Research Article

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Model of electric charge distribution in the trap of a close-contact TENG system

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Abstract: Electron propagation in a trapped state between an insulator and a metal during very close contact in a triboelectric nanogenerator (TENG) system was considered in this study. A single energy level (E_0) was assumed for the trap and wave function inside the trap, which is related to the ground state energy. The phase of the waveform in the metal (neglecting the rebound effect at the wall) was assumed very small ($\delta' \ll 1$) because of the large size of the metal. The contact distance between the trap and metal is very small, which allows us to ignore the vacuum potential. Based on our results, the probability of finding an electron inside the trap as a function of time was found to be in oscillation (*i.e.*, back-and-forth propagation of the electron between the trap and metal leads to an equilibrium state). These results can be used to understand the quantum mechanisms of continuous contact, particularly in sliding-mode TENG systems.

Keywords: wave function, trap, oscillation, triboelectric nanogenerator

1 Introduction

The charge transfer mechanism [1–4] is typically described by two factors: (i) thermionic emission, *i.e.*, temperature-induced electron flow [5, 6] in which penetrating charges take longer to reach thermodynamic equilibrium; (ii) tunneling between the metal and trap sites in the insulator [7–9]. However, in a triboelectric nanogenerator (TENG) system, an external circuit is connected to the triboelectric part, where charge transfer occurs at the interface between the metal and the insulator, and an additional charge transfer to the bottom substrate through the circuit occurs [10]. The sliding TENG system uses a continuous frictional mode, which is different from the contact-

separation mode. Charge transfer can occur between the two triboelectric materials when very close contact is maintained. In the contact-separation mode, an electric field is formed between the two surfaces upon separation, leading to the formation of a vacuum potential through which electrons can tunnel [11]. During contact, the driving force for a charge transfer can be described based on the work function difference between the materials. However, this study describes quantum-mechanical electron propagation from a band-diagram point of view, neglecting the vacuum potential between the two materials. The close-contact model used in this work does not use a potential barrier through which electrons can tunnel owing to the charge neutrality on the contact interface (*i.e.*, zero sum charge). In this model, the probability of an electron transfer has been described by a quantum wave function. The surface state of the insulator, wherein the transferred electrons can accumulate, has been described by a localized state and a trap, which was approximated by a square potential well with a single-electron energy (E_0). As the charge transfer between the metal and the trap can occur at the same energy level, a metal-to-trap and a trap-to-metal transfer have the same probability. To simplify the calculation, the initial wave function was described by the trapped electron, and the electron transfer to the empty metal was subsequently calculated. However, the converse probability process could also be applied to the model system. Mathematically, the one-dimensional time-dependent wave function was calculated by an overlap integral. The result obtained by this model showed that the charge transfer was more similar to a direct propagation, resulting in oscillation, rather than tunneling through the potential barrier of the very-close-contact environment.

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2 Results: Calculation of the time-dependent wave function in a close-contact TENG system

2.1 Wave functions of the system consisting of trap of an insulator and a metal

The wave function u of the potential of the system shown in Figure 1 (a) was considered as follows:

$$u = \begin{cases} D \cdot e^{\mu(x+a)} & (x \leq -a), \\ A \cdot \cos kx & (|x| \leq a), \\ C \cdot \sin k(x - a + \delta') & (x \geq a), \end{cases} \quad (1)$$

where the wave function inside the trap was assumed an even function based on the ground state energy. Here, $\delta' \ll 1$ because of the large size of the metal ($L \gg 1$) (i.e., the rebound effect was neglected). E was assumed a single energy of a specific wave function, which resulted in $k = \sqrt{2mE}/\hbar$ and $\mu = \sqrt{2m(V-E)}/\hbar$, where V is the depth of the potential well. The coefficients D , A , C , and δ' were determined from the boundary conditions, whereby u and $\frac{\partial u}{\partial x}$ are continuous at $x = \pm a$.

