SiC-Based Piezoelectric Energy Harvester for Extreme Environment

Jagan Mohan Reddy Kudimi\textsuperscript{a,b,*}, Faisal Mohd-Yasin\textsuperscript{a,b}, Sima Dimitrijev\textsuperscript{a,b}

\textsuperscript{a}Griffith School of Engineering, Griffith University, Brisbane and 4111, Australia
\textsuperscript{b}Queensland Micro- and Nanotechnology Centre, Griffith University, Brisbane and 4111, Australia

Abstract

This paper explores the feasibility of employing cubic silicon carbide on silicon wafer (3C-SiC-on-Si) as a vertical cantilever for the piezoelectric-based energy harvesting in the $d_{31}$ mode intended for the extreme environments. 100nm thick 3C-SiC layer is plasma-etched out of the $<100>$ silicon (Si) wafer and is employed as a bottom electrode, 1μm thick Aluminum nitride (AlN) as a piezoelectric thin film (active layer) and 50nm thick Molybdenum is sputtered on top of the cantilever structure as a top electrode. The length and width of the cantilever beam are 400μm and 30μm, respectively. The performances of the energy harvester using 3C-SiC and Si as bottom electrode and substrate are simulated and compared. The generated output voltage at 1KΩ load resistance is 7.85 times higher for the 3C-SiC based device. Additional tests at higher temperatures show 3C-SiC superior performances in terms of generated power and material strength.

1. Introduction

The emergence of low power wireless electronics and its applications prompt the active research in finding the alternative power sources to enable long term operations and its employment in remote and hard to reach locations such as internal combustion engines. Different ambient energy sources are available in environment for harvesting energy such as solar, thermoelectric, acoustic and mechanical vibrations. Among these, the mechanical vibration energy source has the highest ability to power low power wireless electronic devices [1].

* Corresponding author. Tel.: +61737358026; fax: +61737358021.

E-mail address: jagan.kudimi@griffithuni.edu.au
Mechanical vibration has three transduction mechanisms namely piezoelectric, electromagnetic and electrostatic [2]. Piezoelectric is the most promising solution for powering low power wireless electronic devices and ability to generate maximum power for a given size [3].

Silicon (Si) based cantilever piezoelectric energy harvesters have been investigated in many research works and some of them are briefly mentioned here. In one such works, Si-based cantilever piezoelectric energy harvester used lead zirconate titanate (PZT) as piezoelectric material, platinum/titanium (Pt/Ti) used as electrode and nickel (Ni) as proof mass, which generates 2.16μW power [4]. Similar work employed the same materials for cantilever array piezoelectric energy harvester to produce 3.98μW power [5]. Two more research works on cantilever piezoelectric energy harvester were also implemented using Si substrate with Si as proof mass and generated 2.15μW [6] and 0.32μW [7].

However, none of the stated research works addressed the issue of extreme environment conditions such as higher loads and temperatures, as conventional Si technology will not be operational beyond 500°C [8]. The ability to withstand these extreme conditions is possible with silicon carbide (SiC). Table 1 shows the material properties of 3C-SiC and Si.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>3C-SiC</th>
<th>Si</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [Kg/m³]</td>
<td>3100</td>
<td>2330</td>
</tr>
<tr>
<td>Young’s Modulus [GPa]</td>
<td>440</td>
<td>160</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>0.14</td>
<td>2.4</td>
</tr>
<tr>
<td>Fracture Toughness [MPa·m₁/₂]</td>
<td>3.3</td>
<td>0.7</td>
</tr>
<tr>
<td>Hardness [GPa]</td>
<td>22.9</td>
<td>12.0</td>
</tr>
<tr>
<td>Ultimate Tensile Strength [MPa]</td>
<td>3440</td>
<td>7000</td>
</tr>
<tr>
<td>Energy Band Gap [eV]</td>
<td>2.4</td>
<td>1.1</td>
</tr>
<tr>
<td>Breakdown Field [MV/cm]</td>
<td>1</td>
<td>0.25</td>
</tr>
<tr>
<td>Mechanical Temperature operating range [°C]</td>
<td>&lt;1300°</td>
<td>&lt;500°</td>
</tr>
<tr>
<td>Electrical Device temperature limitation [°C]</td>
<td>&lt;600°</td>
<td>&lt;150°</td>
</tr>
</tbody>
</table>

