



Atomistic Field Theory for contact electrification of dielectrics

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ABSTRACT

The triboelectrification of conducting materials can be explained by electron transfer between different Fermi levels. However, triboelectrification in dielectrics is poorly understood. The surface dipole formations are shown to be caused by the contact-induced surface lattice deformations. An Atomistic Field Theory (AFT) based formulation is utilized to calculate the distribution of the polarization, electric and potential fields. The induced fields are considered as the driving force for charge transfer. The simulation results show that a MgO/BaTiO₃ tribopair can generate up to 104 V/cm², which is comparable with the data in the published literature.

1. Introduction

The triboelectric effect or contact electrification is an experimentally proven phenomenon [1]. Its occurrence in conducting materials can be explained by electron transfer resulting from the difference in work functions or Fermi levels of the contacting metals. That is, electrons in a metal with a higher energy level lower their energy by moving to a metal with a lower energy level [2,3]. However, when a dielectric material is involved, the essential cause of the charge transfer is largely debatable [1]: is it that rubbing the two surfaces increases the microscopic area of contact, or that it contributes energy to affect the charge transfer [1]. Additionally, the mechanism of the charge transfer is also debatable: is it the migration of electrons [4,5] or ions [6,7] or material "pieces" from one surface to another [8]. Because the fundamental cause and mechanism are not known, the answers to this very question about the exhibited behaviors of tribopairs involving dielectrics remain unclear: For example, there is no definite explanation for which dielectric material will attain a positive or a negative charge when it comes in contact with another. Furthermore, even for a given pair of materials, the direction of charge transfer cannot be reliably predicted [9]. To answer these questions, different empirical Triboelectric Series [10], which present an ordering of the materials depending on their tendency to attain positive or negative charges upon contact, have been developed. However, the actual exhibited behavior can depend on a multitude of factors that are not taken into account when the series are developed, which makes them unreliable [11]. In fact, experiments have shown that factors including the nature of contact [12], temperature [13], surface defects [14], the presence of adsorbates in the air [15] and the material strain [9] greatly affect the

results of triboelectrification experiments.

The occurrence of charge transfer necessitates the occurrence of a difference between the potentials of the surfaces in contact. Assuming defect-free surface lattices, unstrained materials and that the experiment is performed in vacuum; prior to any material, ionic or electronic migrations, the only remaining factor that can affect the surface potentials upon contact would be the formation of surface dipoles [16,17]. Therefore, this work postulates that the cause of triboelectrification or contact electrification in dielectrics is attributed to the contact-induced surface lattice deformations which result in the formation of surface dipoles. Furthermore, an Atomistic Field Theory (AFT) based [18] formulation is presented to efficiently calculate the distribution of the polarization, the electric potential and field and the charge density given the state of the constituent atoms of the surface lattices. MD simulations are used to simulate the lattice deformations resulting from the contact of Perovskite crystalline structure Barium Titanate (BaTiO₃) and Magnesia (MgO) because these materials have well established models in the literature [19,20]. It is shown that lattice deformations occur when the two materials are placed in sufficient proximity for the atomic interactions across the boundary to become strong enough to alter the atomic positions and form the surface dipoles.

Although the detailed mechanism of triboelectrification is still poorly understood, it has been the core of several different applications. Triboelectric Nanogenerators (TENGs) are an application of the triboelectric effect that has recently been drawing a lot of attention [21–24]. A TENG is able to convert mechanical to electrical energy similar to other energy harvesting devices but has a high volume energy density (490 kW/m³ [25]) which makes it an attractive alternative for utilizing wasted mechanical energy. A TENG utilizes dielectric materials, such as

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Perovskite-structure BaTiO₃ [26] and Polytetrafluoroethylene (PTFE) [26,27], as triboelectric pairs which underlines the need to further understand triboelectricity in dielectrics. Being dielectric, the materials trap the induced charge rather than transfer it. Consequently, the trapped charge creates an electric field, which induces electrical charge transfer in neighboring electrodes made of conducting materials [25]. Because of the coarse-grain nature of AFT, the presented formulation has potential to model the actual size of a TENG device (at the μm scale) and strengthens its suitability as a design tool for TENGs and other triboelectric devices.

