Space-charge-limited bipolar flow in a nano-gap

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This paper presents a quantum model of space-charge limited (SCL) bipolar flow in a nano-sized planar gap, including the effects of electron tunneling and exchange-correlation. It is found that the classical scaling of the SCL bipolar flow is no longer valid when the gap spacing D is comparable or smaller than the electron's de Broglie wavelength at gap voltage V_g. The classical value of the SCL bipolar electron flow is greatly enhanced due to the electron tunneling through the space-charge electric potential created by both the electrons and ions. The space-charge effect of ions is less significant (compared to electron tunneling) in the deep quantum regime that the quantum SCL bipolar flow is nearly identical to the unipolar electron flow (or quantum Child-Langmuir law).
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Field emission explosive cathodes have been increasingly popular over the traditional thermionic cathodes for high current and high power applications due to better efficiencies and lower power consumption. However, outgassing, which typically occurs in these high current cathodes, has become a major issue to determine its emission characteristics. Recently, the characteristics of bipolar flow in field emission explosive diodes have also been extensively investigated under the space-charge-limited (SCL) condition.[1–6]

The classical bipolar flow characteristic was first calculated by Langmuir,[7] who found that the SCL bipolar electron flow across a gap would be enhanced by a factor of 1.86 from the well-known one-dimensional (1D) classical Child-Langmuir (CL) law:[8,9]

$$J_{\mathrm{CL}} = \frac{4\epsilon_o}{9}\sqrt{\frac{2e}{m_e}}\frac{V_g^{3/2}}{D^2}, \tag{1}$$

where D is the gap spacing, V_g is the gap voltage, e and m_e are the charge and mass of the electron, respectively, and ϵ_o is the free space permittivity. The amount of ion current density (in terms of electron current density) is $\sqrt{Zm_e/m_i}$, independent of V_g and D, where m_i and Z are the rest mass and positive charge of the ion, respectively.

With the rapid progress in nanoscale fabrication, nanosize gaps[10,11] have been fabricated and utilized in nanodiodes and nano-triodes, which are operated at low voltage $V_g < 40$ V with gap spacing on the order of $D < 100$ nm. Using nano-scale emitters, local current density higher than 10^8 A/cm^2 may be contained with voltages below 20 V at room temperature.[11] Compared to the classical[7] and relativistic models,[12–14] there are no studies of SCL bipolar flow in the regime of low voltage and small spacing, where quantum effects may become important. Recently, the 1D classical CL law has been extended to quantum regime, where quantum effects such as the electron tunneling and many electron exchange-correlation effects are included.[15–17] In the 1D quantum model of unipolar flow, mean field theory was used to calculate the SCL electron current density across a nano-gap for a given D and V_g. New quantum scalings of $V_g^{1/2}$ and D^{-4} have also been calculated[16] and derived.[17] In this letter, we seek to include the effects of ions by developing a quantum model of the SCL bipolar flow in a nano-gap.

Let us consider a 1D planar diode of gap spacing D with a grounded cathode and an anode potential of V_g. Electrons and ions with zero emission energy are injected normally into the gap from the cathode and anode, respectively. Using mean field theory, the 1D time-independent Schrödinger equation, the Poisson equation and charge conservation relation are solved to obtain the maximum electron current density J that can be transported across the gap under the bipolar SCL flow condition. For simplicity, we introduce several normalized parameters:[16] $\bar{x}=x/D$, $\phi=V/V_g$, $\lambda=D/\lambda_o$ is the normalized gap spacing, $\phi_g=eV_g/E_H$ is the normalized gap voltage, $q^2=n/n_o$ is the normalized electron density, q is the normalized wave amplitude, and $\gamma=J/J_{\mathrm{CL}}$ is the normalized electron current density. The normalized scales: $\lambda_o=\sqrt{\hbar^2/2em_eV_g}$ is the electron De Broglie wavelength at V_g, $n_o=2\epsilon_oV_g/3eD^2$ is the density scale, $E_H=e^2/4\pi\epsilon_oa_o=27.2$ eV is the Hartree energy, and $a_o=4\pi\epsilon_o\hbar^2/me^2=0.0529$ nm is the Bohr radius.

In terms of the normalized parameters, the 1D time-independent Schrödinger equation, the Poisson equation and charge conservation relation can be formulated as

$$q'' + \lambda^2\left[\phi - \phi_{xc} - \frac{4}{9}\frac{\gamma^2}{q^4}\right]q = 0, \tag{2}$$

$$\phi'' = \frac{2}{3}q^2 - \frac{1}{4}\frac{\alpha}{\sqrt{1-\phi}}, \tag{3}$$

$$\alpha = s_c^2 + \frac{4}{3}\int_0^1 q^2\phi' d\bar{x}, \tag{4}$$

where the prime denotes the derivative with respect to $\bar{x}$. Here, $\phi_{xc}(<0) \equiv \phi_x + \phi_c = V_{xc}[r_s]/\phi_g$, and $V_{xc}[r_s]$ is the many electron exchange-correlation term based on local density theory [see Eqs. (2) and (3) in Ref. 16]. The parameter $\alpha = 16/9\sqrt{(m_i/Zm_e)}(J_i/J_{\mathrm{CL}})$ is the normalized ion current density J_i. Note in the derivation of Eqs. (2)–(4), we have ig-

