

Theoretical Calculation Of $Q(t)$, (Transferred Charge) In A Contact-Mode Triboelectric Nanogenerator With Variable σ (Triboelectric Charge Density): Dynamic Study (Time-Dependent)

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Abstract: An analytical model for time-dependent transferred charge $Q(t)$ in a contact-mode triboelectric nanogenerator was constructed in this paper. Based on the mathematical model, the variable triboelectric charge density (σ) is used to calculate a first-order ordinary differential equation within tunneling distance. The approach presented here in the first derivation of $Q(t)$ under nanoscale contact electrification.

Keywords: Time-dependent transferred charge, TENG, variable tribocharge, contact mode

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I. Introduction

In general, if a contact-mode triboelectric nanogenerator (TENG) [1-10] is connected to an external circuit with a resistor R , the output characteristics can be described by simple Ohm's law:

$$V = IR = R \frac{dQ(t)}{dt} = -\frac{Q(t)}{S\epsilon_0} \left[\frac{d}{\epsilon} + x(t) \right] + \frac{\sigma x(t)}{\epsilon_0} \dots \dots \dots (1)$$

Eq(1) is a first-order ordinary differential equation with boundary conditions such as $Q(0) = 0$ [11]. When $t=0$, the metal and dielectric layer are in contact with each other for long time. Thus, electrostatic induction is not carried out to induce the transferred charge Q on the bottom metal, indicating that $Q(0) = 0$. However, the tribocharge density σ in Eq(1), which was previously regarded as a constant, has the functions of several parameters such as

$$\sigma = \left[\frac{\frac{W-E_0}{e(1+d/\epsilon x(t))}}{d/\epsilon \cdot \epsilon_0 + \frac{1+d/\epsilon x(t)}{N_s(E) \cdot e^2}} \right] \dots \dots \dots (2)$$

within the tunneling distance between the metal and dielectric [12]. Therefore, this paper presents the theoretical calculation of time-dependent $Q(t)$ in a contact-mode TENG with variable σ within a nanoscale distance. The tunneling distance $x(t)$ can be larger if the electron's kinetic energy is similar to that of the barrier energy between the metal and dielectric layers, as the transmission probability approaches one.

II. Calculation of time-dependent transferred charge $Q(t)$ in a contact-mode TENG

The first-order ordinary differential equation including variable σ can be written as

$$\frac{dQ(t)}{dt} \cdot R = \underbrace{\frac{-Q(t)}{S \cdot \epsilon_0} \left(\frac{d}{\epsilon} + x(t) \right)}_{1st \ part} + \underbrace{\frac{x(t)}{\epsilon_0} \left[\frac{(W - E_0)/e(1 + d/\epsilon x(t))}{d/\epsilon \cdot \epsilon_0 + \frac{1+d/\epsilon x(t)}{N_s(E) \cdot e^2}} \right]}_{2nd \ part} \dots \dots \dots (3)$$

The $x(t)$ is the tunneling distance between the metal and dielectric layer, which is very small, such that the second part on the right in Eq(3) can be expanded by power series as

$$\begin{aligned} & \frac{(-E_0 + W)x(1 + \frac{d}{x\epsilon})}{e(\frac{1+d}{e^2 N_s(E)} + \frac{d}{\epsilon \epsilon_0}) \epsilon_0} \\ &= \frac{(eN_s(E)W - eN_s(E)E_0)x}{\epsilon_0} + \frac{(-e^3 N_s(E)^2 W + e^3 N_s(E)^2 E_0)x^2}{\epsilon_0^2} \\ &+ \frac{(de^5 N_s(E)^3 W - de^5 N_s(E)^3 E_0 + e^3 N_s(E)^2 W \epsilon \epsilon_0 - e^3 N_s(E)^2 \epsilon E_0 \epsilon_0)x^3}{d\epsilon_0^3} + O[x]^4 \dots \dots (4) \end{aligned}$$

with $t < \frac{x_{critical}}{v} = \frac{x_{max}}{v}$.