Section 2 of this work derives the developed atomistic formulation and the approach to obtain the electric characteristics from the simulation results. Section 3 illustrates the atomistic models of the materials utilized in the MD simulation. Section 4 describes, in detail, the simulation procedure. Section 5 discusses the obtained dipole formations and electric characteristics. The conclusions can be found in Section 6.

2. Atomistic formulation for electromechanical coupling

In an MD simulation, atomic forces are calculated at each time step and the positions are updated by time integration. Using these positions, the electrical characteristics (electric field, electric potential and charge density) can be calculated by iterating relevant formulas [28] over all the atoms in the system. To simulate a micro-scale triboelectric layer that is usually employed in a TENG, a relatively large number of atoms is needed that will make the calculation be extremely time consuming.

Chen et al. introduced a concept of dipole formation for lattices at their current state and hypothesized that each lattice can be represented as a dipole [29,30]. In other words, a crystalline structure is approximated as a collection of dipole. This dipole can not only be used for the calculations of the electric characteristics but also related to the Miller indices for crystallines. A perfect lattice in general results to no polarization relative to the center of the lattice. However, if a lattice is perturbed by stimuli, e.g. temperature, mechanical forces or body forces, the motions of all atoms within a lattice consequently produce polarization and the lattice can be considered as a dipole. It should be noticed that this concept is different from a molecular dipole. The dipole for a lattice is defined at its perturbed state while a molecular dipole exists in the ground state of a molecule.

Each consequent dipole represents a lattice and induces an electric field in its proximity. The surface lattices of both materials are interfered by each other when the pair is in close distance during electrification. In this work, the induced field is hypothesized as the driving force for charge transfer.

There are multiple theories to describe the lattice properties. Atomistic Field Theory (AFT) [18] is one approach to efficiently obtain properties from the state of the atoms at a certain time. Solids possess a repetitive pattern of atoms referred to as the Bravais lattice, which is neutrally charged. By placing a node at the center of a representative lattice, the motion of any atom within the lattice can be expressed by Refs. [29,30]:

$$\mathbf{u}(k, \alpha) = \mathbf{u}(k) + \zeta(k, \alpha) \quad (1)$$

where α and k represent the α -th atom in the k -th unit cell, $\mathbf{u}(k)$ is the displacement of the k -th unit cell and $\zeta(k, \alpha)$ is the relative displacement of atom α to the centroid of the k -th unit cell. All the physical quantities can be then expressed in physical and phase spaces, which are connected through the Dirac delta function, δ , and the Kronecker delta function, $\tilde{\delta}$, as

$$A(\mathbf{x}, \mathbf{y}^\alpha, t) = \sum_{k=1}^{N_{uc}} \sum_{\alpha=1}^{N_a} a[\mathbf{r}(t), \mathbf{p}(t)] \delta(\mathbf{R}^k - \mathbf{x}) \tilde{\delta}(\Delta r^{k\zeta} - \mathbf{y}^\alpha) \quad (2)$$

with normalization conditions

$$\int_{V^*} \delta(\mathbf{R}^k - \mathbf{x}) d^3\mathbf{x} = 1 \quad (k = 1, 2, 3, \dots, n) \quad (3)$$

where V^* is the volume of a unit cell; \mathbf{R}^k and \mathbf{x} is the position vector of the k -th unit cell in the phase and physical spaces, respectively. N_{uc} and N_a are the number of unit cells in the system and the number of atoms in the k -th unit cell, respectively.