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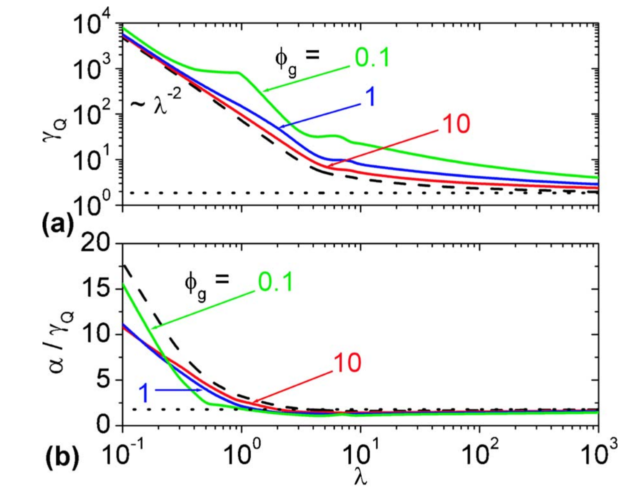

FIG. 1. (Color online) (a) The normalized bipolar SCL electron current density $\gamma_Q = J/J_{CL}$, and (b) the normalized ion current density (in terms of electron current density) α/γ_Q as a function of λ for ϕ_g=0.1, 1, and 10 (solid lines) and $\phi_g \gg 1$ (dashed line). The dotted line is the classical value of (a) γ_Q=1.86 and (b) α/γ_Q=16/9.

nored completely the quantum effects of ions by assuming that the De Broglie wavelength of ion is much smaller than the gap spacing.

The boundary conditions for Eqs. (2)–(4) are $q(1) = \sqrt{2\gamma/3}$, $q'(1)=0$, $\phi(0)=0$, $\phi(1)=1$, $\phi'(1)=0$, and $\phi'(0) = s_c$, where s_c is the surface electric field of the cathode that is numerically calculated for a given γ. With the boundary conditions, we determine the bipolar quantum CL law by calculating the maximum normalized electron current density defined as γ_Q, and its equivalent normalized SCL ion current density α. For $\gamma > \gamma_Q$, solutions to Eqs. (2)–(4) no longer exist. At $\phi_g \gg 1$ and $\lambda \gg 1$, the solution will approach the classical limit of $s_c=0$, $\gamma_Q=1.86$, and $\alpha/\gamma_Q=16/9$. For finite λ but at $\phi_g \gg 1$, we have $\phi_{xc} \to 0$, where the exchange-correlation effect becomes negligible. At $\alpha \to 0$, we will recover the quantum Child-Langmuir law.[16]

Figure 1 illustrates the dependence of γ_Q and α/γ_Q as a function of λ for ϕ_g=0.1 to $\phi_g \gg 1$, where the classical values are also plotted for comparison (dotted lines). For a given ϕ_g, both γ_Q and α increases significantly with decreasing values of λ (<10) in the quantum regime. At very small λ (deep quantum regime), the value of γ_Q is approximately proportional to λ^{-2}. Thus, similar to the quantum CL law,[16] the quantum bipolar electron flow will also has a quantum scaling of $V_g^{1/2}$ and D^{-4} as opposed to the classical scaling of $V_g^{3/2}$ and D^{-2}. The amount of the SCL ion current density (in terms of electron current density) is no longer a constant, which is $\alpha/\gamma_Q=16/9$ predicted by the classical theory.

In Fig. 2(a), we see that the bipolar flow (solid line) always has a potential barrier with a smaller height and a narrower width for the electrons to tunnel through at zero energy level (ϕ=0), as compared to the unipolar flow (dashed lines). At λ=10, the barrier's height (in terms of V_g) and width (in terms of D) for the bipolar flow are decreased from 0.19 to 0.16, and from 0.45 to 0.4, respectively. Due to charge neutralization, electrons in bipolar flow has higher tunneling probability and higher electron current density, which can also be inferred by the higher and broader values of the electron wave amplitude shown in Fig. 2(b). The enhancement of the electron current density will depend on the

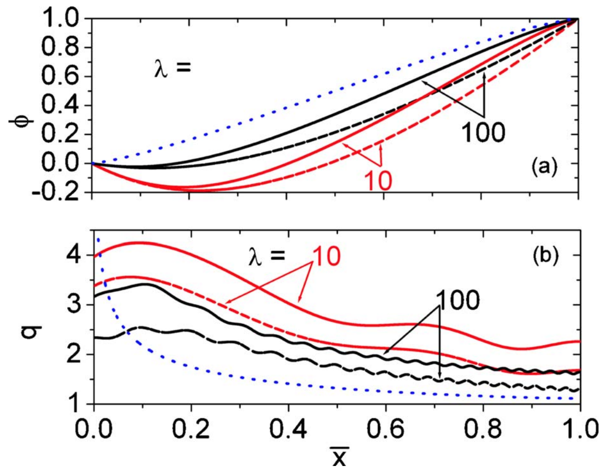

FIG. 2. (Color online) (a) The normalized profile of the electric potential ϕ and (b) wave amplitude q for bipolar (solid lines) and unipolar (dashed lines) flow at ϕ_g=1 for λ=10 (top) and λ=100 (bottom), where the dotted lines represent the classical limits of bipolar flow.