To calculate the overlap integral, an initial wave function $\psi(0)$ inside an isolated trap was first considered [5], as shown in Figure 1 (b), where the trap is far from the metal.

$$\psi(0) = \begin{cases} F \cdot \cos k_0 x & (|x| \leq a), \\ G e^{-\mu_0|x-a|} & (|x| \geq a), \end{cases} \quad (2)$$

where

$$F = \sqrt{\frac{\mu_0}{1 + \mu_0 a}}, \quad G = \frac{k_0 \cdot F}{\sqrt{k_0^2 + \mu_0^2}}, \quad (3)$$

$$k_0 = \frac{\sqrt{2mE_0}}{\hbar}, \quad \mu_0 = \frac{\sqrt{2m(V-E_0)}}{\hbar}.$$

Applying the boundary conditions for the electron wave function inside the trap that is very close to the metal, resulted in the following relations:

$$\begin{aligned} D &= A \cos ak, \\ \mu D &= k \cdot A \sin ak, \\ A \cos ka &= C \cdot \sin k\delta', \quad -k \cdot A \sin ka = k \cdot C \cos k\delta'. \end{aligned} \quad (4)$$

Assuming $\delta' \ll 1$ in Eq. (4) gave the following relations:

$$\begin{aligned} \mu &= k \cdot \tan ak, \\ \delta' &= -\frac{1}{k \cdot \tan ka} = -\frac{1}{\mu}, \end{aligned} \quad (5)$$

$$\frac{A}{C} = -\frac{1}{\sin ka} = -\frac{1}{\sin\left(\frac{\sqrt{2mE}}{\hbar} \cdot a\right)}$$

when C was set to 1,

$$A = -\frac{1}{\sin\left(\frac{\sqrt{2mE}}{\hbar} \cdot a\right)}. \quad (6)$$

2.2 Overlap integral $a(E)$

An overlap integral was defined as follows:

$$\begin{aligned} a(E) &= \int_{-\infty}^{\infty} \psi(0) \cdot u^*(E) dx \\ &= \int_{-\infty}^{\infty} F \cos k_0 x \cdot A \cdot \cos kx dx \\ &= F \cdot A \int_{-\infty}^{\infty} \cos^2 k_0 x dx \\ &= F \cdot A(E) \left\{ a + \frac{\sin 2k_0 \cdot a}{2k_0} \right\}, \end{aligned} \quad (7)$$

where the resonance condition at $k \approx k_0$ was used.

2.3 Time-dependent wave functions $\psi(x, t)$

To calculate the time-dependent wave function inside the trap, the following formula was used:

$$\begin{aligned} \psi(x, t) &= \int_{-\infty}^{\infty} a(E) \cdot u(E) e^{-iEt/\hbar} \cdot N(E) dE \\ &= \int_{-\infty}^{\infty} NF \cdot A(E) \cdot \left\{ a + \frac{\sin 2k_0 a}{2k_0} \right\} \cdot A(E) \cos kx \\ &\quad \cdot e^{-iEt/\hbar} \cdot dE = NF \cdot \left\{ a + \frac{\sin 2k_0 a}{2k_0} \right\} \\ &\quad \cdot \left[\int_{-\infty}^{\infty} A^2(E) \cdot \cos kx \cdot e^{-\frac{iEt}{\hbar}} dE \right]. \end{aligned} \quad (8)$$

Considering the resonance to occur at $k \approx k_0$, then

$$\begin{aligned} \psi(x, t) &\cong NF \cdot \left\{ a + \frac{\sin 2k_0 a}{2k_0} \right\} \cos k_0 x \\ &\quad \cdot \left[\int_{-\infty}^{\infty} \frac{e^{-\frac{iEt}{\hbar}}}{\sin^2\left(\frac{\sqrt{2mE}}{\hbar} \cdot a\right)} dE \right]. \end{aligned} \quad (9)$$

When E was changed to $-E$ in the integral, then

$$\psi(x, t) = NF \cdot \left\{ a + \frac{\sin 2k_0 a}{2k_0} \right\} \cos k_0 x \quad (10)$$

$$\cdot \left[\int_{-\infty}^{\infty} \frac{e^{iEt/\hbar}}{\sin^2 \left(\frac{\sqrt{2mE}}{\hbar} \cdot ai \right)} dE \right] \\ = NF \cdot \left\{ a + \frac{\sin 2k_0 a}{2k_0} \right\} \cos k_0 x \\ \cdot \left[\int_{-\infty}^{\infty} \frac{e^{\frac{iEt}{\hbar}}}{-\sin h^2 \left(\frac{\sqrt{2mE}}{\hbar} \cdot a \right)} dE \right]$$

