Finite-element modelling of triboelectric nanogenerators accounting for surface roughness

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Abstract

Triboelectric nanogenerators (TENG) transform mechanical energy into electrical energy as a result of contact between suitably chosen surfaces. Surface roughness plays a key role in the performance of contact-separation TENG, defining the ratio of real contact area to the apparent one for a given contact force. We develop a novel numerical approach for coupling mechanical contact and electrostatics equations to simulate TENG behaviour using the finite-element library MoFEM. Good qualitative agreement is found between the numerical predictions of the proposed method, available experimental data and approximate analytical models. The developed finite-element framework can be used for further study of the effect of various TENG parameters on the output performance.

Key words: *triboelectric nanogenerator; surface roughness; mechanical contact; electric field; finite-element method*

1 Introduction

Triboelectric nanogenerators (TENG) are modern devices which use the effect of contact electrification and electrostatic induction to transform mechanical energy into electrical energy during repeated cycles of contact between suitably chosen surfaces [1]. These devices have attracted great attention as autonomous sources of clean energy for various applications, from miniature wearable systems to ocean wave energy harvesting; they can also be employed as sensors [2].

Since tribo-charges only appear in zones of the real contact between two surfaces, recent studies have been devoted to the effect of the surface roughness, which defines the ratio of real contact area to the apparent one for a given external load, on the output performance of contact-separation TENG. In [1], an experiment has been reported which demonstrated the dependence of the open-circuit voltage of the TENG on the external load. Furthermore, an approximate analytical formula has been derived in the same paper, which showed good qualitative agreement with the experimental data. Recently, numerical simulations were used to compute the real contact area and the equivalent capacitance of TENG in case of patterned surfaces [2].

However, simulation of TENG accounting for microscale surface roughness is associated with considerable computational difficulties and has not been reported yet. In this study we develop a novel approach for coupling mechanical contact and electrostatics equations using the finite-element library MoFEM [3], permitting simulation of TENG with representative surface roughness taken into account.

2 Coupled problem statement

We consider a contact-separation TENG with tribo-layers made of PET and PDMS materials, see Fig. 1(a), which is the same setup as was used in experiment reported in [1]. The simulation is performed in two stages: contact stage and separation stage. To set up the former, we consider a representative element of the device, see Fig. 1(b), and compute the equivalent surface heights distribution as $h_0(x,y) = h_1(x,y) + h_2(x,y)$, where $h_1(x,y)$ and $h_2(x,y)$ are roughness measurements

