Dynamics of a Field Emitted Beam From a Microscopic Inhomogeneous Cathode

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Abstract—We investigate by molecular dynamics simulations (Torfason et al., 2015; 2016) a beam of electrons released via field emission from a planar cathode surface of 1 μm² with an inhomogeneous two-level work function, φlow and φhigh. A rectangular grid, where each cell can have one out of two values of the work function, is used as a model. The number of cells in the grid ranges from 6 × 6 to 96 × 96. We compare a periodic checkerboard arrangement with disordered distributions of patches. We perform multiple simulations and randomize the pattern each time. We study the beam behavior by calculating the position and velocity of each electron, r.m.s. emittance, and the brightness of the electron beam. The emittance increases while brightness decreases, with the mean distance between patches with φlow when they are in minority, and they switch the behavior versus the mean distance between patches with φhigh when these patches are in minority, respectively. The Coulomb interaction between all particles is fully included in our simulations.

Index Terms—Diode physics, electron sources, field emission, space–charge, vacuum electronics.

I. INTRODUCTION

FIELD emitted electrons have a wide range of use, such as in microwave tubes, electron microscopes, vacuum channel transistors [3], [4], ultrafast diodes [5]–[7], and space propulsion systems [8]. For many of these applications, it is important to understand and control electron beam dynamics. The dynamics of the beam are strongly affected by the conditions at the point of emission, and hence, the emitting surface influences the properties of the electron beam greatly. The effects of the cathode surface on the beam can be via the shape of the surface [2], [9], roughness or imperfections [10]–[12], temperature [13], or material properties such as the work function [14].

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In practice, a cathode is never completely homogeneous and includes a certain amount of randomness or disorder. It is, therefore, important to evaluate the effects of an imperfect cathode on the quality of the beam. In particular, low emittance and high brightness are often desired in many-electron devices [12], [15], [16]. Jensen et al. [14] used a general emission model, incorporating thermal, field, and photoemission, and a particle-in-cell approach to study the consequences of cathode nonuniformity due to work function variation. One of the findings was that the beam emittance is more sensitive to such imperfections than the current itself. In a recent article, we considered a microscopic vacuum diode with a field emission mechanism and an inhomogeneous cathode comprised of four active patches separated by inactive areas [17]. We found that the mutual space–charge effects set in rapidly when the distance between the emitting patches is considerably shorter than the diode gap.

In the present work, we consider a microscopic planar diode, with a square emitting area on the cathode split into checks with different work functions. We study how the work function distribution affects the current, the emittance, and the brightness. We build upon previous work [1], [2], using our molecular dynamics (MDs) code where the Coulomb interaction between all electrons is fully incorporated. The MD approach takes the discrete emission of electrons into account and allows us to track individual electron trajectories. This allows us to calculate quantities that characterize the beam quality, such as velocity, density, current, emittance, and brightness. The simulations use both designed surfaces and randomly generated ones for the cathode.

Section II gives a description of the methodology and the model used. Results are presented in Section III with a short summary and conclusion in Section IV.

II. METHODOLOGY

Fig. 1 shows the system being modeled, a planar vacuum diode with gap spacing d. The cathode in the system is grounded, and the potential V₀ is applied to the anode, which creates an electric field that is strong enough to cause field emission. The emission is only allowed to take place on
a square area with side lengths $L$ and is described by the Fowler–Nordheim law. The equation for it is

$$J = \frac{A}{t^2(\ell)\phi} F^2 e^{-v(\ell)B\phi^3/F}$$  \hspace{1cm} (1)$$

where $\phi$ is the work-function and $F$ is the field at the surface of the cathode, taken to be positive. $A = e^2/(16\pi^2\hbar) \, [\text{eV} \, \text{V}^{-2}]$ and $B = 4/(3h)(2m_e e)^{1/2}$ \, [eV$^{-3/2}$ V m$^{-1}$] are the first and second Fowler–Nordheim constants, while $v(\ell)$ and $t(\ell)$ are called the Nordheim functions arising due to the image charge [18], and $\ell = eF/(4\pi\epsilon_0\phi^2)$ is the scaled barrier field.