The first term on the right in Eq(4) is substituted into the second part of Eq(3), then Eq(3) can be rewritten as

$$\frac{dQ(t)}{dt} \cdot R \cong -\frac{Q(t)}{S \cdot \epsilon_0} \left(\frac{d}{\epsilon} + x(t) \right) + \left[\frac{-e \cdot E_0 \cdot N_s(E) + eN_s(E) \cdot W}{\epsilon_0} \right] x(t) \dots \dots \dots (5)$$

$$\cong -\frac{Q(t)}{S \cdot \epsilon_0} \cdot \frac{d}{\epsilon} + x(t) \left[\frac{N_s(E) \cdot e \cdot (W - E_0)}{\epsilon_0} - \frac{Q(t)}{S \cdot \epsilon_0} \right] \dots \dots \dots (6)$$

Eq(6)describes the transferred charge with time change and varying tunneling distance $x(t)$, which is associated with the work function difference $(W - E_0)$ and the averaged surface density of state $N_s(E)$ of the dielectric material. In Eq(4), more than the first term on the right is neglected.

The solution of Eq(6) can be obtained as follows:

$$Q(t) = -e \int_1^t \frac{e^{-\frac{d-\epsilon x [K[1]]}{RS\epsilon_0}} dK[1]}{\left(\int_1^0 \frac{e^{-\frac{d-\epsilon x [K[1]]}{RS\epsilon_0}} dK[1]}{RS\epsilon_0} (-eE_0N_s(E)S\epsilon x[K[2]] + eN_s(E)SW\epsilon x[K[2]]) dK[2] \right)} - \int_1^t \frac{e^{-\frac{d-\epsilon x [K[1]]}{RS\epsilon_0}} dK[1]}{RS\epsilon_0} (-eE_0N_s(E)S\epsilon x[K[2]] + eN_s(E)SW\epsilon x[K[2]]) dK[2] \dots \dots \dots (7)$$

Substituting vt into $x(t)$ in Eq(7) with a boundary condition, $Q(0) = 0$, it can be rewritten as

$$Q(t) = -\frac{1}{2\sqrt{R}\sqrt{v}\epsilon\sqrt{\epsilon_0}} e^{\frac{t^2v}{2RS\epsilon_0} - \frac{d^2}{2RSv\epsilon^2\epsilon_0} - \frac{dt}{RS\epsilon_0}} N_s(E)\sqrt{S}(E_0 - W) \left(2e^{\frac{t^2v}{2RS\epsilon_0} + \frac{d^2}{2RSv\epsilon^2\epsilon_0} + \frac{dt}{RS\epsilon_0}} \sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0} - 2e^{\frac{d^2}{2RSv\epsilon^2\epsilon_0}} \sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0} + d\sqrt{2\pi}\text{Erfi}\left[\frac{d}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}}\right] - d\sqrt{2\pi}\text{Erfi}\left[\frac{d + tv\epsilon}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}}\right] \right) \dots \dots \dots (8)$$

Simplifying Eq(8) leads to

$$Q(t) = \frac{1}{2\sqrt{R}\sqrt{v}\epsilon\sqrt{\epsilon_0}} e^{\frac{(d+tv\epsilon)^2}{2RSv\epsilon^2\epsilon_0}} N_s(E)\sqrt{S}(E_0 - W) \left(2\left(e^{\frac{d^2}{2RSv\epsilon^2\epsilon_0}} - e^{\frac{(d+tv\epsilon)^2}{2RSv\epsilon^2\epsilon_0}} \right) \sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0} - d\sqrt{2\pi}\text{Erfi}\left[\frac{d}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}}\right] + d\sqrt{2\pi}\text{Erfi}\left[\frac{d + tv\epsilon}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}}\right] \right) \dots \dots \dots (9)$$

with $t < \frac{x_{max}}{v}$

$\text{Erfi}(z) = \text{erf}(iz)/i$, which is defined as an imaginary error function

$$\text{erfi}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt \dots \dots \dots (9-2)$$