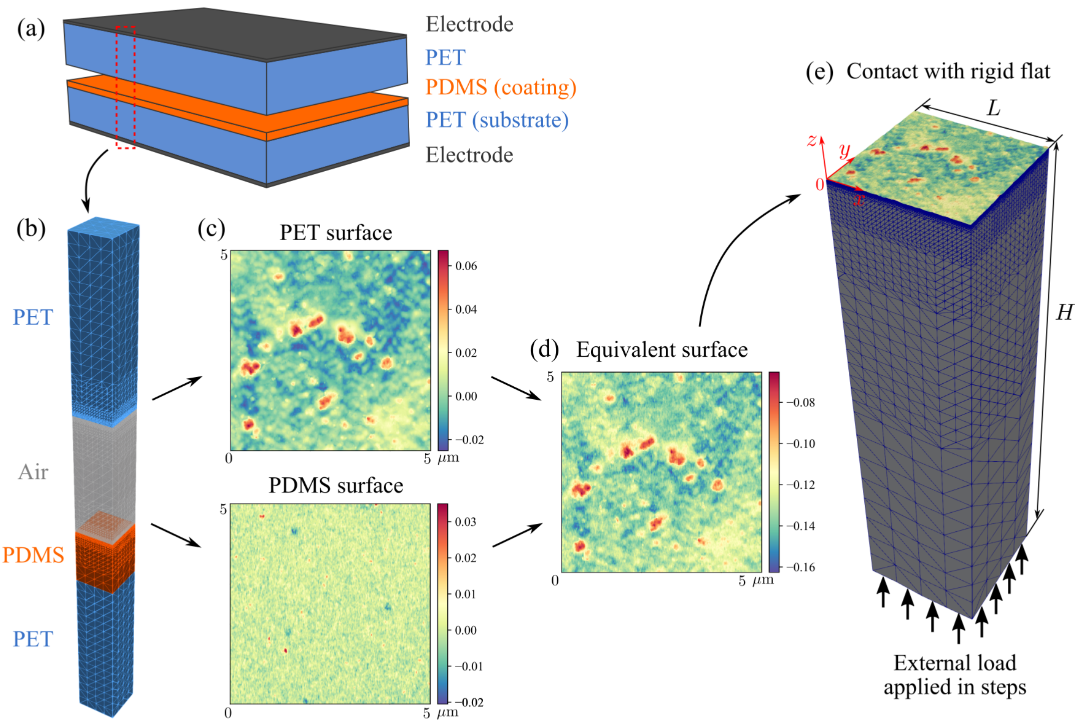

Figure 1: (a) Schematic of the contact-separation TENG; (b) sketch of the representative element; (c) examples of surface roughness measurements; (d) equivalent surface height distribution; (e) contact problem setup: $L = 5\,\mu$m, $H = 20\,\mu$m, $E_0 = 1.53$ MPa, $\nu_0 = 0.4$, see [1].

of PET and PDMS surfaces, respectively, see Fig. 1 (c) and (d). Note that consideration of the contact between a rigid flat and a deformable solid with equivalent surface roughness and elastic properties (Young's modulus E_0 and Poisson coefficient ν_0) is valid under assumptions of small deformations and small slopes of the surface profile, relevant for the application under study [4]. Introducing $\mathbf{u} = [u_x, u_y, u_z]^\intercal$ as the displacement field and $\boldsymbol{\sigma}$ as the stress tensor, the contact problem is governed by:

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}) = 0 & \text{in } (0,L)\times(0,L)\times(-H,0) \quad (1a)\\ g(\mathbf{u}) \geq 0,\ \sigma_n(\mathbf{u}) \leq 0,\ g(\mathbf{u})\,\sigma_n(\mathbf{u}) = 0 & \text{on } \Gamma^{\mathrm{c}} \quad (1b)\\ \sigma_{zz}\big|_{z=-H} = -p_{\mathrm{ext}} & (1c)\\ u_x\big|_{x=0} = u_x\big|_{x=L} = u_y\big|_{y=0} = u_y\big|_{x=L} = 0, & (1d) \end{cases}$$

where (1a) is the balance of momentum equation (volumetric forces are neglected), (1b) are the unilateral contact constraints, σ_n is the negative of the contact pressure, g is gap, i.e. signed distance between potential contact surface Γ^{c} and surface $z = 0$. The contact is enforced by the external load (1c) applied in steps, while on the vertical walls of the solid we consider symmetry boundary conditions (1d), see Fig. 1(e).
The solution of the contact problem provides the distribution of the contact pressure and the real contact area for each load step, see Fig. 2 (a) and (b), which is used as the input for the second (separation) stage. In particular, we consider the tribo-charges density $\sigma(x, y)$ equal to $\sigma_0 = 40.7\,\mu\mathrm{C/m}^2$ [1] if point belongs to the real contact area and zero otherwise.
Denoting the electric potential as $\phi(x, y, z)$, the electric field as $\mathbf{E} = [E_x, E_y, E_z]^\intercal = -\nabla\phi$, and the electric permittivity as $\epsilon(z)$, see Fig. 2(c), the electrostatics problem for a representative element