This article explains the development of cantilever piezoelectric energy harvester based on two different substrates and to compare their performances. Section 2 presents mathematical modeling for cantilever beam to determine the generated output voltage. Section 3 discussed about finite element simulation setup in detail for modeling the 3D cantilever beam. Section 4 compares the performance of cantilever piezoelectric energy harvester based on 3C-SiC and Si substrates. Finally this paper is concluded based on the best performance of cantilever piezoelectric energy harvester at extreme environment conditions.

2. Mathematical Modeling

![Unimorph piezoelectric cantilever structure in 2 Dimensional](image-url)
2D unimorph piezoelectric cantilever beam is shown in fig.1, consisting of three layers i.e., piezoelectric layer, substrate/bottom electrode and top electrode. Cantilever is fixed at one end at x=0 and free at another end at x=L. The length of cantilever is ‘L’ and width of the cantilever is ‘w’. The length and width of the cantilever is identical for all three layers except for their thicknesses. The thickness of the substrate/bottom electrode, the piezoelectric and the top electrode layers are denoted as \( t_s \), \( t_p \) and \( t_e \), respectively. The direction of the length is poled along the x-axis and the thickness is poled along the z-axis. The neutral plane of the cantilever is denoted as \( n \). The Young’s modulus of the substrate/bottom electrode, the piezoelectric and the top electrode are represented as \( E_s \), \( E_p \) and \( E_e \), respectively. The constant force, \( F \) is applied on the cantilever tip or the free end of the cantilever in \( d_{31} \) vibrational mode. The neutral plane position [9] is shown as

\[
\int_{\text{Min}}^{\text{Max}} E \left( \frac{z-t_n}{r} \right) \, dz = 0
\]  

where ‘\( r \)’, the radius curvature of the cantilever is shown as

\[
t_n = \frac{-E_s t_s^2 + E_p t_p^2 + E_e (t_e^2 - t_t^2)}{2(E_s t_s + E_p t_p + E_e (t_e - t_p))}
\]

The bending modulus per unit width [9] of the cantilever is expressed as

\[
D = \int_{\text{Min}}^{\text{Max}} E(z - t_n)^2 dz
\]

\[
D = \frac{2}{3}\left( E_s t_s^3 + E_p t_p^3 + E_e (t_e^3 - t_t^3) \right) + t_n \left( E_s t_s^2 - E_p t_p^2 - E_e (t_e^2 - t_t^2) \right) + t_n^2 \left( E_s t_s + E_p t_p + E_e (t_e - t_p) \right)
\]

The generated electric field ‘\( E_g \)’ in z-direction [10] is expressed as

\[
E_g(x, z) = g_{31} \sigma
\]

where ‘\( g_{31} \)’ is piezoelectric coefficient related to piezoelectric strain coefficient, dielectric constant of piezoelectric and free space permittivity and ‘\( \sigma \)’ is lateral stress in piezoelectric layer. Finally, the Unimorph piezoelectric cantilever generated output voltage per unit force is shown as

\[
V_{avg} = \frac{L}{2} g_{31} \frac{E_p}{wD} \left( \frac{r}{2} - t_n t_p \right)
\]

Equation (6) states that the generated output voltage is purely depending on the cantilever beam dimensions, the material properties and also the applied force.

3. Finite Element Simulation

Two application modes are employed to model the cantilever piezoelectric energy harvester; the first is the structural mechanics and the second is piezoelectric. Both modes are crucial to analyze the cantilever beam in different environment conditions and also to determine the generated output voltage.

3.1. Geometry

The 3D cantilever structure is shown in fig.2, which consists of three layers and the proof mass that is placed at the free end. The length and the width of the cantilever are 400\( \mu \)m and 30\( \mu \)m, respectively, whereas the thicknesses are varying for each layer including the proof mass that is poled along the z-axis.
The substrate/bottom electrode has 100nm thickness, the piezoelectric layer has 1μm thickness, while the top electrode has 50nm thick layer. In our design, the proof mass is added mainly to increase the generated output power, while decreasing the resonance frequency. The dimensions for the proof mass are 30μm×30μm×20μm.

