AIP ADVANCES **7**, 065307 (2017)

Exact analytical theory for inverse tunneling of free vacuum electrons into a solid

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(Received 28 April 2017; accepted 2 June 2017; published online 13 June 2017)

This paper presents an exact analytical theory for the inverse tunneling of free vacuum electrons through a triangular potential barrier into a metal. It is found that the inverse tunneling probability is the same as that of the field emission of electrons from metal into vacuum, for the same incident electron energy, metal properties (work function, Fermi energy), and applied electric field strength. For incident electrons with velocities not normal to the vacuum-metal interface, the three-dimensional (3D) oblique tunneling is equivalent to the one-dimensional (1D) normal tunneling, by considering only the longitudinal energy of the electrons normal to the vacuum-metal interface. [http://dx.doi.org/10.1063/1.4986220]

I. INTRODUCTION

The field emission heat engine (FEHE) is a novel thermionic converter to directly convert heat into electricity with high efficiency. It operates with strong electric fields applied on the anode and/or cathode to set up quantum tunneling barriers, so that electrons (in a hot cathode) with energies lower than the surface vacuum level can escape the cathode, transit the vacuum gap, and "inverse tunnel" into the cooler anode.[1,2] This process produces a voltage and provides useful power output when the converter is connected through an external circuit or load.

The power density and efficiency of a thermionic converter is typically limited by the work function of the anode.[3] In FEHE, an electric field is applied near the anode to suppress the thickness of the potential barrier, so that vacuum electrons with total energy less than the anode surface vacuum level can still enter the anode via quantum tunneling. This process is similar to field emission in reverse, so is called "inverse tunneling".[2] The difference is that in field emission, low-energy electrons circumvent the work function surface potential barrier, travelling from the solid into vacuum. In contrast, in the anode side of the FEHE, low-energy electrons circumvent the work function surface potential barrier by travelling from into vacuum into the solid.

An analogous physical effect to inverse tunneling is used in vacuum electronics to generate ions via field desorption (also called field ionization) where an electric field is used to induce electron tunneling into a metal. Field desorption is commercially used to ionize analytes in mass spectroscopy.[4] However, in field desorption, the electron which tunnels into the solid is originally bound to an atom or molecule in vacuum. In contrast, in the FEHE, the tunneling electrons start as free electrons in the vacuum.

Figure 1 shows the two types of electron tunneling: field emission with electrons tunneling from metal to vacuum (Fig. 1a) and inverse tunneling of free vacuum electrons into a metal (Fig. 1b). For one-dimensional (1D) field emission, the incident electrons impinge normally onto the front of the potential barrier (i.e. the metal-vacuum interface); whereas in inverse tunneling, the electrons impinge obliquely on the front of the potential barrier, when their velocity is assumed to be perpendicular

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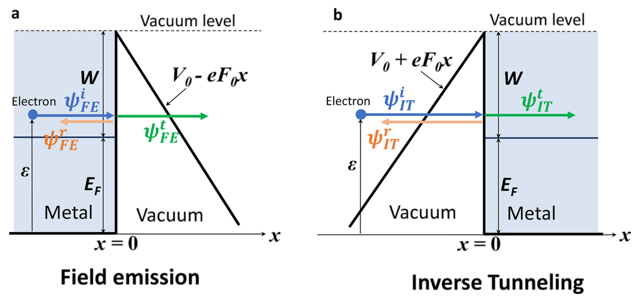

FIG. 1. (a) Field emission, and (b) Inverse tunneling. The metal-vacuum interface is located at $x = 0$. The metal has Fermi level E_F and work function W, with $V_0 = E_F + W$. The external DC electric field is F_0. The initial electron energy is at ε. The incident electron wave is ψ^i, the transmitted and reflected electron waves are ψ^t and ψ^r respectively.

to the vacuum-metal interface. Despite recent experimental demonstration of inverse tunneling,[2,5] there is still a lack of theoretical model to accurately describe inverse tunneling.

This paper provides an *exact* 1D theory for inverse tunneling of vacuum electrons into a metal, and its straightforward extension to the more general three-dimensional (3D) model, where the electron travels at arbitrary direction with an oblique angle to both the front and the back of the potential barrier (Fig. 4).