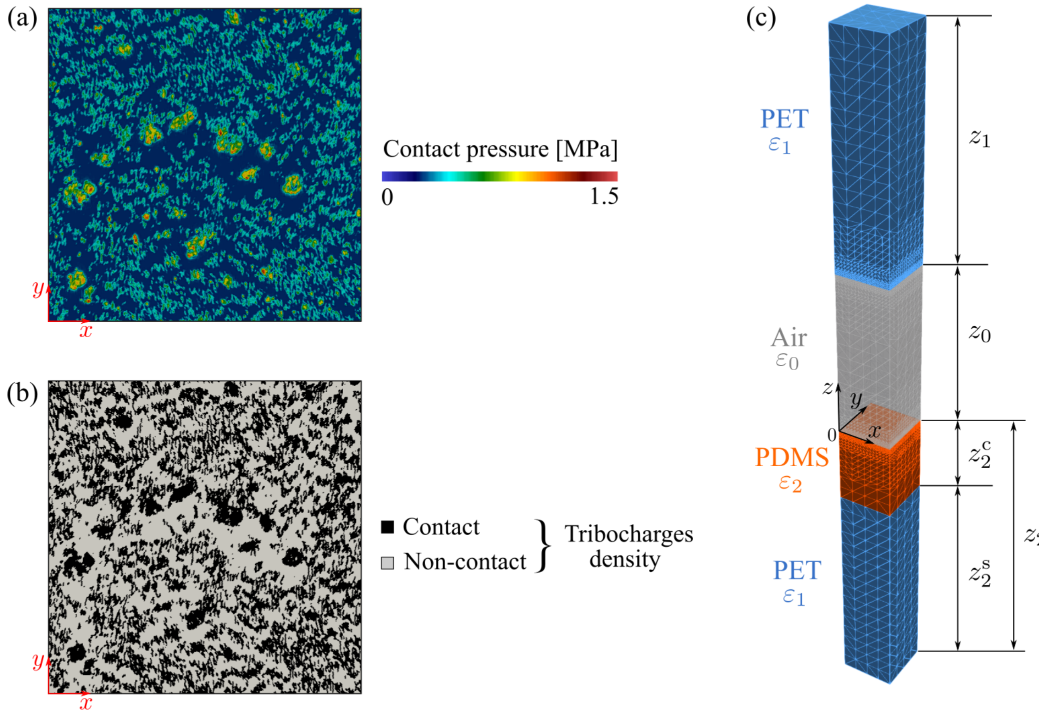

Figure 2: Output of the contact stage for $p_{\text{ext}} = 0.08\,\text{MPa}$: the distribution of (a) the contact pressure and (b) the contact area. (c) Setup of the separation stage: $\epsilon_0 = 8.85 \times 10^{-9} \mu\text{F/mm}$, $\epsilon_1 = 3.3\,\epsilon_0$, $\epsilon_2 = 2.72\,\epsilon_0$, $z_0 = 1.3\,\text{mm}$, $z_1 = z_2^s = 0.127\,\text{mm}$, $z_2^c = 0.02\,\text{mm}$, see [1].

of the TENG reads (note that volumetric charges are not considered):

$$\begin{cases} \epsilon(z)\,\nabla \cdot \mathbf{E} = 0 & \text{in } (0,L)\times(0,L)\times(-z_2, z_0+z_1) & \text{(2a)} \\ [\![\epsilon(z)\,E_z]\!]_{z=0} = [\![\epsilon(z)\,E_z]\!]_{z=z_0} = \sigma(x,y) & & \text{(2b)} \\ \phi|_{z=-z_2} = 0, \;\; \phi|_{z=z0+z1} = \text{const} & & \text{(2c)} \\ E_x|_{x=0} = E_x|_{x=L} = E_y|_{y=0} = E_y|_{x=L} = 0. & & \text{(2d)} \end{cases}$$

Interface conditions are imposed in (2b), where $[\![\cdot]\!]$ denotes the jump of the argument across the interface and $\sigma(x,y)$ is the tribo-charges density. Eq. (2c) corresponds to equipotential surfaces arising from the presence of electrodes, and (2d) enforces symmetry. The open-circuit voltage, which as a measurable parameter of the TENG performance, is recovered as $V_{\text{OC}} = \phi|_{z=z0+z_1}$.