As $a \ll 1$, the denominator in the integral could be expanded by a power series, such that

$$\sinh^2 \left(\frac{\sqrt{2mE}}{\hbar} \cdot a \right) \approx \frac{2Ema^2}{\hbar^2} + \frac{4E^2 \cdot m^2 \cdot a^4}{3\hbar^4} + \dots \quad (11)$$

The integral in Eq. (10) could then be rewritten as

$$\int_{-\infty}^{\infty} \left[\frac{-e^{iEt/\hbar}}{\frac{2Ema^2}{\hbar^2} + \frac{4E^2 \cdot m^2 \cdot a^4}{3\hbar^4}} \right] dE. \quad (12)$$

This integral could be solved using a contour integral and the residue theorem with two branch poles.

$$\text{Poles} = \begin{cases} 0 \\ \frac{-3\hbar^2}{2a^2 \cdot m} \end{cases} \quad (13) \\ \text{Residues} = \begin{cases} \frac{-\hbar^2}{2a^2 \cdot m} \\ \frac{\hbar^2 e^{-3it\hbar/2a^2 m}}{2a^2 \cdot m} \end{cases}$$

The value of the integral in Eq. (10) was then obtained as

$$\pi i \left[\frac{-\hbar^2}{2a^2 \cdot m} + \frac{\hbar^2 e^{-3it\hbar/2a^2 m}}{2a^2 \cdot m} \right] \\ = \left[\frac{i \left(-1 + e^{-3it\hbar/2a^2 m} \right) \pi \hbar^2}{2a^2 \cdot m} \right]. \quad (14)$$

Therefore, $\psi(x, t)$ could be restated under the condition $a \ll 1$, as

$$\psi(x, t) \cong N\sqrt{\mu_0} \cdot a \cos k_0 x \\ \cdot \left\{ \frac{i \left(e^{-\frac{3it\hbar}{2a^2 m}} - 1 \right) \pi \hbar^2}{2a^2 \cdot m} \right\}. \quad (15)$$

The probability of finding an electron inside the trap was then obtained as

$$|\psi(x, t)|^2 \cong N^2 \cdot \mu_0 \cdot a^2 \cdot \cos^2 k_0 x \\ \cdot \left[\frac{\pi^2 \hbar^4 \sin^2 \left(\frac{3t\hbar}{4a^2 \cdot m} \right)}{a^4 \cdot m^2} \right], \quad (16)$$

where N is the density of states in the metal and is given by $mL/\pi\hbar^2 k_0$ [5].

Substituting N , μ_0 , and k_0 into Eq. (16) led to the following relation:

$$|\psi(x, t)|^2 \quad (17) \\ \cong \left[\frac{L^2 \sqrt{m(V - E_0)} \cdot \hbar \cdot \cos^2 \left[\frac{\sqrt{2mE_0}}{\hbar} \cdot x \right] \cdot \sin^2 \left(\frac{3t\hbar}{4a^2 \cdot m} \right)}{16 \cdot \sqrt{2} \cdot a^2 \cdot E_0 \cdot m \cdot \pi^4} \right].$$

Selecting the time and space information from Eq. (17), we obtained

$$|\psi(x, t)|^2 \sim \cos^2 \left[\frac{\sqrt{2mE_0}}{\hbar} \cdot x \right] \cdot \sin^2 \left(\frac{3t\hbar}{4a^2 \cdot m} \right) \quad (18)$$

where E_0 is the initial single-electron energy inside the isolated trap.

Therefore, the triboelectric charge density formed on the interface could be described as

$$\sigma = |\psi(x, t)|^2 \cdot n \cdot e, \quad (19)$$

where e is the elementary charge and n is the surface density of the traps contained on the surface of the insulator (in units of $\#/m^2$).

Furthermore, $V - E_0$ was the work function of the insulator ϕ_{I_0} , and Eq. (17) could be restated as

$$|\psi(x, t)|^2 \quad (20) \\ \cong \left[\frac{L^2 \sqrt{m\phi_{I_0}} \cdot \hbar \cdot \cos^2 \left[\frac{\sqrt{2mE_0}}{\hbar} \cdot x \right] \cdot \sin^2 \left(\frac{3t\hbar}{4a^2 \cdot m} \right)}{16 \cdot \sqrt{2} \cdot a^2 \cdot E_0 \cdot m \cdot \pi^4} \right] \\ \sim \sqrt{\phi_{I_0}}$$