When $t > \frac{x_{max}}{v}$, the tunneling distance x equals to x_{max} . Then, Eq(6) can be restated as

$$RQ'[t] = \frac{(-eE_0N_s(E) + eN_s(E)W)x_{max}}{\epsilon_0} - \frac{(x_{max} + \frac{d}{\epsilon})Q[t]}{S\epsilon_0} \dots \dots \dots (10)$$

From Eq(10) with the boundary condition $Q(x_{max}/v) = Q_0$, $Q(t)$ can be obtained as

$$Q(t) = -\frac{1}{d + x_{max}\epsilon} e^{-\frac{t(d+x_{max}\epsilon)}{RS\epsilon_0}} \left(-d e^{\frac{x_{max}(d+x_{max}\epsilon)}{RSv\epsilon_0}} Q_0 - e^{\frac{x_{max}(d+x_{max}\epsilon)}{RSv\epsilon_0}} Q_0 x_{max}\epsilon + e e^{\frac{t(d+x_{max}\epsilon)}{RS\epsilon_0}} E_0 N_s(E) S x_{max}\epsilon - e e^{\frac{x_{max}(d+x_{max}\epsilon)}{RSv\epsilon_0}} E_0 N_s(E) S x_{max}\epsilon - e e^{\frac{t(d+x_{max}\epsilon)}{RS\epsilon_0}} N_s(E) S W x_{max}\epsilon + e e^{\frac{x_{max}(d+x_{max}\epsilon)}{RSv\epsilon_0}} N_s(E) S W x_{max}\epsilon \right) \dots \dots \dots (11)$$

Eq(11) can be simplified as

$$Q(t) = \frac{1}{d + x_{\max} \epsilon} e^{-\frac{t(d+x_{\max} \epsilon)}{RS\epsilon \epsilon_0}} \left(d e^{-\frac{x_{\max} (d+x_{\max} \epsilon)}{RSv\epsilon \epsilon_0}} Q_0 + \left(e^{-\frac{x_{\max} (d+x_{\max} \epsilon)}{RSv\epsilon \epsilon_0}} (Q_0 + eN_s(E)S(E_0 - W)) - e e^{-\frac{t(d+x_{\max} \epsilon)}{RS\epsilon \epsilon_0}} N_s(E)S(E_0 - W) \right) x_{\max} \epsilon \right) \dots \dots \dots (12)$$

In Eq(12), Q_0 can be calculated by substituting $t = \frac{x_{\max}}{v}$ into Eq(9).

$$Q_0 = \frac{1}{2\sqrt{R}\sqrt{v}\epsilon\sqrt{\epsilon_0}} e e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} N_s(E)\sqrt{S}(E_0 - W) \left(2 \left(e^{-\frac{d^2}{2RSv\epsilon^2\epsilon_0}} - e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} \right) \sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0} - d\sqrt{2\pi}\text{Erfi} \left[\frac{d}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] + d\sqrt{2\pi}\text{Erfi} \left[\frac{d + x_{\max} \epsilon}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] \right) \dots \dots \dots (13)$$

Eq(13) can be simplified as

$$Q_0 = \frac{1}{2\sqrt{R}\sqrt{v}\epsilon\sqrt{\epsilon_0}} e e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} N_s(E)\sqrt{S}(E_0 - W) \left(2 \left(e^{-\frac{d^2}{2RSv\epsilon^2\epsilon_0}} - e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} \right) \sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0} - d\sqrt{2\pi}\text{Erfi} \left[\frac{d}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] + d\sqrt{2\pi}\text{Erfi} \left[\frac{d + x_{\max} \epsilon}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] \right) \dots \dots \dots (14)$$

