Effects of mechanical deformation on energy conversion efficiency of piezoelectric nanogenerators

This content has been downloaded from IOPscience. Please scroll down to see the full text.
2015 Nanotechnology 26 275402
(http://iopscience.iop.org/0957-4484/26/27/275402)

View the table of contents for this issue, or go to the journal homepage for more

Download details:

IP Address: 1.233.212.154
This content was downloaded on 14/07/2015 at 06:48

Please note that terms and conditions apply.
Effects of mechanical deformation on energy conversion efficiency of piezoelectric nanogenerators

Jinho Yoo¹, Seunghyeon Cho², Wook Kim¹, Jang-Yeon Kwon³, Hojoong Kim³, Seunghyun Kim⁴, Yoon-Suk Chang⁴, Chang-Wan Kim² and Dukhyun Choi¹,⁵

¹ Department of Mechanical Engineering, College of Engineering, Kyung Hee University, 1732, Deogyeong-daero, Giheung, Yongin, Gyeonggi, 446-701, Korea
² School of Mechanical Engineering, Konkuk University, Gwangjin-gu, Seoul, 143-701, Korea
³ School of Integrated Technology, Yonsei University, 162-1, Songdo-dong Yeonsu-gu, Incheon, 406-840, Korea
⁴ Department of Nuclear Engineering, College of Engineering, Kyung Hee University, 1732, Deogyeong-daero, Giheung, Yongin, Gyeonggi, 446-701, Korea
⁵ Industrial Liaison Research Institute, Kyung Hee University, 1732, Deogyeong-daero, Giheung, Yongin, Gyeonggi, 446-701, Korea

E-mail: goodant@konkuk.ac.kr and dchoi@khu.ac.kr

Received 15 March 2015, revised 10 May 2015
Accepted for publication 26 May 2015
Published 18 June 2015

Abstract
Piezoelectric nanogenerators (PNGs) are capable of converting energy from various mechanical sources into electric energy and have many attractive features such as continuous operation, replenishment and low cost. However, many researchers still have studied novel material synthesis and interfacial controls to improve the power production from PNGs. In this study, we report the energy conversion efficiency (ECE) of PNGs dependent on mechanical deformations such as bending and twisting. Since the output power of PNGs is caused by the mechanical strain of the piezoelectric material, the power production and their ECE is critically dependent on the types of external mechanical deformations. Thus, we examine the output power from PNGs according to bending and twisting. In order to clearly understand the ECE of PNGs in the presence of those external mechanical deformations, we determine the ECE of PNGs by the ratio of output electrical energy and input mechanical energy, where we suggest that the input energy is based only on the strain energy of the piezoelectric layer. We calculate the strain energy of the piezoelectric layer using numerical simulation of bending and twisting of the PNG. Finally, we demonstrate that the ECE of the PNG caused by twisting is much higher than that caused by bending due to the multiple effects of normal and lateral piezoelectric coefficients. Our results thus provide a design direction for PNG systems as high-performance power generators.

Online supplementary data available from stacks.iop.org/NANO/26/275402/mmedia

Keywords: piezoelectric nanogenerator, energy conversion efficiency, mechanical deformation, numerical simulation

(Some figures may appear in colour only in the online journal)
1. Introduction

Piezoelectric nanogenerators (PNGs) have attracted great interest for use in self-powered systems for medical science, defense technology, and personal electronics due to their capability to convert a variety of mechanical energies such as blood flow, sounds, and human movements into electricity [1–5]. PNGs can also serve as a ‘gate’ voltage to effectively tune/control the charge transport across an interface/junction; electronics based on such a mechanism are referred to as piezotronics, with applications such as electronic devices that are triggered or controlled by force or pressure, sensors, logic units, and memory [6–13]. The development of transparent, flexible/wearable, and biocompatible PNGs could lead to further applications in smart wearable systems and implantable telemetric devices [14–17].

The basic mechanism to produce electricity from PNGs is based on a piezoelectric potential, called piezopotential, created by deformation of a piezoelectric active layer, which is caused by mechanical strain [18, 19]. The piezopotential is critically affected by the piezoelectric coefficients fundamentally determined by the crystal structure of the material. These crystal structures can be modified by doping and alloying. Therefore, many researches have focused on the design and synthesis of new piezoelectric materials to improve the output power of PNGs [20–23]. A piezopotential that is created by the polarization of a dipole can be reduced by surface defect charges. Such defect charges can be eliminated by surface treatments or interfacial controls, resulting in enhanced piezopotential [24, 25].