II. ONE-DIMENSIONAL (1D) MODEL

A. Field emission

The textbook model for field emission of electron tunneling through a triangular barrier[6–10] is shown in Fig. 1a. All electric fields are assumed to be perpendicular to the metal surface. The incident electron has an energy of ϵ, whose velocity is perpendicular to the metal surface. The electrons in the metal would see a potential barrier across the metal-vacuum interface,

$$\Phi_{FE}(x) = \begin{cases} 0, & x < 0; \\ V_0 - eF_0 x, & x \geq 0, \end{cases} \tag{1}$$

where $V_0 = E_F + W$, with E_F and W being the Fermi energy and the work function of the metal respectively, F_0 is the applied electric field, and e is the electron charge. To calculate the emission probability, we solve the 1D time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + [\Phi(x) - \epsilon]\,\psi(x) = 0, \tag{2}$$

where $\psi(x)$ is the complex electron wave function, m is the electron mass, and the potential $\Phi(x) = \Phi_{FE}(x)$ is given in Eq. (1). For $x < 0$, the solution to Eq. (2) may be written as,

$$\psi_{FE}(x) = \psi^i_{FE}(x) + \psi^r_{FE}(x) = e^{ik_0 x} + R_{FE}e^{-ik_0 x}, \qquad x < 0 \tag{3}$$

which is the superposition of an unit amplitude incident plane wave and a reflected wave with reflection amplitude R_{FE}, where $k_0 = \sqrt{2m\epsilon/\hbar^2}$. For $x \geq 0$, as done by Fowler and Nordheim,[6] Eq. (2) can be reduced to,

$$d^2\psi/d\eta_{FE}^2 + \eta_{FE}\psi = 0, \qquad x \geq 0 \tag{4a}$$

with

$$\eta_{FE} \equiv \left(\frac{2emF_0}{\hbar^2}\right)^{1/3}\left(x + \frac{\epsilon - V_0}{eF_0}\right), \tag{4b}$$

whose solution are Airy functions. The transmitted wave function for $x \geq 0$ is,

$$\psi^t_{FE}(x) = T_{FE}[Ai(-\eta_{FE}) - iBi(-\eta_{FE})], \tag{5}$$

where T_{FE} is the transmission amplitude, and Ai and Bi are the Airy function of the first kind and second kind, respectively. Note that in writing the solution in Eq. (5) [as well as in Eq. (3), we assume

$\psi(x) \sim e^{-i\frac{\epsilon}{\hbar}t}$ dependence, where t is time, so that Eq. (5) represents an outgoing wave traveling to the right.[7,11]

The solutions in Eqs. (3) and (5) are matched at the metal-vacuum interface from the conditions that both ψ and $d\psi/dx$ are continuous at $x = 0$. It is easy to show that the transmission amplitude T_{FE} is

$$T_{FE} = \frac{2}{\left[Ai(-\eta_{FE0}) + \frac{k_e}{k_0}Bi'(-\eta_{FE0})\right] + i\left[\frac{k_e}{k_0}Ai'(-\eta_{FE0}) - Bi(-\eta_{FE0})\right]}, \tag{6}$$

where $\eta_{FE0} \equiv k_e[(\epsilon - V_0)/eF_0]$, $k_e \equiv (2emF_0/\hbar^2)^{1/3}$, and a prime denotes the derivative with respect to the argument. The barrier transmission function is defined as $D_{FE}(\epsilon) \equiv J_t(\epsilon)/J_i(\epsilon)$, which is the ratio of the transmitted current density over the incident current density, calculated by using the probability current density $J = (i\hbar/2m)(\psi\nabla\psi^* - \psi^*\nabla\psi)$. The barrier transmission function is found to be[7]

$$\begin{aligned} D_{FE}(\epsilon) &= \frac{1}{\pi}\frac{k_e}{k_0}|T_{FE}|^2 \\ &= \frac{4}{\pi}\frac{k_e}{k_0}\frac{1}{\left[Ai(-\eta_{FE0}) + \frac{k_e}{k_0}Bi'(-\eta_{FE0})\right]^2 + \left[\frac{k_e}{k_0}Ai'(-\eta_{FE0}) - Bi(-\eta_{FE0})\right]^2}, \ \textbf{exact solution} \end{aligned} \tag{7}$$

where we have used Eq. (6) and the Wronskian property $Ai(x)Bi'(x) - Bi(x)Ai'(x) = 1/\pi$. Equation (7) is the *exact* transmission function for tunneling of electrons normally incident on the metal-vacuum interface through a triangular barrier (i.e. field emission), as shown in Fig. 1a. In the limit of small electric field, we have $-\eta_{FE0} \gg 1$, and $Ai(-\eta_{FE0}), Ai'(-\eta_{FE0}) \ll Bi(-\eta_{FE0}), Bi'(-\eta_{FE0})$, thus, Eq. (7) is reduced to

