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Full paper

Comprehensive contact analysis for vertical-contact-mode triboelectric nanogenerators with micro-/nano-textured surfaces

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ABSTRACT

The triboelectric nanogenerator (TENG) is a new energy technology to convert mechanical energy into electricity based on contact charging and electrostatic induction. To increase the effective power generation in a limited device size, micro-/nano-textures are often designed at the contact surfaces. As the contact region decreases to micro/nano scale, adhesive forces such as van der Waals and electrostatic forces become dominant. However, there is currently no comprehensive model including micro-/nano-textures and the above adhesive forces, and thus the selection and design of textures are still lack of theoretical guidance. In this paper, the numerical contact and electrical models considering van der Waals and electrostatic forces are established, and the computational methods such as inexact Newton method, bi-conjugate stabilized (Bi-CGSTAB) method and fast Fourier transform (FFT) technique are employed to quantitatively analyze the effects of charge densities, applied loads, texture shapes and sizes on both contact and electrical performance. It is shown that the electrostatic force can be ignored when the charge density is small, while with large charge density, the electrical performance is significantly overestimated if the electrostatic forces are neglected. Among the four selected types of textures (pyramid, cone, cylinder and cube), the pyramid and cube textures are found to provide the larger output voltage under different applied loads, and also the optimal sizes for high voltage are presented, respectively. This study can provide the guideline for the texture design of high power generation TENGs.

1. Introduction

Triboelectric nanogenerator (TENG) invented by Zhonglin Wang's group is a new energy technology to convert mechanical energy into electricity based on contact charging and electrostatic induction [1]. The vertical-contact-mode TENG has attracted enormous amount of attention due to its simple structure, high energy conversion and broad application areas [2]. And the output performance of TENG can be improved by various methods, in which selecting a proper charging material and increasing the contact area are the two common methods [3–6]. To increase the effective contact area in a limited device size, micro-/nano-textures are often designed at the contact surfaces [7–9]. For example, Fan et al. [9] fabricated three kinds of regular and uniform polymer patterned arrays, i.e., line, cube, and pyramid micropatterns and found that the power generations of TENGs with micropatterned surfaces are significantly larger than those with flat surfaces.

A key factor that dictates the performance of the TENG is the amount of induced charge which depends on surface charge density and contact area. Therefore, contact electrification of TENGs with textures is closely related to the contact mechanics, the core of which is to establish the relationship between the applied load and effective contact area. In the attempt to reveal the connection between contact mechanics and electrical performance of TENGs with textured surfaces, Seol et al. [10] analyzed the deformation behavior of micro pyramid textures during contact process based on elastic deformation theory, and the expressions between the applied pressure, effective contact area and open-circuit voltage of TENGs with pyramid textures were presented. It was shown that the open-circuit voltage was sensitive to the applied pressure change under low pressure while the sensitivity significantly decreased under high applied pressure. However, for TENGs with micro-/nano-textures, as the contact regions shrinks to micro/nano scales, the surface-to-volume ratio increases and the effects of adhesive forces (such as van der Waals, electrostatic forces) become significant compared with those of body forces (gravity and inertia). In addition, for the material commonly used as the textured dielectric layer in TENGs, such as polydimethylsiloxane (PDMS), the ratio of elastic deformation energy to surface energy is rather large and thus adhesive forces should be included in contact models for TENGs with

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micro-/nano-textures. Jin et al. [11] established a numerical contact model of TENG considering van der Waals interaction based on Derjaguin approximation [12] and Lennard–Jones surface force law [13] to predict the contact area and open-circuit voltages under different applied loads. However, when the electrode and the dielectric layer of TENG come into contact, in addition to the van der Waals interactions, electrostatic interactions arise due to the electric field formed by the contact charges and become rather important because of the retained charges in dielectric layer [14]. In fact, it has been found in experiments that during some contact electrification processes, the influence of electrostatic forces on contact performance is even more significant than that of van der Waals forces [15–17]. For example, it was shown that 80% of adhesion force between mica and silicon sheets came from the electrostatic force due to contact electrification [15], and the electrostatic force generated by contact between polystyrene and graphite significantly changed the surface adhesive force [16]. However, as to TENGs commonly with metal and polymer in contact, the contribution of electrostatic force induced by contact charges to adhesive force and the electrical performance has not been well understood. In addition, there has been no theoretical analysis on the effects of texture shapes under different applied load on both the adhesive contact and electrical performance of TENGs, and thus the optimal shapes for high power generation TENGs still remain unclear.

Therefore, the present paper will focus on the above issues and establish the numerical contact model considering both van der Waals and electrostatic forces to investigate the effects of charge densities, applied loads, texture shapes and sizes on the contact and electrical performance of vertical-contact-mode triboelectric nanogenerators.

2. Theoretical model and numerical algorithm

Fig. 1(a) and (b) are the schematic diagrams of the typical contact and separation states of a spring-based TENG with textured surfaces, respectively, where $V(t)$ represents the voltage between the two electrodes. As described in the introduction, to obtain the voltage $V(t)$, contact mechanics analysis between the contact electrode and the textured dielectric layer is required. Fig. 1(c1) and (c2) shows the schematic drawings of contact and separation between the contact electrode and a unit block of the textured dielectric layer with the height of $S_p(x,y)$, respectively, where h denotes the surface gap of contact electrode and textured dielectric layer. α is the approach between the bottom of the electrode and the plane of $z = 0$, when the electrode is located above the plane of $z = 0$, α is negative, otherwise α is positive. Ω represents the contact region between the two surfaces.