In this work, the emission area on the cathode has a work function that varies with position, $\phi(x, y)$. A rectangular grid is created where each square check can have its own work function. A Metropolis–Hastings (MH) like algorithm is used to determine where electron emission occurs. The exponential

$$D_F = \exp\left(-v(\ell)B\phi^3/F\right)$$  \hspace{1cm} (2)$$
of the Fowler–Nordheim function is the escape probability for incoming electrons at the Fermi level and is used as a probability distribution for the MH algorithm. This makes both the field and the work function affect the placement of electrons on the cathode. The part in front of the exponent

$$J_{\text{supp}} = \frac{A}{t^2(\ell)\phi} F^2$$  \hspace{1cm} (3)$$
is interpreted as the electron supply. It is integrated [19] over the surface of the cathode to obtain the number of electrons coming to the surface. The variation of the field and work function are both taken into account in this integration. Once a suitable location for emission has been found for an electron using the MH algorithm, a uniform random number is generated between 0 and 1. That number is then compared with (2) to determine if emission occurs at that location or not. Electrons are emitted with vanishing initial velocity. Simulations confirm that the effects of scattering dominate the effect of lateral emission velocity on the emittance, and that typical longitudinal emission velocity is also of low importance.

We use the Velocity–Verlet algorithm to update each electron’s position and velocity in every time step of the simulation. The force on each electron in the diode gap is calculated using Coulomb’s law. From these three quantities, the code can calculate various properties of the electron beam. Such as current, emittance, brightness, and density. The current is calculated using the Shockley–Ramo theorem [20], [21]. Where we sum over the contribution from all electrons to the total current. The equation is

$$I = \frac{q}{d} \sum_i v_{z,i}$$  \hspace{1cm} (4)$$

where $q$ is the electron charge, $v_z$ the $z$-component of the instantaneous velocity (with $z$ being normal to the cathode), and $d$ the gap spacing. To describe the spread of the electron beam at the anode, we calculate the transverse emittance of the beam in the $x$- and $y$-directions. To describe the spread of the electron beam at the anode, we calculate the transverse emittance of the beam in the $x$- and $y$-directions. We use the statistical emittance [22], [23], $\epsilon_x = (x^2)(x^2) - (x)(x)^2)^{1/2}$. The $x$-position and the slope of the electron trajectory $x' = dx/dz \approx v_x/d$ are recorded when the electrons pass through the anode. The slope is calculated using the velocity of the electrons. The emittance in the $y$-direction is calculated in the same way. Another quality factor characterizing the beam is brightness [22] which is calculated from the emittance and current using

$$B = \frac{2I}{\pi^2 \epsilon_x \epsilon_y}$$  \hspace{1cm} (5)$$

where $I$ is the current and $\epsilon_x, \epsilon_y$ are the emittance in the $x$- and $y$-directions, respectively.

### III. RESULTS

All the simulations were performed for the gap voltage and gap spacing fixed at $V_0 = 2 \, \text{kV}$ and $d = 1 \, \mu\text{m}$, respectively. The emitter side length is set to $L = 1 \, \mu\text{m}$. We studied systems with two different work function values, which we set to $\phi_{\text{low}} = 2.0 \, \text{eV}$ and $\phi_{\text{high}} = 2.5 \, \text{eV}$, forming either a checkerboard pattern on the cathode’s surface or randomly distributed patches on a square lattice.

### A. Checkerboard Pattern

Fig. 2 shows the emitting area of the cathode with a $6 \times 6$ checkerboard pattern with the corresponding phase space diagram for $x$–$x'$, shown below. As seen in Fig. 2(b) each column forms its own S-shaped pattern in the phase space, i.e., locally every column acts as a single periodic emitter with its own emittance that contributes to the total emittance. The angular range of the S-shaped pattern depends on the column’s position with respect to the center of the cathode. The electrons...
Fig. 3. Electron density through a single row on the checkerboard in Fig. 2. The density for 2.0 eV (blue solid line) and 2.5 eV (orange dashed line) are scaled such that the area under each curve is 1. The boxes at the bottom of the graph represent the checkerboard row. Red boxes show the location of checks with work function 2.5 eV and gray boxes with 2.0 eV.