3.2. Subdomain Settings

The material selection is the main novelty of this design. Two different materials are employed for the cantilever piezoelectric energy harvester as the substrate/bottom electrode, namely the 3C-SiC and Si. The piezoelectric thin film is used as the active material with major advantages such as the generation of large motions, low hysteresis and high sensitivity with wide dynamic ranges [11]. Three major piezoelectric thin films are lead zirconate titanate (PZT), zinc oxide (ZnO) and aluminum nitride (AlN). AlN is chosen for this design due to its best compatibility and less risk of line contamination of the clean room. The material chosen for the top electrode and the proof mass is molybdenum (Mo), which has high density and ability to provide more displacement. The body load condition [12] is applied in each layer of the cantilever beam with an acceleration of 2.25ms⁻² [13] in d₃₁ mode.

3.3. Boundary Settings

The boundary settings is concerned with the constraint condition, the surface load and the electric boundary condition. A fixed constraint is used at one end of cantilever beam and the proof mass load is applied on top surface of the electrode. The floating potential and ground are assigned to the top and the bottom surfaces of the piezoelectric material, respectively and both surfaces are connected to the load resistance of 1KΩ with the help of SPICE netlist. The remaining surfaces of the piezoelectric layer are assigned as zero charge/symmetry.

3.4. Mesh Settings

In the mesh settings, the free mesh parameters option is chosen to mesh the 3D cantilever beam. Based on computational problem, the mesh size has been chosen as extreme coarse. The total number of mesh elements being arranged for this cantilever beam is 7118.
4. Results and Discussion

The mathematical modeling has been performed for the 2D cantilever beam without the proof mass. Equation (6) is used to determine the generated output voltage per unit force for 3C-SiC and Si substrates, which are $6.14 \times 10^6 \text{ VN}^{-1}$ and $5.91 \times 10^6 \text{ VN}^{-1}$, respectively.

![Fig. 3 Cantilever piezoelectric energy harvester](image)

Two types of analysis are carried out namely the Eigen and the frequency response. The performance of the cantilever piezoelectric energy harvester using 3C-SiC and Si as the substrates/bottom electrodes are compared. The resonant frequency of the structure is 5.401 KHz and 4.702 KHz for 3C-SiC and Si, respectively. The maximum displacements at these resonance frequencies for 3C-SiC and Si are 6.21μm and 1.31μm, respectively, as shown in fig.3(a). The generated output voltage at 1KΩ load resistance at the input acceleration of $2.25 \text{ m/s}^2$ are 6.04μV and 0.769μV for the 3C-SiC and Si, respectively.

A parametric sweep has been performed at different surface loads and temperatures to analyze the cantilever piezoelectric energy harvester at extreme environment with respect to the generated power and the strength, under resonance condition. Fig. 3(b) shows the generated power of the piezoelectric energy harvester at the applied surface load of 0Nm$^{-2}$ to 100Nm$^{-2}$ on top electrode. Fig. 3(c) and 3(d) show the generated power and the material strength of both 3C-SiC and Si-based cantilever piezoelectric energy harvester at the temperature range of 273.15K to 1273.15K. It should become very apparent that the results from these four figures demonstrate that the 3C-SiC based energy harvester has superior performance over Si based energy harvester.
Based on the mathematical and the finite element simulation results, we found that the 3C-SiC based cantilever piezoelectric energy harvester performs better in all aspects such as the displacement, the generated output voltage as well as extreme environments.

5. Conclusion

Piezoelectric-based energy harvesters are promising energy sources for powering low power wireless electronics. This paper performs the mathematical analysis and the finite element simulation modelling of cantilever structure on two different substrates, namely 3C-SiC and Si. The mathematical modelling demonstrates that the generated output voltage per unit force depends on cantilever beam dimensions, material properties and the applied force. Our calculation shows that the generated output voltage per unit force for 3C-SiC is 1.04 times higher than Si. The finite element simulation is then performed on the cantilever piezoelectric energy harvester with the proof mass to determine the generated output voltage at extreme environments. The generated output voltage at 1KΩ load resistance is 7.85 times higher for the 3C-SiC based cantilever energy harvester compared to Si based device. 3C-SiC based energy harvester also outperforms Si-based prototype in extreme environment conditions.