3 Discussion

In a close-contact model, the trap present on the surface of an insulator was assumed to be defined by the surface density of states, which was determined by the quantum square well potential. The electronic potential energy as a function of position for this close-contact model is shown in Figure 1 (a). As the distance between the trap and the metal is approximately zero, the image potential on the metal side was not considered, and there was no potential barrier (i.e., there is no decay of the wave function). However, the potential changes discontinuously as the distance approaches zero (i.e., close contact). A calculation of the wave function considering the distance between the insulator and metal was provided by Lowell [5]. Here, the wave functions were calculated for a complete system consisting of a metal and trap on an insulator. Subsequently, the time dependent method was used to calculate the time-evolution wave functions [5, 12]. The probability of a charge transfer can be applied equally to both

Figure 1: (a) Electron potential energy along the x -axis from the center of the trap potential (i.e., a square potential with a depth of V and a width of $2a$) in the insulator. The potential is assumed to be closely defined by the trap and the metal (a contact line is shown). The shape of the potential energy wave functions is shown. (b) The isolated potential energy of an electron in the trap is shown as a function of position x .

cases, i.e., metal-to-trap and trap-to-metal. The initial electron wave function is described by the electron trapped inside the isolated quantum well, which propagates towards the metal with time. It is assumed that the Fermi energy of the trap is greater than that of the metal. The wave function inside the trap is not influenced by the metal, which is located far from it. This structure can lead to the formation of a localized wave function with ground state energy (i.e., an even function), as shown in Figure 1 (b).

When the metal is approaching or is in contact with the trap, electron tunneling through the barrier is not considered because of the instantaneous nature of the contact. During contact, the wave function inside the trap is assumed identical to that of the isolated trap. This resonance condition was used to calculate the overlap integral $a(E)$, which is maximized when the wave function inside the trap is approximately equal to that of an isolated trap (i.e., $E \approx E_0$). Otherwise, for very small values of $a(E)$, the filled electron state of the trap gradually propagates into

Figure 2: Plot of the time component of $|\psi(x, t)|^2$

Figure 3: Three-dimensional plot of both time and spatial components of $|\psi(x, t)|^2$

Figure 4: Plot of $|\psi(x, t)|^2$ as a function of Φ_{I_0}

the empty metal. Figure 2 shows the time component of the probability of finding an electron, i.e., $\sin^2\left(\frac{3t\hbar}{4a^2 \cdot m}\right)$. This figure implies that the electron probability inside the trap oscillates. Conversely, the electron probability in the metal is given by $1 - |\psi(x, t)|^2$, which is also an oscillation pattern. In other words, the electron charge density as a function of time alternates between the metal and the trap. Figure 3 shows the distribution of both time and spatial components inside the trap, i.e., $\cos^2\left[\frac{\sqrt{2mE_0}}{\hbar} \cdot x\right] \cdot \sin^2\left(\frac{3t\hbar}{4a^2 \cdot m}\right)$

(the time component shows the oscillation). The results obtained for the close-contact-mode TENG system showed the oscillation of electron propagation, which is driven by the work function difference between the trap and the metal. It is evident from Eq. (20) that the electron charge density inside the trap is proportional to the square root of the work function of the insulator ($\sqrt{\phi_{I_0}}$), as shown in Figure 4.

4 Conclusion

The charge transfer between the trap in the insulator and the metal in a close-contact-mode TENG system was described using quantum mechanics. Our physical system was described by close contact model between the metal and the trap in the insulator as in, for example, sliding-mode triboelectric nanogenerator where contact and separation were not repeated, but close contact was maintained. Once the contact and separation occur, there exists a vacuum region between the metal and the insulator that can form a potential barrier [11]. After electron transfer, due to the accumulated charges the electric field can be formed which can lead to the formation of sloped potential barrier. In this model system, the vacuum potential barrier was not considered due to the absence of the vacuum where electron can transfer or tunnel through it. Instead, in this region electron can freely transfer back and forth that was modeled as non-tunneling region. Furthermore, it was assumed that the trap was located close to the surface that was directly connected with the surface of the metal for simple calculation. The trap potential was assumed a square potential. The time-dependent wave function, which is related to the probability of finding electrons (or the electron density) inside the trap, was found to be in oscillation. This implies that, with the metal in close contact, the charge density inside the trap flows back and forth. The results were analytically investigated.

Conflict of Interests: The authors declare that there are no conflicts of interest.

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