As mentioned above, the piezopotential is intrinsically determined by material properties, so that many previous researches have focused on material syntheses and interfacial controls. However, it is more significantly dependent on external deformations, an extrinsic parameter [26]. Greater strain can be produced on PNGs by providing higher mechanical energies. Furthermore, the strain distributions on a piezoelectric active layer can be changed by the type of mechanically driven deformation such as bending and twisting [27]. To date, some studies by bending have been performed, but no one has studied such an effect of the twisting deformation on the performance of PNGs. Although the total strain energy as an input energy is the same, the output power from PNGs may differ based on the strain distribution on the piezoelectric active layer caused by the type of mechanical deformation.

In this study, we investigate the effect of mechanical deformation on energy conversion efficiency (ECE) of PNGs with experiments and numerical simulation. We simply prepare zinc oxide (ZnO)–based PNGs to examine ECE according to bending and twisting mechanical deformations. We also suggest a method to determine the ECE of PNGs. The output power from PNGs is calculated using the output voltage and current signals. The input energy is determined through numerical simulation based on the given deformation conditions of the ZnO active layer. We determine that the ECE of PNGs by twisting is much higher than that by bending due to the different strain distributions. The results may provide an effective design of PNG systems for high-performance power generators.
2. Experiments

Figure 1(a) shows the different mechanical deformations for bending and twisting of a PNG based on a ZnO piezoelectric film. The details of the ZnO-based PNG are illustrated in figure 2. As shown in figure 1(a(i)), the PNG is subject to bending deformation, where the critical parameter is the radius of the curvature ($\rho$) which is the distance from the center of the curvature to the neutral axis of the film (see figure S1). By decreasing the distance ($L$) between the zigs, the bending deformation increases, resulting in a decreased radius of curvature. Since the bending curvature ($\kappa$) is inversely related to the radius of curvature (i.e., $\kappa = 1/\rho$), $\kappa$ increases with increasing bending deformation. For bending tests, we utilized a bending tester (JIBT-210) which can hold a sample of a length 10 to 100 mm, a width 10 to 100 mm and a thickness of 2 mm at a speed ranging from 1 to 100 mm s$^{-1}$. In our bending tests, the bending distances ($L_0-L$) were 10, 20, 30, and 40 mm, and the corresponding bending curvatures ($\kappa$) were determined to be 0.13, 0.16, 0.2, and 0.24 cm$^{-1}$. The bending rate was fixed at 30 mm s$^{-1}$ for all bending tests. Figure 1(a(ii)) shows the twisting deformation of our PNG. We twisted the PNG by varying the twist angle ($\theta$) at each zig, resulting in a total twisting angle ($\theta_t$) of 2$\theta$. To evaluate the output performance under twisting deformation, we used a twisting tester (JITT-400) which has the operation twist angle between $-50$ and $-50^\circ$ and the maximum sample size of a length 25 to 95 mm and a thickness 1.5 mm at a speed ranging from 1 to 100 mm$^2$/s. For the twisting tests, the total twisting angles ($\theta_t$) were 20, 40, 60, and 80$^\circ$ (i.e. twist angle 10$^\circ$ to 40$^\circ$). The twisting rate was fixed at 40$^\circ$/s for all twisting tests. To measure the output voltages and currents from PNGs according to the mechanical deformation, we used a Keithley 2182A nanovoltmeter and Keithley 6485 picoammeter. Depending on the mechanical deformations, the strain distributions are significantly different, as shown in figure 1(b). Thus, the output power and ECE must differ according to the type of mechanical deformation.

We fabricated the PNG based on a ZnO thin film (see figure 2). First, we prepared a 50 nm-thick indium tin oxide (ITO)-coated polyethylene terephthalate (PET) substrate (figure 2(a(i))). In order to provide an effective mechanical deformation, we designed the PET substrate with an 8 cm length and 1 cm width. The thickness of a PET film was 125 $\mu$m. After etching out the half of the ITO layer on a PET substrate (figure 2(a(ii))), a 200 nm-thick ZnO (figure 2(a(iii))) was deposited by using a radiofrequency (RF) magnetron sputter with a ZnO target. The RF power was 200 W, and the working pressure was 5 mTorr in an Ar and O$_2$ mixture gas during ZnO deposition, maintaining the oxygen partial pressure of $\sim$3% [O$_2$/(Ar + O$_2$) = 3%]. Finally, a silver (Ag) top electrode of 100 nm thickness was deposited by thermal evaporation, as shown in figure 2(a(iv)). As shown in the photograph of figure 2(b), the active area where all layers are overlapped was 5 mm $\times$ 4 mm. Copper wires were connected to the top and bottom electrodes (i.e., Ag and ITO, respectively) of PNGs with the measurement instruments.

