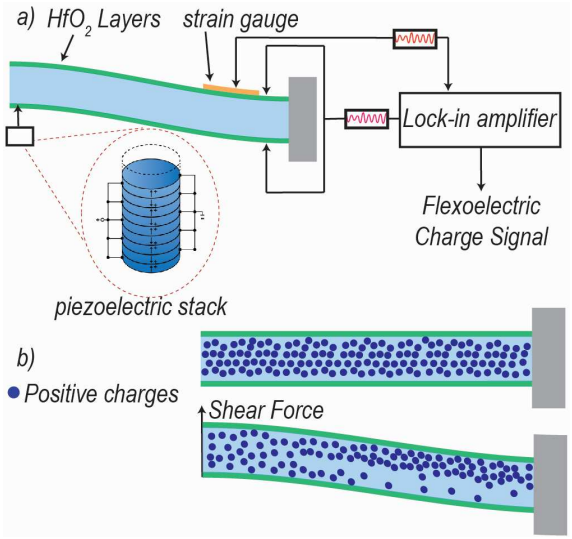

Figure 2. a) Experimental setup for measuring flexoelectric coefficient of doped silicon beam. A 4 Hz AC voltage applied to a piezoelectric stack drive the free end of the beam. The strain gauge, connected to a lock-in amplifier, measures the strain on the surface of the flexoelectric structure. A current amplifier measures the charge from the top electrode, phase-matched by the lock-in amplifier, to generate an output signal. b) Free carriers (holes in p-doped silicon beam) accumulate at the upper surface due the electric field induced by the flexoelectricity.

30 nm thickness on both sides. For this experiment, the beam was p-doped (doped with boron) with a resistivity of $\sim 1 - 10\ ohm - cm$, and the dopant concentration was $1.4 \times 10^{15} atom/cm^3$ to $1.5 \times 10^{16} atom/cm^3$. The 30 nm of undoped, amorphous HfO_2 onto both surfaces was deposited via ALD.

Using the measurement set up in Figure 2, the effective flexoelectric coefficient was found to be 4.9±0.4 μC/m (see Figure 3). The measured value for the effective flexoelectric coefficient is higher than the predictions based on the linear response theory of flexoelectricity verifying an enhancement from the doping [13]. Compared to one value of the flexoelectric coefficient of silicon as reported in the literature ($0.4 \times 10^{-9} C/m$) [13], the results depicted in Figure 2 indicate an approximately $10^4 X$ enhancement. The ability to explore this intriguing experimental result through physics-based simulations

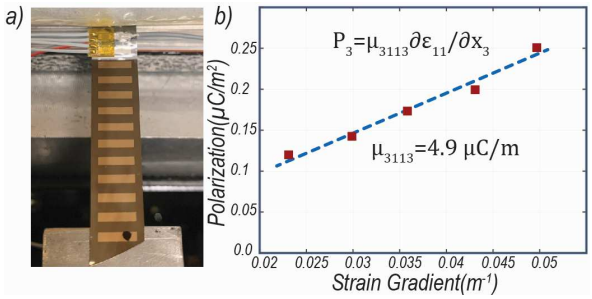

Figure 3. a) 500 μm doped silicon flexoelectric beam with a width of 1 cm and a length of 5 cm. A 30 nm thick insulating HfO2 layer is deposited on both silicon surfaces. b) Experimental measurement of effective flexoelectric coefficient for the doped silicon beam.

could elucidate the mechanism and inform optimizations. However, due to the challenging nature of simulating realistic inhomogeneous flexoelectric systems, there is a lack of accessible computational tools to support the study of the underlying physics in these materials. Therefore, developing a computational system that can accurately predict the flexoelectricity in semiconductors is of great value.

NUMERICAL MODELING AND RESULTS

Equation (2) with the appropriate Dirichlet boundary conditions and Neumann boundary conditions which can be found in [13], [14] can be solved analytically only for very simple models, such as the Euler–Bernoulli beam [8], [9]. For more complicated models, a computational model must be utilized. A mixed formulation was developed in FEniCSx open software to solve the partial differential equation system in Equation (2). The material properties for the silicon are listed in Table 1 [8].

Table 1: Material properties for silicon.

Physical property	symbol	Value
Elastic stiffness constants	c_{1111} c_{1122}	$166 \times 10^9\ N/m^2$ $63.9 \times 10^9\ N/m^2$
Dielectric susceptibility	χ	$0.107 \times 10^{-9}\ C/mV$
Flexoelectric constants	μ_{3113}	$0.5 \times 10^{-6}\ C/m$
Hole mobility	μ_{11}^{hole}	$450 \times 10^{-4}\ \frac{m^2}{V \bullet s}$
Diffusion constant of holes	D_{ij}^{hole}	$12 \times 10^{-4}\ \frac{m^2}{V \bullet s}$

The model accurately forecasts the redistribution of free charges within a beam, as illustrated in Figure 4. When subjected to mechanical stress, holes within the material relocate owing to the electric field generated through flexoelectric coupling. At the upper surface of the beam, positive perturbations in carrier concentration are observed, indicative of the anticipated accumulation of holes in that region.