$$D_{FE}(\epsilon) \cong 4\frac{\sqrt{\epsilon(E_F + W - \epsilon)}}{E_F + W}\exp\left[-\frac{4}{3}\frac{\sqrt{2m}}{\hbar}\frac{(E_F + W - \epsilon)^{3/2}}{eF_0}\right], \tag{8}$$

where we have used the asymptotic expressions of $Bi(-\eta_{FE0}) \simeq \pi^{-1/2}|\eta_{FE0}|^{-1/4}\exp\left[\frac{2}{3}(-\eta_{FE0})^{3/2}\right]$, and $Bi'(-\eta_{FE0}) \simeq \pi^{-1/2}|\eta_{FE0}|^{+1/4}\exp\left[\frac{2}{3}(-\eta_{FE0})^{3/2}\right]$ in the limit of $-\eta_{FE0} \to \infty$. Equation (8) is the familiar transmission function for the Fowler-Nordheim field emission.[6,7]

B. Inverse tunneling

As shown in Fig. 1b, consider free vacuum electrons of energy ϵ propagating towards the vacuum-metal interface, where a reverse triangular potential barrier is present due to the different bias of the grid on the left (not shown) and the solid. The velocity of the incident electron is assumed to be perpendicular to the vacuum-metal surface. The vacuum free electrons would see a potential barrier near the vacuum-metal interface,

$$\Phi_{IT}(x) = \begin{cases} V_0 + eF_0x, & x < 0; \\ 0, & x \geq 0, \end{cases} \tag{9}$$

where $V_0 = E_F + W$, with E_F and W being the Fermi energy and the work function of the metal respectively. The electrons would initially propagate above the potential barrier ($\epsilon > \Phi_{IT}(x)$), and then tunnel through a surface barrier ($\epsilon < \Phi_{IT}(x)$) before entering the metal. This is quite different from the traditional field emission (Fig. 1a), as the electron impinges on a tilted surface barrier. That is, the velocity of the electron is not normal to the front of the potential barrier (even though it is normal to the vacuum-metal interface). However, the electron tunneling problem can still be easily solved by using Airy functions.

Similar to the field emission, we solve the 1D time-independent Schrödinger equation, Eq. (2), to obtain the transmission probability, where the potential $\Phi(x) = \Phi_{IT}(x)$ is now given by Eq. (9). For $x < 0$, Eq. (2) with Eq. (9) can be reduced to,

$$d^2\psi/d\eta_{IT}^2 - \eta_{IT}\psi = 0, \qquad x < 0 \tag{10a}$$

with

$$\eta_{IT} \equiv \left(\frac{2emF_0}{\hbar^2}\right)^{1/3}\left(x - \frac{\epsilon - V_0}{eF_0}\right), \tag{10b}$$

whose solution are precisely Airy functions. In the vacuum region $x < 0$, the solution to Eq. (10) may be written as,

$$\psi_{IT}(x) = \psi^i_{IT}(x) + \psi^r_{IT}(x), \quad x < 0 \tag{11a}$$

$$\psi^i_{IT}(x) = Ai(\eta_{IT}) + iBi(\eta_{IT}), \tag{11b}$$

$$\psi^r_{IT}(x) = R_{IT}[Ai(\eta_{IT}) - iBi(\eta_{IT})], \tag{11c}$$

which is the superposition of the incident wave ψ^i_{IT} and a reflected wave ψ^r_{IT} with the reflection amplitude R_{IT}. The solutions in Eq. (11) are constructed by assuming $\psi(x) \sim e^{-i\frac{\epsilon}{\hbar}t}$ dependence, so that Eq. (11b) represents an incident wave traveling to the right, and Eq. (11c) a reflected wave traveling to the left. For $x \geq 0$, the transmitted wave is

$$\psi^t_{IT}(x) = T_{IT}e^{ik_0 x}, \tag{12}$$

where T_{IT} is the transmission amplitude, $k_0 = \sqrt{2m\epsilon/\hbar^2}$, and ψ^t_{IT} is traveling to the right with $e^{-i\frac{\epsilon}{\hbar}t}$ dependence.