Acknowledgements

This work is supported by Queensland Micro- and Nanotechnology Centre (QMNC) and Griffith School of Engineering.

References

Appendix A. Generated voltage derivation for Cantilever piezoelectric energy harvester

Neutral plane position is determined by [9]

\[ \int_{\text{min}}^{\text{max}} E \left( \frac{z-t_n}{r} \right) dz = 0 \]  \hspace{1cm} (1)

\[ \int_{-t_s}^{0} E_s \left( \frac{z-t_n}{r} \right) dz + \int_{0}^{t_p} E_p \left( \frac{z-t_n}{r} \right) dz + \int_{t_p}^{t_e} E_e \left( \frac{z-t_n}{r} \right) dz = 0 \]  \hspace{1cm} (2)

where ‘r’ radius curvature of the cantilever shown in equation (3)

\[ \frac{1}{r} = -\frac{F}{wD}(L-x), \quad 0 < x < L \]  \hspace{1cm} (3)

\[ \frac{E_s}{r} \int_{-t_s}^{0} (z-t_n) dz + \frac{E_p}{r} \int_{0}^{t_p} (z-t_n) dz + \frac{E_e}{r} \int_{t_p}^{t_e} (z-t_n) dz = 0 \]  \hspace{1cm} (4)

\[ E_s \int_{-t_s}^{0} (z-t_n) dz + E_p \int_{0}^{t_p} (z-t_n) dz + E_e \int_{t_p}^{t_e} (z-t_n) dz = 0 \]  \hspace{1cm} (5)

\[ E_s \left( \frac{z^2}{2} - t_n z \right)_{-t_s}^{0} + E_p \left( \frac{z^2}{2} - t_n z \right)_{0}^{t_p} + E_e \left( \frac{z^2}{2} - t_n z \right)_{t_p}^{t_e} = 0 \]  \hspace{1cm} (6)

\[ E_s \left( -\frac{t_s^2}{2} - t_n t_s \right) + E_p \left( \frac{t_p^2}{2} - t_n t_p \right) + E_e \left( \frac{t_e^2}{2} - t_n t_e - \frac{t_p^2}{2} + t_n t_p \right) = 0 \]  \hspace{1cm} (7)

\[ -\frac{E_s t_s^2}{2} + \frac{E_p t_p^2}{2} + \frac{E_e t_e^2}{2} = E_s t_n t_s + E_p t_n t_p + E_e t_n t_e - E_e t_n t_p \]  \hspace{1cm} (8)

Therefore position of the neutral plane is expressed as

\[ t_n = -\frac{E_s t_s^2 + E_p t_p^2 + E_e (t_e - t_p)}{2 (E_s t_s + E_p t_p + E_e (t_e - t_p))} \]  \hspace{1cm} (9)

Bending modulus per unit width of the cantilever is expressed as [9]

\[ D = \int_{\text{min}}^{\text{max}} E(Z-t_n)^2 dz \]  \hspace{1cm} (10)

\[ D = \int_{-t_s}^{0} E_s (z-t_n)^2 dz + \int_{0}^{t_p} E_p (z-t_n)^2 dz + \int_{t_p}^{t_e} E_e (z-t_n)^2 dz \]  \hspace{1cm} (11)

\[ D = E_s \int_{-t_s}^{0} (z^2 - 2zt_n + t_n^2) dz + E_p \int_{0}^{t_p} (z^2 - 2zt_n + t_n^2) dz + E_e \int_{t_p}^{t_e} (z^2 - 2zt_n + t_n^2) dz \]  \hspace{1cm} (12)

\[ D = E_s \left( \frac{z^3}{3} - 2zt_n + t_n^2 \right)_{-t_s}^{0} + E_p \left( \frac{z^3}{3} - 2zt_n + t_n^2 \right)_{0}^{t_p} + E_e \left( \frac{z^3}{3} - 2zt_n + t_n^2 \right)_{t_p}^{t_e} \]  \hspace{1cm} (13)