Therefore, Eq(12) can be rewritten as

$$Q(t) = \frac{1}{d + x_{\max} \epsilon} e^{-\frac{t(d+x_{\max} \epsilon)}{RS\epsilon \epsilon_0}} \left(\frac{1}{2\sqrt{R}\sqrt{v}\epsilon\sqrt{\epsilon_0}} d e^{-\frac{x_{\max} (d+x_{\max} \epsilon)}{RSv\epsilon \epsilon_0}} e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} N_s(E)\sqrt{S}(E_0 - W) \left(2 \left(e^{-\frac{d^2}{2RSv\epsilon^2\epsilon_0}} - e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} \right) \sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0} - d\sqrt{2\pi}\text{Erfi} \left[\frac{d}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] + d\sqrt{2\pi}\text{Erfi} \left[\frac{d + x_{\max} \epsilon}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] \right) + x_{\max} \epsilon \left(-e e^{-\frac{t(d+x_{\max} \epsilon)}{RS\epsilon \epsilon_0}} N_s(E)S(E_0 - W) + e^{-\frac{x_{\max} (d+x_{\max} \epsilon)}{RSv\epsilon \epsilon_0}} \left(eN_s(E)S(E_0 - W) + \frac{1}{2\sqrt{R}\sqrt{v}\epsilon\sqrt{\epsilon_0}} e e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} N_s(E)\sqrt{S}(E_0 - W) \left(2 \left(e^{-\frac{d^2}{2RSv\epsilon^2\epsilon_0}} - e^{-\frac{(d+x_{\max} \epsilon)^2}{2RSv\epsilon^2\epsilon_0}} \right) \sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0} - d\sqrt{2\pi}\text{Erfi} \left[\frac{d}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] + d\sqrt{2\pi}\text{Erfi} \left[\frac{d + x_{\max} \epsilon}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] \right) \right) \right) \right) \dots \dots \dots (15)$$

Eq(15) can be simplified as

$$\begin{aligned}
 Q(t) = & \frac{1}{2\sqrt{R}\sqrt{v}\epsilon(d+x_{\max}\epsilon)\sqrt{\epsilon_0}} e^{\frac{(d+x_{\max}\epsilon)(d+2tv+x_{\max}\epsilon)}{2RSv\epsilon^2\epsilon_0}} N_s(E)\sqrt{S}(E_0) \\
 & - W \left(2\sqrt{R}\sqrt{S}\sqrt{v}\epsilon \left(d \left(-e^{\frac{(d+x_{\max}\epsilon)(d+3x_{\max}\epsilon)}{2RSv\epsilon^2\epsilon_0}} + e^{\frac{d^2+2dx_{\max}\epsilon+2x_{\max}^2\epsilon^2}{2RSv\epsilon^2\epsilon_0}} \right) \right. \right. \\
 & \left. \left. + \left(-e^{\frac{(d+x_{\max}\epsilon)(d+2tv+x_{\max}\epsilon)}{2RSv\epsilon^2\epsilon_0}} + e^{\frac{d^2+2dx_{\max}\epsilon+2x_{\max}^2\epsilon^2}{2RSv\epsilon^2\epsilon_0}} \right) x_{\max}\epsilon \right) \sqrt{\epsilon_0} \right. \\
 & - d e^{\frac{x_{\max}(d+x_{\max}\epsilon)}{RSv\epsilon_0}} \sqrt{2\pi}(d+x_{\max}\epsilon) \operatorname{Erfi} \left[\frac{d}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] \\
 & \left. + d e^{\frac{x_{\max}(d+x_{\max}\epsilon)}{RSv\epsilon_0}} \sqrt{2\pi}(d+x_{\max}\epsilon) \operatorname{Erfi} \left[\frac{d+x_{\max}\epsilon}{\sqrt{2}\sqrt{R}\sqrt{S}\sqrt{v}\epsilon\sqrt{\epsilon_0}} \right] \right) \dots \dots \dots (16)
 \end{aligned}$$

III. Results and analysis.

The transferred charge $Q(t)$ is the charge flow quantity through an external circuit that includes a resistor R connected to the contact-mode TENG, as shown in Fig.1. In this calculation, $x(t)$ is a time-varying tunneling distance whose magnitude is very small; hence, we used approximation to derive Eq(9), although $x(t)$ shown in Fig.1 is a bit exaggerated. Eq(9) can be simplified as

$$Q(t) = N_s(E)(E_0 - W) f(R, v, \epsilon, \epsilon_0, S, d; t) \dots \dots \dots (9-3)$$

According to Eq(9-3), the time-dependent transferred charge $Q(t)$ is absolutely proportional to both $N_s(E)$ and $E_0 - W$ with the top electrode moving with v within a tunneling distance. Other parameters such as dielectric constant ϵ and structural parameters (S, d) are intertwined with time.