It is straightforward to define polarization density, $\mathbf{p}(\mathbf{x}, \mathbf{y}^\alpha, t)$, of ζ -th atom within k -th unit cell as

$$\mathbf{P}(\mathbf{x}, \mathbf{y}^\alpha, t) = \sum_{k=1}^{N_{uc}} \sum_{\alpha=1}^{N_a} q^\zeta(\mathbf{R}^k + \Delta r^{k\zeta}) \delta(\mathbf{R}^k - \mathbf{x}) \tilde{\delta}(\Delta r^{k\zeta} - \mathbf{y}^\alpha) \quad (4)$$

By averaging over the unit cells results in the homogeneous field, the polarization density, $\mathbf{P}(\mathbf{x}, t)$, for the unit cell at the position \mathbf{x} is given by Refs. [29,30]:

$$\mathbf{P}(\mathbf{x}, t) = \sum_{k=1}^{N_{uc}} \sum_{\alpha=1}^{N_a} q^\alpha \mathbf{d}^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \quad (5)$$

where q^α is the charge of atom α and $\mathbf{d}^{k\alpha}$ is the displacement (relative to the center of the lattice) of the α -th atom in the k -th unit cell.

When the lattices of the two materials approach each other, the constituent atoms of both lattices interact (repulse/attract) according to the assumed interatomic potential. Such atomistic motions result in dipole formation on the surface. The electric potential density at the position \mathbf{z} due to the unit cell at \mathbf{x} could be calculated from Refs. [29–31]:

$$V(\mathbf{z}, \mathbf{x}, t) = \sum_{k=1}^{N_{uc}} \sum_{\alpha=1}^{N_a} q^\alpha \mathbf{d}^{k\alpha} \cdot \frac{(\mathbf{z} - \mathbf{x})}{|\mathbf{z} - \mathbf{x}|^3} \delta(\mathbf{R}^k - \mathbf{x}) \quad (6)$$

N_{uc} is the number of unit cells in the system instead of the atoms, which considerably improves the calculation performance. Consequently, the induced electric field density at the position \mathbf{z} by a unit cell located at \mathbf{x} can be calculated from by using $E = -\nabla_z V$ [29–31]:

$$\mathbf{E}(\mathbf{z}, \mathbf{x}, t) = \sum_{k=1}^{N_{uc}} \sum_{\alpha=1}^{N_a} q^\alpha \mathbf{d}^{k\alpha} \cdot \left(\frac{3(\mathbf{z} - \mathbf{x}) \otimes (\mathbf{z} - \mathbf{x})}{|\mathbf{z} - \mathbf{x}|^5} - \frac{\mathbf{I}}{|\mathbf{z} - \mathbf{x}|^3} \right) \delta(\mathbf{R}^k - \mathbf{x}) \quad (7)$$

where \mathbf{I} is the identity matrix. The electric field at position \mathbf{z} induced by all unit cells can be found by integrating Equation (7) over all unit cells as [29,30].

$$\mathbf{E}(\mathbf{z}, t) = \int \sum_{k=1}^{N_{uc}} \sum_{\alpha=1}^{N_a} q^\alpha \mathbf{d}^{k\alpha} \cdot \left(\frac{3(\mathbf{z} - \mathbf{x}) \otimes (\mathbf{z} - \mathbf{x})}{|\mathbf{z} - \mathbf{x}|^5} - \frac{\mathbf{I}}{|\mathbf{z} - \mathbf{x}|^3} \right) \delta(\mathbf{R}^k - \mathbf{x}) d^3\mathbf{x} \quad (8)$$

3. Material choice

The test case involves a Perovskite crystalline structure barium titanate (BaTiO₃), and a rocksalt crystalline structure magnesia (MgO). Both are modeled using the Coulomb-Buckingham potential [19,32–34]:

$$U^{ij}(r^{ij}) = \frac{q^i q^j}{r^{ij}} + A e^{-\frac{r^{ij}}{\rho}} - \frac{C}{r^{ij6}} \quad (9)$$

where U^{ij} is the potential, r^{ij} is the interatomic distance, q^i is the charge of the i -th atom and A and ρ and C are species-to-species dependent parameters [19].

Chen and Lee [20] showed that for the original Coulomb-Buckingham potential shown in Equation (9), an unphysical collision between oxygen atoms (Buckingham Catastrophe) can occur when the interatomic distance becomes lower than a critical value. Therefore, the modification suggested by Chen and Lee [20] is included: The addition of a Lennard-Jones r^{ij-12} repulsive term. The final form of the potential becomes:

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