Fig. 4. Emittance (red solid line), brightness (blue dashed line), and current (green dash dotted line), as a function of \( n \) of the checkerboard size \( n \times n \).

originating from the central columns are symmetric in phase space with respect to line \( x' = 0 \) and span the shortest range of angles (slightly exceeding 20 mrad). The angular dispersion of the S-shaped pattern increases with the distance from the cathode’s center. It is shifted toward higher or lower values depending on whether the column is situated to the right or left of the cathode center, respectively. The electrons from the edge columns are unconstrained by the vacuum outside the boundary of the emitter, while the spread in the opposite direction is hindered by the particles emitted from the internal columns. As a result, the angular spread outward from the edge is much larger than inward from the edge. Toward the center of the cathode, the space-charge becomes more symmetric, and thus the S-shaped patterns become more symmetric. The corresponding phase-space diagram for the \( y \) coordinate (\( y'-y'' \)) looks the same and, therefore, is not shown.

Another quantity strongly affected by the work function distribution is the electron density. In Fig. 3, we show a cross-sectional slice of the electron density taken through the third row from the top in Fig. 2. Each curve was scaled such that the area under it is equal to 1. As a result, they show the distribution of particles emitted from different work function regions separately. If the density of electrons emitted from the areas of higher work function were scaled with respect to the one describing the electrons released from those of lower work function, then it would be so small that its shape would not be visible. The density of electrons emitted from lower work function areas forms maxima of a different height, which considerably decreases in magnitude toward the cathode center. These electrons spread out above the areas of higher work function to such a degree that they overlap. Even greater spreading takes place to the vacuum outside the cathode and leads to the shift of the density peak associated with the edge patch away from the center of that check. The same features occur in the density of electrons emitted from the patches of higher work function but are much weaker, i.e., the density of electrons above the central areas is only slightly lower than above the edge one, the spreading of these beamlets is much smaller. The difference in the beamlets’ qualitative structure from low and high work function is because space-charge effects are more pronounced for the areas with low work function, as the corresponding current density is much greater.

The high edge emission due to decreased space charge effects on the sides of the uniform cathodes has been described previously [1], [24]. In the case of checkerboard systems, this effect is seen not only at the outer edges of the emitter but also in each of the low work function checks so that the current density at the edge of those checks is greater than in their interior. An increase of the number of checks results in an increase of emitted current as seen in Fig. 4, as the larger number of checks result in the increase of the total length of the edges, and thus the areas of the strongest emission. However, as the number of checks is increased while keeping the total emitter size unchanged, an increase in the number of checks corresponds to a decreased distance between checks of low work function. This leads to increased mutual space-charge effects between those checks, which has the effect of decreasing the emitted current from each of them [17]. Eventually, the competing effects of enhanced edge emission and mutual space-charge interaction lead to the current leveling off at a value below that of a corresponding emitter of uniformly low work function.

In Fig. 4, we also see the \( x \) component of emittance’s dependence on the number of checks on the emitter (the \( y \) component behaves similarly due to symmetry). The reason for the emittance decreasing with the increasing number of checks is the following. When the checks are sufficiently large, they behave nearly like independent emitters, and the beam consists of small beamlets centered below low work function checks, distributed periodically over the entire emitter. Electrons emitted from the edge of each low work function check experience a transverse force due to higher space-charge above the check’s interior than over the adjacent high work function check. As the checks become smaller and more numerous, the distance between the low work function checks decreases, and the asymmetry in the transverse space-charge force is reduced, which in turn reduces the transverse component of electrons emitted from the check edges. Thus, emittance decreases with increasing check number. A competing effect is that with greater current density
Fig. 5. (a) $12 \times 12$ lattice with work function 2.5 eV where 14 randomly distributed patches with a lower work function 2.0 eV have been placed on it. Patches with work function 2.5 eV are shown in red while patches in other colors correspond to the work function 2.0 eV. (b) $x'-x$ phase space diagram for the pattern shown in a. The colors show which patch the electrons where emitted from.

(or simply greater electron density near the cathode), scattering increases, leading to greater emittance. Thus the growth in current with increasing the check number causes the emittance to grow. Hence, the emittance initially drops with increasing check number but then asymptotically reaches a constant value. The decrease of emittance accompanied by the increase of the emitted current results in an increase of the brightness (blue line Fig. 4). The finer the work function grid on the cathode’s surface, the better quality of the emitted beam is obtained. It is interesting to note that the brightness of a fine-grained emitter, with alternating checks of high and low work function, can be considerably higher than that of an emitter with uniformly low work function, even with a moderate reduction in current, as can be seen by comparison of Fig. 4 with Figs. 6 and 8.