The solutions in Eqs. (11) and (12) are matched at the vacuum-metal interface from the conditions that both ψ and $d\psi/dx$ are continuous at $x = 0$. It is easy to show that the transmission amplitude T_{IT} is

$$T_{IT} = \frac{2}{\pi}\frac{1}{\left[\frac{k_0}{k_e}Ai(\eta_{IT0}) + Bi'(\eta_{IT0})\right] + i\left[Ai'(\eta_{IT0}) - \frac{k_0}{k_e}Bi(\eta_{IT0})\right]}, \tag{13}$$

where $\eta_{IT0} \equiv k_e[(V_0 - \epsilon)/eF_0]$, and $k_e \equiv (2emF_0/\hbar^2)^{1/3}$, and a prime denotes the derivative with respect to the argument. The barrier transmission function for the inverse tunneling is defined as $D_{IT}(\epsilon) \equiv J_t(\epsilon)/J_i(\epsilon)$, which is the ratio of the transmitted current density over the incident current density, calculated by using the probability current density $J = (i\hbar/2m)(\psi\nabla\psi^* - \psi^*\nabla\psi)$. The barrier transmission function is found to be

$$D_{IT}(\epsilon) = \pi\frac{k_0}{k_e}|T_{IT}|^2 = \frac{4}{\pi}\frac{k_e}{k_0}\frac{1}{\left[Ai(\eta_{IT0}) + \frac{k_e}{k_0}Bi'(\eta_{IT0})\right]^2 + \left[\frac{k_e}{k_0}Ai'(\eta_{IT0}) - Bi(\eta_{IT0})\right]^2}, \quad \textbf{exact solution} \tag{14}$$

where we have used Eq. (13) and the Wronskian property $Ai(x)Bi'(x) - Bi(x)Ai'(x) = 1/\pi$. Equation (14) is the *exact* transmission function for the inverse tunneling of free vacuum electrons normally propagating towards the vacuum-metal interface through a reverse triangular barrier, as shown in Fig. 1b.

Since $\eta_{IT0} = -\eta_{FE0}$, it is interesting to note that the expression for $D_{IT}(\epsilon)$ in Eq. (14) is *identical* to that for $D_{FE}(\epsilon)$ in Eq. (7), even though the electron wave functions are very different (Eqs. (4) and (5) vs. Eqs. (11) and (12), also c.f. Fig. 2). This result may be expected from the WKBJ approximation[12–14] for electron tunneling through a potential barrier, where the transmission probability is a function of the "area under the barrier" only, and the local "shape" of the barrier is not important, with $D_{WKBJ}(\epsilon) = \exp\left[\left(-\frac{2\sqrt{2m}}{\hbar}\right)\int_{x_1}^{x_2}\sqrt{\Phi(x) - \epsilon}\,dx\right]$, where x_1 and x_2 are the two roots of $\Phi(x) - \epsilon = 0$. Note that it is well known in the theory of ballistic transport through nanoscale devices, the tunneling coefficient going from left to right and right to left are equal to each other.[12–14] It is demonstrated here for the first time for the case of direct and inverse tunneling of free vacuum electrons into a metal.

In terms of nondimensional quantities, $\bar{\epsilon} = \epsilon/W$, $\overline{E_F} = E_F/W$, length scale $\lambda_0 = \sqrt{\hbar^2/2mW}$, $\bar{x} = x/\lambda_0$, $\overline{F_0} = F_0 e\lambda_0/W$, the transmission function for both field emission, Eq. (7), and inverse tunneling, Eq. (14), becomes,

$$D_{IT}(\bar{\epsilon}) = D_{FE}(\bar{\epsilon}) = \frac{4}{\pi}\frac{\overline{F_0}^{1/3}\sqrt{\bar{\epsilon}}}{\left[\sqrt{\bar{\epsilon}}Ai(\beta) + \overline{F_0}^{1/3}Bi'(\beta)\right]^2 + \left[\overline{F_0}^{1/3}Ai'(\beta) - \sqrt{\bar{\epsilon}}Bi(\beta)\right]^2}, \quad \textbf{exact solution} \tag{15}$$