In order to compare the numerically predicted results with the experimental results in Figure 3, the effective flexoelectric coefficient was calculated from the differential charge accumulation at the top and bottom of the beam. The charge accumulation in the current flexoelectric semiconductor beam can be calculated as

$$Q = q \int_{\Omega} (\Delta p) d\Omega \tag{4}$$

From the experimental set up, the charge per unit area is

$$D_3 = -\mu_{3113} \eta_{113} \tag{5}$$

Finally, from Equation (4), at any location through the beam length, the amount of charge accumulated at the top surface per unit area can be calculated as

$$P^* = q \Delta p \frac{h}{2} \tag{6}$$

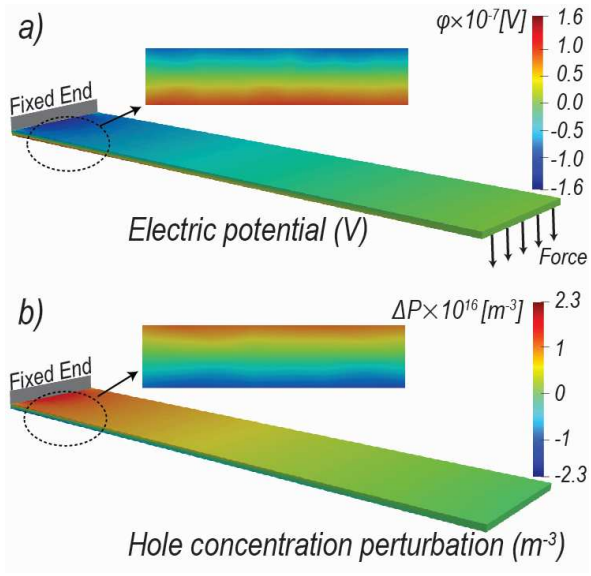

Figure 4. Simulation results for a doped silicon beam with force applied to the free end resulting in a strain gradient through the thickness of the beam. a) Distribution of the electric potential and, b) redistribution of free carriers in the doped silicon beam.

P^*, is the induced polarization due to free charge redistribution. P^* was calculated for different strain gradient values to obtain the effective flexoelectric coefficient of the doped silicon beam; this enables comparison of the numerical results with the experimental results in Figure 3. Figure 5 shows the calculated polarization as a function of strain gradient for different values of the flexoelectric coefficient in undoped silicon. (The different strain gradients occur at different locations along the length of the beam.) The slope of each line in Figure 5 indicates the effective flexoelectric coefficient of the doped silicon structure that includes the enhancement due to the free charge redistribution. The results in Figure 5 indicate approximately $10X$ enhancement in the effective flexoelectric coefficient due to the doping of the silicon.

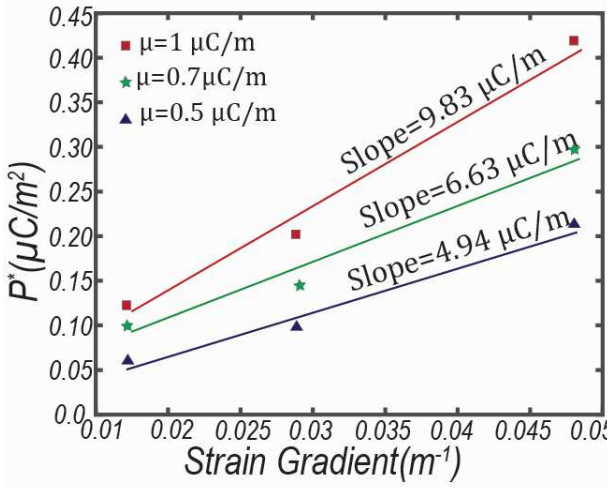

Figure 5. Induced polarization due to free charge redistribution in doped silicon.

For the case of $\mu = 0.5\mu C/m$, the numerical results match the results in Figure 3. We should note that there are few reports of the flexoelectric coefficient of undoped silicon in the literature and these reports vary widely, from $10^{-9}C/m$ [13] to $10^{-6}C/m$ [15]. The value of $0.5\mu C/m$ is at the at the very high end of what is reported in the literature leading to some skepticism in the accuracy of the numerical results. Thus, further investigation is needed to determine the flexoelectric coefficient of undoped silicon and the exact cause and magnitude of the observed effective flexoelectric effect.

CONCLUSIONS

In this paper, the hypothesis that strain gradients induce charge redistribution in semiconductors, resulting in electrical polarization, was tested. The experiments confirmed significant induced polarization in doped silicon beams (1 cm x 5 cm x 520 μm) with 30 nm insulating HfO_2 layers. To further amplify this effect and attain a higher effective flexoelectric coefficient, the interplay between mechanical fields and mobile charges in these materials was explored using a 3D numerical model that integrates the principles of flexoelectricity and the drift-diffusion theory of semiconduction. The effective flexoelectric coefficient was calculated and matched experimental data for $\mu = 0.5\mu C/m$, but this value exceeds most flexoelectric coefficients reported for silicon. Further investigation is needed to determine the exact magnitude and nature of the observed enhancement due to the space charge effect.

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