In order to analyze the asymptotic behavior of Eq(9), five parameters— $R, \epsilon, d, S,$ and v —were investigated. Firstly, when R approaches infinity or an appropriately larger value, $Q(t)$ reaches following

$$Q(t) = -\frac{eN_s(E)t^2v(E_0-W)}{2R\epsilon_0} \dots \dots \dots (17)$$

$Q(t)$ is linearly proportional to $N_s(E), E_0 - W,$ and $v,$ but is directly proportional to the square of t and inversely proportional to $R.$ This means that a larger R can also suppress the asymptotic quantity of $Q(t),$ making an open-circuit condition. When R reaches zero, the imaginary part of $Q(t)$ was obtained, indicating that it is not a physically acceptable quantity.

Secondly, when ϵ is large, it means that one of the triboelectric layers is a high- κ material, $Q(t)$ can then be approaching the following relation asymptotically:

$$Q(t) = e \left(-1 + e^{-\frac{t^2v}{2RS\epsilon_0}} \right) N_s(E)S(E_0 - W) \dots \dots \dots (18)$$

Eq(18) also approaches asymptotically the following relation if $v \rightarrow$ infinity or R or $S \rightarrow$ zero:

$$Q(t) = -N_s(E)S(E_0 - W)e \dots \dots \dots (19)$$

In other words, high velocity of the top electrode, longer duration, very small resistance, or small surface area allows $Q(t)$ to be Eq(19). With ϵ approaching zero, the imaginary part of $Q(t)$ was obtained, which was non-physical. Thirdly, when d reaches a very large value (thick dielectric layer), the imaginary part of $Q(t)$ was obtained, indicating a non-physical quantity. However, when d approaches zero (thin dielectric layer), the asymptotic behavior of $Q(t)$ was the same as that of a high- κ material case ($\epsilon \rightarrow \infty$), as shown in Eq(18). This implies that thin and high- κ dielectric materials can have the proper asymptotic behavior of a function of $Q(t)$ in this case.

Fourthly, if the surface area of S is very large (i.e., scalable), then $Q(t)$ reaches

$$Q(t) = -\frac{eN_s(E)t^2v(E_0-W)}{2R\epsilon_0} \dots \dots \dots (20)$$

This asymptotic behavior is the same as that for very large resistance ($R \rightarrow \infty$), as shown in Eq(17). However, there was no physics with S approaching zero.

Lastly, if the velocity of the top electrode is very high, then $Q(t)$ is

$$Q(t) = -e e^{\frac{(d+tv\epsilon)^2}{2RSv\epsilon^2\epsilon_0}} \left(-1 + e^{\frac{(d+tv\epsilon)^2}{2RSv\epsilon^2\epsilon_0}} \right) N_s(E)S(E_0 - W) \dots \dots \dots (21)$$

When v approaches zero (very low speed), then $Q(t)$ is

$$Q(t) = \frac{eN_s(E)Sv(E_0-W)\epsilon(-dt + (1 - e^{-\frac{dt}{RS\epsilon_0\epsilon}})RS\epsilon_0\epsilon)}{d^2} \dots\dots\dots (22)$$