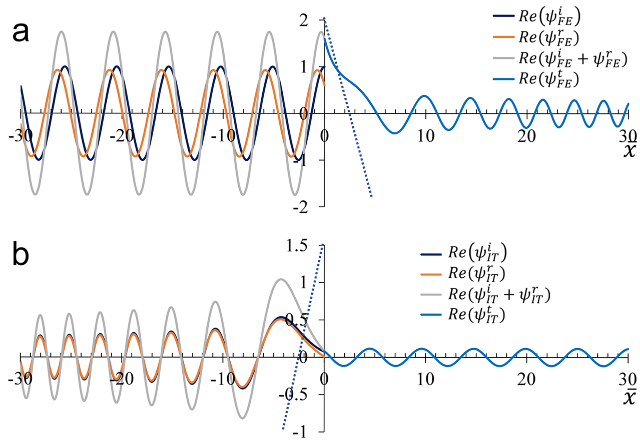

FIG. 2. Electron wave function for (a) Field emission, from Eqs. (4) and (5), and (b) Inverse tunneling, calculated from Eqs. (11) and (12). In the calculation, we assume $\overline{E_F}=1$, $\bar{\epsilon}=\overline{E_F}+0.5$, and $\overline{F_0}=0.2$. The incident electron wave is ψ^i, the transmitted and reflected electron waves are ψ^t and ψ^r respectively. The dashed lines indicates the location of the potential barrier.

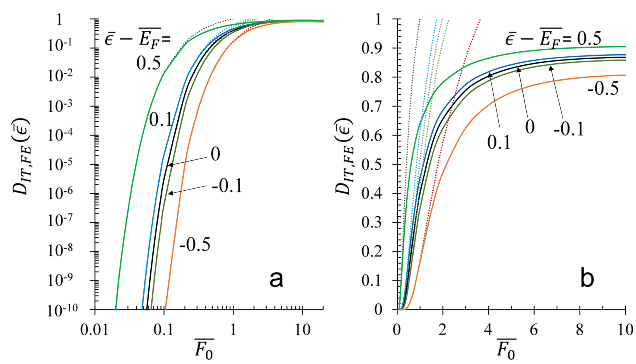

FIG. 3. The transmission function for both inverse tunneling and field emission, $D_{IT}(\bar{\epsilon})=D_{FE}(\bar{\epsilon})$ calculated from Eq. (15) (solid lines), as a function of the electric field $\overline{F_0}$, for different incident electron energy $\bar{\epsilon}-\overline{E_F}$, in (a) log scale, and (b) linear scale. The dashed lines are from the approximate solution, Eq. (16). In the calculation, we assume the solid is copper (work function $W=4.7$eV, Fermi level $E_F=7.0$eV).

where $\beta=\left(1+\overline{E_F}-\bar{\epsilon}\right)/\overline{F_0}^{2/3}$. In the limit of small electric field, $\beta\to\infty$, Eq. (15) reduces to,

$$D_{IT}(\bar{\epsilon}) = D_{FE}(\bar{\epsilon}) \cong 4\frac{\sqrt{\bar{\epsilon}\left(1+\overline{E_F}-\bar{\epsilon}\right)}}{1+\overline{E_F}}\exp\left[-\frac{4}{3}\frac{\left(1+\overline{E_F}-\bar{\epsilon}\right)^{\frac{3}{2}}}{\overline{F_0}}\right], \tag{16}$$

which is also the normalized form of Eq. (8).

Examples of the electron wave functions for the field emission and the inverse tunneling are shown in Fig. 2. It is clear that both the wave function ψ and its first derivative $d\psi/dx$ are continuous across the metal-vacuum interface $x=0$. The transmission function, Eq. (15), and the approximate solution, Eq. (16), are shown in Fig. 3, as a function of electric field, for the special case of copper ($W=4.7$eV, $E_F=7.0$eV), for various incident electron energy relative to the Fermi level, $\bar{\epsilon}-\overline{E_F}$. The transmission probability increases significantly as the incident electron energy increases.

III. THREE-DIMENSIONAL (3D) MODEL

For the more general case when the electron velocity is not normal to the vacuum-metal interface, it is necessary to generalize the above 1D theory into 3D. Consider the inverse tunneling barrier near