3 Numerical results

The computational framework for solving the coupled problem defined in (1)-(2) was developed using the finite-element method and was implemented as an open-source module of MoFEM [3]. To verify the proposed methodology, we performed simulations using the TENG parameters and 8 samples of the surface measurements corresponding to the experiment reported in [1]. In Fig. 3(a) we show the evolution of the real contact area with the increasing external load (output of the contact stage). Numerical results are in good agreement with Persson's formula, see [1], however, the analytical formula underestimates the contact area for small and medium loads compared to the numerical simulation, which has been already reported in studies of contact between rough surfaces using the boundary element method [5]. Since the real contact area value can have strong influence on the output performance of TENG, the observed results underline the importance of using the numerical simulation (e.g. FEM) to obtain more precise predictions.

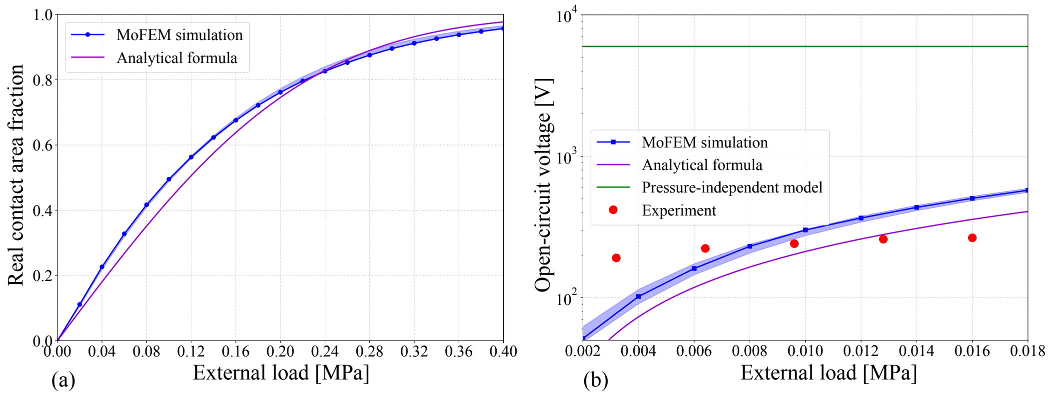

Figure 3: Evolution of (a) the fraction of the real contact area and (b) the open-circuit voltage under increasing external load. Curves corresponding to the simulation represent median values computed over 8 surface roughness profiles; interquartile ranges are shown as shaded regions.

In Fig. 3(b) we show the evolution of the open-circuit voltage (output of the separation stage) with respect to the external load used in the contact stage. Novel numerical results are in the same qualitative agreement with the experimental data as the approximate analytical solution proposed in [1]. At the same time, the analytical formula shows lower open-circuit voltage for the same external load than the numerical result, which is also in agreement with the difference in predictions of the real contact area between the two methods, presented in Fig. 3(a).

4 Conclusions

We proposed a methodology for numerical simulation of contact-separation TENG, which requires coupling of mechanical contact and electrostatic equations. The distinctive feature of this work is consideration of surface topography of the tribo-layers provided by the roughness measurements. The obtained numerical results show agreement with both experimental observations and available analytical formulas regarding the effect of the surface roughness on the output performance of the TENG. At the same time, the developed coupled finite-element framework permits extensions accounting for non-linear (e.g. elastoplastic) material behaviour of tribo-layers and/or interfacial friction during the contact stage. Moreover, the proposed framework allows to consider heterogeneous materials and predict the effect of inclusions in the tribo-layers on the output performance, facilitating the optimization and design of new TENG.

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