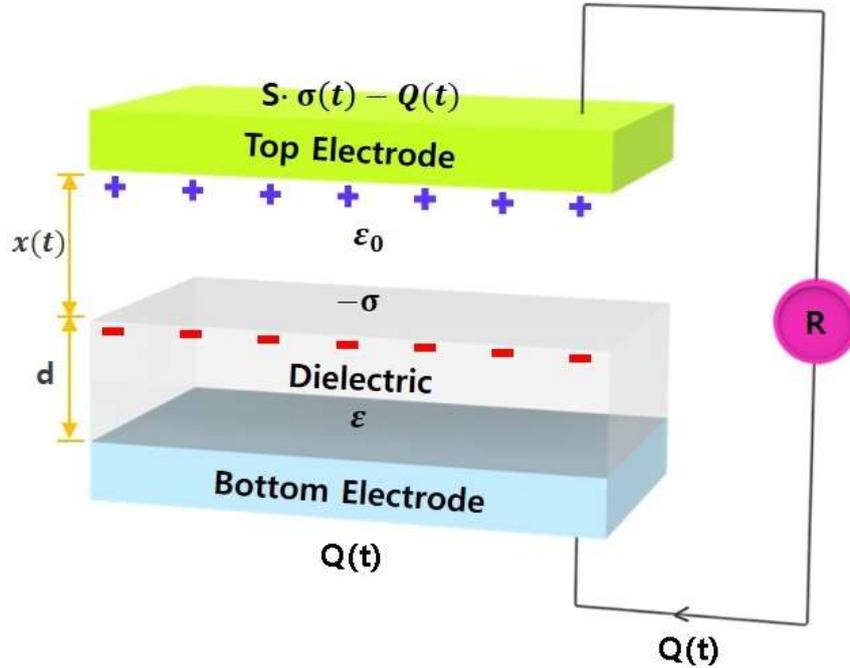


Figure 1: Illustration of triboelectrification with tunneling distance $x(t)$, tribocharge density σ , induced charges on the top electrode $S\sigma(t)-Q(t)$, and transferred charges on the bottom electrode $Q(t)$

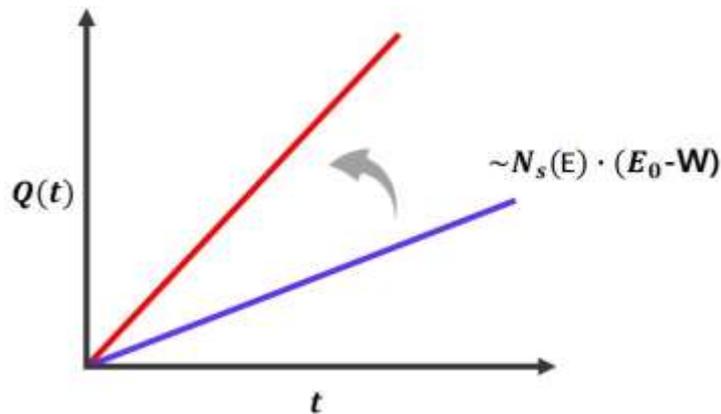


Figure 2: A schematic plot of $Q(t)$ vs. time. $Q(t)$ is directly proportional to both $N_s(E)$ and $E_0 - W$

Table 1: Parameter limit table

		R	ϵ	d	s	v
limit	Large ($\rightarrow +\infty$)	O	O	X	O	O
	Small ($\rightarrow +0$)	X	X	O	X	O

O : Physically acceptable

X : unacceptable

IV. Conclusion

We have investigated important parameters related to the time-dependent transferred charge $Q(t)$, namely R , ϵ , $N_s(E)$, $E_0 - W$, d , S , and v . In particular R , ϵ , d , S , and v were selected to analyze the asymptotic behavior of $Q(t)$. The results show that $Q(t)$ was proportional to both $N_s(E)$ and $E_0 - W$, as shown in Fig.2. In many cases, in order to increase $Q(t)$, the surface density states of dielectric material and the effective work function difference between the metal electrode and dielectric, should increase. When calculating the asymptotic behavior of a function $Q(t)$ with various parameters, the imaginary part of $Q(t)$ obtained was disregarded owing to the fact that it was physically unacceptable, as shown in Table 1.

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