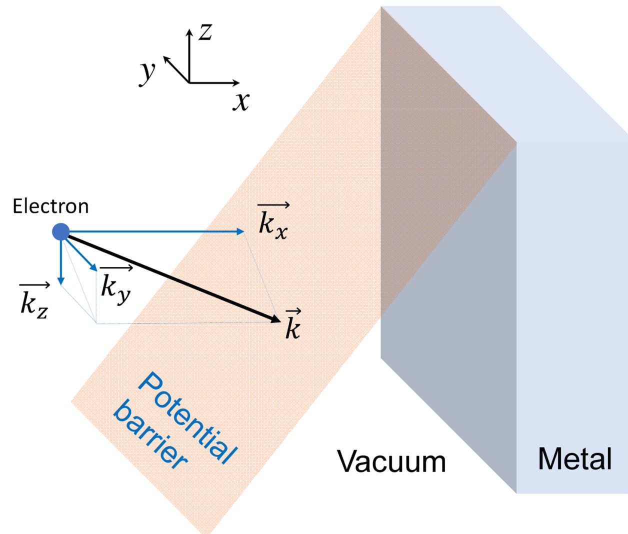

FIG. 4. Inverse tunneling with incident electron velocity not normal to the vacuum-metal interface. The total wave vector may be decomposed as $\vec{k} = \overrightarrow{k_x} + \overrightarrow{k_y} + \overrightarrow{k_z}$, where $\overrightarrow{k_x}$, $\overrightarrow{k_y}$, and $\overrightarrow{k_z}$ are the wave vector along the three axes.

the vacuum-metal interface, where the incident electron velocity has an arbitrary direction, as shown in Fig. 4.

The 3D Schrodinger equation reads,

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + [\Phi(\vec{r}) - \epsilon]\psi(\vec{r}) = 0, \tag{17}$$

where the electron has a total energy of ϵ and the potential profile $\Phi(\vec{r}) = \Phi(x)$ is assumed to have only x-dependence (Fig. 4). Thus, the electron wave function may assume the general form $\psi(\vec{r}) = \psi(x)\, e^{ik_y y} e^{ik_z z}$, which is inserted into Eq. (17) to obtain,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + [\Phi(x) - \epsilon_x]\,\psi(x) = 0, \tag{18}$$

where $\epsilon_x = \epsilon - \frac{\hbar^2}{2m}k_y^2 - \frac{\hbar^2}{2m}k_z^2$ is the longitudinal energy with velocity perpendicular to the vacuum-metal interface. Equation (18) is in the same form as Eq. (2) for the 1D case. Therefore, the 3D oblique tunneling is equivalent to the 1D normal tunneling, with electron of reduced effective energy of $\epsilon - \frac{\hbar^2}{2m}k_y^2 - \frac{\hbar^2}{2m}k_z^2$. This is true for arbitrary x-dependent potential landscape $\Phi(x)$, including both field emission and inverse tunneling. Note this is equivalent to the statement that the effective height of the barrier has increased by the amount $\frac{\hbar^2}{2m}k_y^2 + \frac{\hbar^2}{2m}k_z^2$, therefore the probability of penetration of the electron is smaller than when both k_y and k_z are zero.[15] It is also important to note also that this is a different effect from the "refraction" of electrons during emission, which comes purely from conservation of energy and momentum.[16]

IV. CONCLUSION

In summary, we have developed an exact analytical theory for the inverse tunneling of free vacuum electrons through a potential barrier into a solid. It is found that the inverse tunneling probability is the same as that of the field emission of electrons from metal into vacuum, for the same incident electron energy, metal properties (work function, Fermi energy), and applied electric field strength. This is consistent with the WKBJ approximation that only the "area under the curve", not the particular shape of the potential barrier determines the tunneling probability, and consistent with the principle of microscopic reversibility. As well known in ballistic transport through nanoscale semiconductor devices, it is demonstrated here for the first time for the case of direct and inverse tunneling of free vacuum electrons into a metal. The electron wave functions are compared for field emission and inverse tunneling. For incident electrons with velocities not normal to the vacuum-metal interface, the 3D oblique tunneling is equivalent to the 1D normal tunneling, with a reduced effective energy being the longitudinal electron energy normal to the vacuum-metal interface. This study may provide guideline for the design of field emission heat engines[2,17,18] and other novel devices[19–21] involving inverse tunneling of free vacuum electrons into a solid. Next steps to further improve the model can include adding the image force in the potential, a.k.a. the Schottky-Nordheim barrier,[22,23] which will increase the transmission probability. Another step is to take into account electron occupancy and density-of-states in the solid, which can decrease transmission probability, since there needs to be available states in the solid for incoming electrons to occupy in order for electron absorption to take place via inverse tunneling. The variation in effective mass has to be considered for inverse tunneling into a semiconductor.

ACKNOWLEDGMENTS

P. Zhang was supported by AFOSR Grant No. FA9550-14-0309 through a subcontract from the University of Michigan.

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