\[ D = E_s \left( \frac{t_s^3}{3} + t_s^2 t_n + t_n^3 t_s \right) + E_p \left( \frac{t_p^3}{3} - t_p^2 t_n + t_n^3 t_p \right) + E_e \left( \frac{t_e^3}{3} - t_e^2 t_n - t_n^3 t_e \right) \]  \hspace{1cm} (14)

\[ D = \frac{1}{3} (E_s t_s^3 + E_p t_p^3 + E_e (t_e^3 - t_p^3)) + t_n (E_s t_s^2 - E_p t_p^2 - E_e (t_e^2 - t_p^2)) + t_n^2 (E_s t_s + E_p t_p + E_e (t_e - t_p)) \]  \hspace{1cm} (15)
The lateral strain in cantilever at position \((x, z)\) is
\[
\varepsilon = -\frac{z-t_n}{r}
\] (16)

\[
\varepsilon = \frac{F}{wD} (L - x)(z - t_n) \quad \text{for} \quad 0 < x < L
\] (17)

The lateral stress in the piezoelectric layer and shown in equation
\[
\sigma = \varepsilon E_p
\] (18)

\[
\sigma = \frac{F E_p}{wD} (L - x)(z - t_n) \quad \text{for} \quad 0 < x < L
\] (19)

In thickness direction, the generated electric field in the piezoelectric layer at \((x, z)\) is [10]
\[
E_g(x, z) = g_{31} \sigma
\] (20)

\[
E_g(x, z) = \frac{F E_p}{wD} (L - x)(z - t_n) \quad \text{for} \quad 0 < x < L
\] (21)

where \(g_{31}\) is the piezoelectric coefficient related to piezoelectric strain coefficient \(d_{31}\), dielectric constant of the piezoelectric material \(\varepsilon_r\) and free space permittivity \(\varepsilon_0\).

\[
g_{31} = \frac{d_{31}}{\varepsilon_r \varepsilon_0}
\] (22)

Generated voltage is obtained by integrating the generated electric field with respect to \(z\)
\[
V(x) = \int_0^{t_p} E_g(x, z) dz
\] (23)

\[
V(x) = \int_0^{t_p} g_{31} \frac{F E_p}{wD} (L - x)(z - t_n) dz
\] (24)

\[
V(x) = g_{31} \frac{F E_p}{wD} (L - x) \int_0^{t_p} (z - t_n) dz
\] (25)

\[
V(x) = g_{31} \frac{F E_p}{wD} (L - x) \left( \frac{z^2}{2} - t_n z \right)_0^{t_p}
\] (26)

\[
V(x) = g_{31} \frac{F E_p}{wD} (L - x) \left( \frac{t_p^2}{2} - t_n t_p \right)
\] (27)

From the above equation states that the generated output voltage is purely depending on the cantilever beam dimensions, the material properties and also the applied force. The charge produced from piezoelectric material is distributed on both electrode surfaces. The generated voltage between top and bottom surface is equal to average of \(V(x)\) over length of piezoelectric layer \(L\).

\[
V_{avg} = \frac{1}{L} \int_0^L V_{in} dx
\] (28)

\[
V_{avg} = \frac{1}{L} \int_0^L g_{31} \frac{F E_p}{wD} (L - x) \left( \frac{t_p^2}{2} - t_n t_p \right) dx
\] (29)

\[
V_{avg} = \frac{1}{L} g_{31} \frac{F E_p}{wD} \left( \frac{t_p^2}{2} - t_n t_p \right) \int_0^L (L - x) dx
\] (30)

\[
V_{avg} = \frac{1}{L} g_{31} \frac{F E_p}{wD} \left( \frac{t_p^2}{2} - t_n t_p \right) \left( L^2 - \frac{x^2}{2} \right)_0^L
\] (31)

\[
V_{avg} = \frac{L}{F} \frac{E_p}{wD} \left( \frac{t_p^2}{2} - t_n t_p \right)
\] (32)

Therefore generated output voltage per unit force by cantilever piezoelectric energy harvester shown in equation (32)