values of D and V_g, which is no longer equal to the classical limit of 1.86 [see Figs. 1(a) and 3(a)]. The classical profiles of the bipolar flow are also plotted (dotted lines) in the figure for comparison.

In order to see the degree of charge neutralization in various λ and ϕ_g, the ratio of SCL electron current density of the bipolar flow to the unipolar flow, $\beta = \gamma_Q/\gamma_Q(\alpha=0)$ is plotted in Fig. 3(a). In the quasi-classical regime (λ=1000), β approaches the classical limit of 1.86 as expected. At small λ<0.1, β decreases to about 1.15 (for ϕ_g=1 and 10) in the deep quantum regime. In the range of 0.1<λ<100, the ratio depends explicitly on the values of λ and ϕ_g, which is due the exchange-correlation effects, especially for small ϕ_g. Thus, we may conclude that the space-charge effects of ions may be negligible at small λ<0.1, where the electron tunneling is more significant and the bipolar flow is nearly identical to the unipolar flow (or quantum CL law)[16] with a small

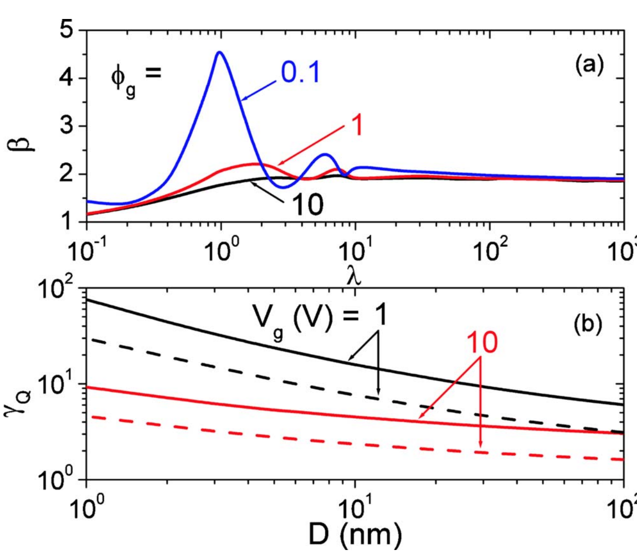

FIG. 3. (Color online) (a) Ratio of the bipolar electron current density to the unipolar electron current density $\beta = \gamma_Q/\gamma_Q(\alpha=0)$ as a function of λ for ϕ_g=0.1, 1, and 10. (b) The normalized bipolar SCL electron current density γ_Q as a function of D=1–100 nm at V_g=1 V (top) and V_g=10 V (bottom) for the bipolar (solid lines) and unipolar flows (dashed lines).

enhancement of 1.15 that is even *smaller* than the classical limit of 1.86.

In Fig. 3(b), γ_Q for the bipolar flow (solid lines) and unipolar flow (dashed lines) are plotted in the range of $D = 1-100$ nm at $V_g=1$ V (top) and 10 V (bottom) to illustrate some practical parameters that can be fabricated with the current nano-fabrication technology. For a given V_g, γ_Q increases with decreasing D (from 100 to 1 nm) and it increases more rapidly for small V_g and D. At $D=100$ nm and $V_g=1$ V, γ_Q for the bipolar and unipolar flow are 6.05 and 3.11, respectively. At $D=1$ nm and $V_g=1$ V, the values are increased to 75.9 and 29.7. Thus, it is expected that the SCL electron current density in a nano-gap will be increased by a factor of about 2 or more (due to charge neutralization) in the range of 1 nm$<D<$100 nm and 1 V$<V_g<$10 V.

In conclusion, we have formulated a new quantum model for the SCL bipolar flow in a planar nano-gap with small gap voltage, which includes the effects of electron tunneling and exchange-correlation. It is found that the classical model[7] is no longer valid in quantum regime, where quantum effects become important. Compared to the quantum CL law,[16] the SCL electron current density for the quantum bipolar flow is higher by a factor of 2 or more in the practical parameters, and it has the same quantum scaling of $V_g^{1/2}$ and D^{-4}. Smooth transition between the classical and the quantum regimes is demonstrated. Note the applicability of the quantum SCL bipolar flow model may be tested with explosive field emission cathode[1–3] in the range of nano-gap[11] with significant outgassing from anode. By controlling the degree of outgassing, it may be possible to study the transition of quantum CL law[16] to the SCL bipolar flow presented here.

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