In order to understand the deformation-induced performance of PNGs, we determined the ECE of PNGs as the ratio of output energy to input energy, where we suggest that the input energy should be considered by the strain energy of the only piezoelectric layer (the detailed reason will be discussed in the results and discussion section). To determine the strain energy of the piezoelectric layer, we calculated the strain energy using numerical simulation of bending and twisting of the PNG. Such a numerical simulation for the strain energy of the only ZnO layer is critically important because we could not determine the strain energy for the ZnO layer by experiments or the other theoretical relationships. Thus, the strain energy on the ZnO layer in a PNG device, which is calculated only within the elastic deformation range, was determined using the finite element method (FEM) and the commercial finite element software.
FEM software ABAQUS. Figure 3(a) shows the three-dimensional (3D) FEM model of our PNG. PET and ZnO are modelled with a solid element and shell element, respectively. We ignored the ITO and the top Ag electrode layers since their thicknesses (50 and 100 nm) are too small compared with that (125 μm) of PET. The detailed reasons are further introduced in the supplementary information (see figure S2).

In order to minimize the edge effects from the numerical simulation, we modeled the ZnO layer with the size of 10 × 8 mm² on PET and extracted the strain energy of the ZnO active area with 5 × 4 mm². In this calculation, we assumed that our materials are all homogenous. Figure 3(b) shows the total strain energy distributions on the PET film, including the ZnO layer at the center according to bending and twisting deformation. The strain energy \( U \) for the elastic range is defined as \( U = \frac{1}{2} \int \sigma^T \epsilon \, dV \), where \( V \) is the volume of the PNG device, \( \{\sigma\} \) is the stress vector, and \( \{\epsilon\} \) is the strain vector. The details for the strain energy calculation can be found in the supplementary information. After we performed the total numerical calculations for the 3D models for the PNG, we determined the strain energy of the ZnO active area as the input energy. The unit of the strain energy \( (U) \) was \( \mu J \).

3. Results and discussion

Figure 4 shows the crystal structure and electrical property of the sputtered ZnO thin film. The x-ray diffraction (XRD) pattern of the ZnO film demonstrates adequate growth along the (002) direction (c-axis) [28–30]. The structure of ZnO is composed of a number of alternating planes composed of tetrahedrally coordinated \( O^{2-} \) and \( Zn^{2+} \) ions, stacked alternatively along the c-axis. The oppositely charged ions produce positively charged (002)-Zn and negatively charged (002)-O polar surfaces, resulting in a normal dipole moment and spontaneous polarization along the c-axis. This c-axis growth of the ZnO thin film was also noted in the field emission scanning electron microscope (FE-SEM) image in the inset of figure 4(a). Figure 4(b) shows the I-V characteristic of our PNG device, as well as the electrical properties of the ZnO film and the device conditions. We controlled the sweep voltage from \(-5 \) to \( 5 \) V. The I-V curve showed a weak diode characteristic in our device. The resistance of the ZnO film was \( \sim M \Omega \), and the Schottky barriers between the ZnO film and Ag electrodes were low, resulting in a weak Schottky diode characteristic in our PNG. By bending our ITO/ZnO/Ag PNG system, a negative piezopotential \( (V^-) \) is formed at the ITO–ZnO interface surface, which drives the piezoelectric-induced electron flow from the ITO electrode to an Ag electrode through an external load resistor, giving rise to a positive current and voltage pulse. Due to the Schottky barrier between ZnO and Ag, the electrons accumulate at the interface region between Ag and ZnO. However, the Schottky barrier at the interface between ZnO and Ag is weak, so that some electrons flow in ZnO and screen the positive piezopotential \( (V^-) \). Thus, the output performance of our system was low. However, it is not within the scope of the study to optimize the ZnO film or the circuit design (i.e., interfacial control or electrode design) for improved output power. We instead focused on the effect of
Figures 5 and 6 show the PNG output voltages (figures 5(a) and 6(a)) and currents (figures 5(b) and 6(b)) of the bending and twisting tests. Figures 5(c) and 6(c) provide the experimental photographs of bending curvatures ($\kappa_1 \sim \kappa_4$) and twisting angles ($\theta_1 \sim \theta_4$), respectively. The bending tests showed that the output voltage increased from 0.3 to 2.2 mV and the output current increased from 25 to 100 nA with increased bending curvature. The output voltage and output current from the twisting tests also increased from 0.8 to 5.2 mV and 25 to 150 nA with increased twisting angle, respectively. We verified that the output signals were from a piezopotential based on switching polarity tests (see figure S3). Based on the output performance, the twisting deformation produced higher output power than the bending deformation. However, since the deformation rate could not be quantitatively compared for bending and twisting, we could not conclude that twisting deformation is more effective for producing electrical power from a PNG. Furthermore, the output power can be increased by higher input energy, indicating the need for study of the ECE of PNGs according to the input mechanical deformations in order to determine which mechanical deformation is more efficient for power generation.