The surface gap h between the bottom of the contact electrode and the textured dielectric layer can be expressed as:

$$h(x, y) = -\alpha - S_p(x, y) + u(x, y) \tag{1}$$

For TENGs, four kinds of textures are commonly applied, that is, pyramid, cone, cube and cylinder, as shown in Fig. 2. The expressions for each texture height distribution $S_p(x,y)$ are also presented, in which a, b, c are the length, height and pitch of the textures, respectively.

$u(x,y)$ in Eq. (1) denotes the elastic deformation of the textured layer and can be evaluated using the Boussinesq integral [18]:

$$u(x, y) = \frac{1}{\pi E^*} \iint \frac{p_{ah}(\xi, \eta)\mathrm{d}\xi\mathrm{d}\eta}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} \tag{2}$$

where $E^* = E/(1\text{-}\nu^2)$, E and ν is the elastic modulus and poisson ratio, respectively. $p_{ah}(x, y)$ is the local pressure distribution between the two contact surfaces which mainly includes van der Waals attractive interaction $p_{vdW}(x,y)$, electrostatic attractive interaction $p_{ele}(x,y)$ and repulsive contact interaction $p_{rep}(x,y)$. Van der Waals interaction originates from the inherent polarization of molecules in materials and thus commonly exists in the whole region. Although the fundamental mechanisms for the occurrence of van der Waals forces are of electrostatic nature, it is regarded as non-electrostatic interaction in the adhesive contact [14]. Repulsive contact interaction arises from the overlapping of atoms electron clouds [19,20]. Normally, the van der Waals interaction and the repulsive contact interaction are considered together based on the Lennard–Jones interatomic potential $w(l)$, which is a pair potential described the potential energy of interaction between two non-bonding molecules [20]. Lennard–Jones interatomic potential is widely used because of its simple expression: $w(l) = B/l^{12}\text{-}C/l^6$, where the repulsive term B/l^{12} represents the repulsive potential and the attractive term $-C/l^6$ is van der Waals potential, l is the distance between molecules and constants B,C are related to such bulk properties as their dielectric constants and refractive indices. Lifshitz-Hamaker approach [20,21], which obtains the van der Waals interaction and the repulsive contact interaction between macroscopic bodies by the pairwise

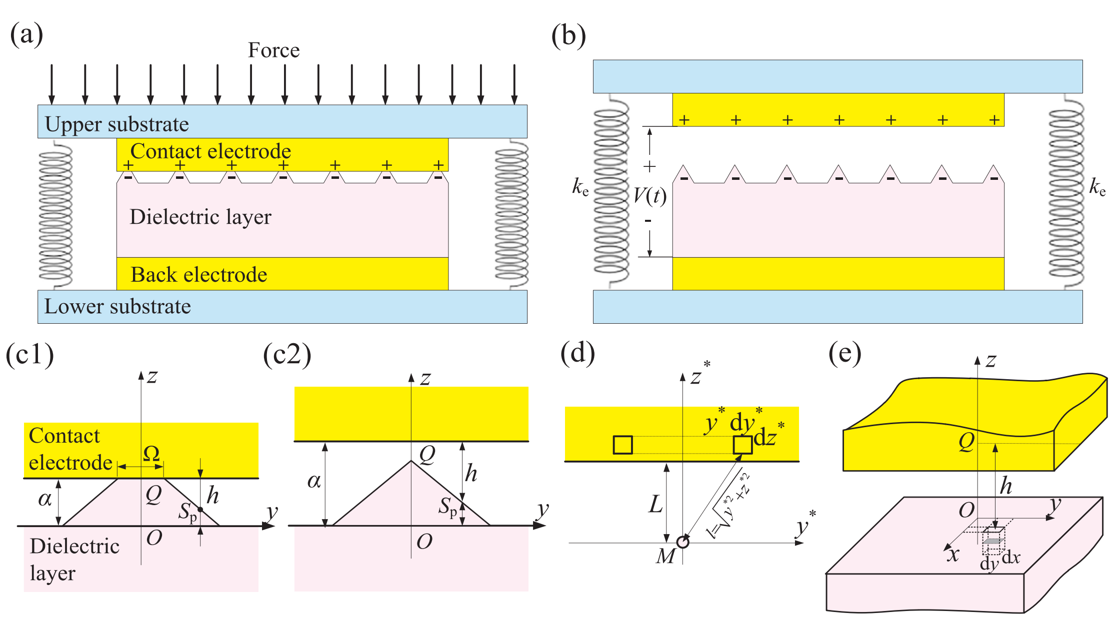

Fig. 1. Schematic diagrams of (a) contact and (b) separation states of a spring-based TENG, (c) the adhesive contact and separation between the electrode and textured layer, (d) adhesive contact between the electrode and a molecule in the dielectric layer, (e) adhesive contact between the electrode and a micro-element body on the textured dielectric layer with textures omitted.