Generally, ECE ($\eta$) can be determined as the ratio ($\eta = E_o/E_i$) of output energy ($E_o$) to input energy ($E_i$). From PNGs, we can determine the output electrical energy as $E_o = \int VdI dt$, where the maximum output energy should be determined by the maximum power from the voltage and current signals according to the resistance. However, the behaviors of maximum output power could be understood by using the peak values of the voltages and the currents [31]. Thus, we simply utilized the peak values to understand the behaviors of ECE. Here, the key issue is the determination of input energy. The source of the input energy for PNGs is mechanical...
deformation, so the input energy should be the strain energy of PNGs. As shown in figure 2, a basic PNG device consists of several layers: a flexible substrate, top/bottom electrodes, and a ZnO thin film. Every layer incurs strain energy by bending; however, we suggest that the input energy should consider only the strain energy from the ZnO layer to understand the ECE of a PNG by external mechanical deformations because the electrical output power is only generated from the piezopotential of the ZnO layer.

The strain energy $U$ was calculated for the ZnO layer on the PET substrate with the size of $8 \times 1 \text{ cm}^2$. We extracted the only strain energy of the ZnO layer by FEM simulations. Figure 7 shows the strain energy distribution on the ZnO active area according to the bending curvatures and the twisting angles. The strain energy distributions were significantly different depending on the type of mechanical deformation. The strain energy caused by bending was maximal at the center and decreased toward the edges. On the other hand, the strain energy caused by twisting was maximal at the edges and minimal at the center. These different strain distributions according to the type of mechanical deformation might provide different output powers from PNGs. In detail, the strain distribution caused by bending is only one directional. In other words, the ZnO layer under bending is subject to compressive stress in the thickness direction ($zz$ direction in the simulation). Therefore, the major piezopotential occurs by $E = d_{zz} \varepsilon_{zz}$ where $E$ is a piezoelectric field, $d_{zz}$ is a piezoelectric coefficient in the thickness direction, and $\varepsilon_{zz}$ is the strain in the thickness direction. On the other hand, the ZnO layer under twisting is subject to mixed stress (i.e. both normal stress and shear stress). Therefore, $d_{zz}$ (the thickness direction) and $d_{xy}$ (the lateral direction) work together to induce piezoelectric potential in the ZnO layer. Since $d_{xy}$ is comparable or in some cases larger than $d_{zz}$, we guess that such higher output performance by twisting could be obtained, compared with that by bending.

Figure 8(a) shows the total strain energies on the ZnO active area for each mechanical deformation. Strain energies in the range of the bending curvatures were linearly increased, but those caused by twisting angle showed a slightly non-linear increase. The strain energies by twisting of a PNG device were much smaller than those by bending because the low strain was distributed at the ZnO active area by twisting. Figure 8(b) is the normalized ECE as a function of input strain energy for each mechanical deformation. We determined the normalized ECE using the relative ECE based on the reference value for the lowest ECE in our experimental conditions, which was the ECE at a bending curvature ($\kappa$) of $0.13 \text{ cm}^{-1}$. As shown in figure 8(b), the normalized ECEs caused by twisting deformation were much higher than those caused by bending since the input energy by twisting was smaller than that by bending, but the output power by twisting was higher than that by bending. Particularly, the ECE at similar strain energies (see figure 8(b)) was over 30 times higher when caused by twisting than when caused by bending. Although the strain rates were not the same in the bending and twisting tests, the 30-fold enhancement was attributed to the type of mechanical deformation based on the previous literature [31]. Thus, twisting deformation is very effective to produce electrical energy from PNGs.

4. Conclusions

In this study, we first investigated the effects of mechanical deformation on the ECE of PNGs using bending and twisting tests. In order to determine the ECE of PNGs, we suggested that the input energy should be considered as the strain energy on the ZnO layer in a PNG device since the output energy is generated from the piezopotential by the ZnO layer. We thus determined the strain energies of the ZnO layer in PNGs using numerical simulations according
to the mechanical deformation. Based on the normalized ECE caused by mechanical deformation in PNGs, twisting was much more effective for generating electrical power than bending. The main reason for this might be the significantly different strain distributions on a ZnO film according to the type of mechanical deformation. Our results thus could provide an effective system design of PNGs as next-generation power generators driven by mechanical energies.

**Acknowledgments**

This research was financially supported by the Fundamental Technology Research Program (2014M3A7B4052202) and by the Basic Science Research Program (2013R1A1A2063798 and 2012R1A2A2A04047240) through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Science, ICT and Future Planning (MSIP).
References

[17] Yuan M et al 2014 Biocompatible nanogenerators through high piezoelectric coefficient 0.5Ba(Zr0.2Ti0.8)O3-0.5(Ba0.5Ca0.5)TiO3 nanowires for in vivo applications Adv. Mater. 26 7432–7