B. Random Pattern

We also examined a random distribution of patches on a square $12 \times 12$ lattice. An example containing 14 patches of lower work function is shown in Fig. 5(a), and the corresponding phase-space diagram below in Fig. 5(b). Every single area of lower work function induces a similar S-shaped pattern in the phase-space diagram (shown in the same color as the corresponding patch). The center and shape depend on the particular check position with respect to other low work function patches. For instance, in the second column from the left of Fig. 5(a), there are three patches with low work function. The S-shaped patterns in phase space, due to electrons from these patches, mostly overlap as none of the low work function patches has a similar low work function patch adjacent to it in the first or third column. By comparison, in the fifth column from the left, there are two low work function patches. The upper one is surrounded by a high work function emitting area, whereas the lower (in green) one has two immediate neighbors of low work function, which affect it via space-charge forces. As a result, the green S-shape in phase space is skewed and shifted considerably to lower values of $x'$.

We performed simulations for 6, 14, 28, and 56 randomly distributed patches of either lower or higher work function on the same $12 \times 12$ lattice. For a fixed number of patches, 50 simulations were conducted, each with new random distribution and thus a different mean distance between the minority patches. Fig. 6 shows the current as a function of the mean distance between all pairs of minority work function patches and the reference values of the current from the uniform cathodes with the two work function values used. When the low work function patches are in the minority, the current is always between the values corresponding to uniform cathodes and strongly increases with the number of low work function areas. The decrease of work function from 2.5 to 2.0 eV results in a considerable increase of current from uniform cathodes and also from individual patches. As a result, the incorporation of even a few low work function patches against a high work function background increases the current.

Importantly, the increase in current is not proportional to the total area of low work function patches, e.g., the
introduction of six patches increases the current by about 2.7×. In comparison, the change from 28 to 56 patches increases the current by about 1.6×. For fixed number of minority checks the current increases slightly with the mean distance of added patches. The space-charge effects between patches decrease with increasing distance between low work function areas allowing them to emit more current. Moreover, the rate of increase becomes greater for a larger number of randomly distributed low work function checks. When there are only six low work function patches on the 12 × 12 emitter, then most arrangements are such that the low work function patches are essentially uncoupled, and the increase with the mean distance is very weak. The situation changes when the number of low work function patches increases because the areas may cluster together and be strongly coupled. This is seen for 56 patches when the lowest current is obtained when the minority checks are close to each other. The increase of the mean distance reduces the mutual space-charge effects between the low work function patches, leading to an increase of emission from them, thus increasing the total current. An interesting effect occurs for the opposite case, i.e., when the high work function checks are the minority ones. A few such patches can increase the current above the level of a uniform cathode with the lower value of work function. As the number of high work function patches increases, the total current will drop down because the increase of current resulting from the reduction of space-charge effects becomes dominated by the decrease in current due to a larger fraction of the total area emitting low current.

Contrary to the uniform and checkerboard systems, the emittance components in the x- and y-direction of the beam emitted from the cathodes containing randomly distributed minority patches are not the same. To capture the emittance for both directions in a single number, we multiply the two components and take their square root, \( \epsilon_x \epsilon_y \). In Fig. 7, we plot this quantity as a function of the mean distance between all pairs of minority work function patches, and for reference, we show the emittance of the uniform cathodes. The emittance of the high work function uniform cathode is much lower than in the other cases, as is the current, Fig. 6. In this case, the beam consists of a few electrons separated from each other by distances at which the Coulomb repulsion is relatively weak, with minimal scattering. Thus their trajectories are mostly normal to the surface. Adding even a few low work function patches results in an increase of the emittance, which generally exceeds the low work function uniform cathode’s emittance, Fig. 7(a). These checks provide the great majority of electrons in the beam. With greater spacing between the low work function patches, the beamlets have more room to expand transversely, which leads to greater emittance. Additionally, with greater spacing between low energy patches, the mutual space-charge coupling between them decreases, and the current density in the beamlets emanating from these patches is increased. With increased current density comes increased scattering, and in turn, increased emittance. For the opposite case, i.e., when the high work function patches are the minority ones, their presence increases the emittance beyond the value for the low work function uniform cathode. Still, their impact decreases when their number is reduced and the separation increased, Fig. 7(b). Agglomerated patches of higher work function increase the beam’s inhomogeneity. The effect is reduced when the additional checks are distributed more uniformly.

Finally, in Fig. 8, we show the beam brightness versus the mean distance between pairs of minority work function patches. This quality factor is proportional to the ratio between the emitted current and the product of emittance components [(5)]. In the case of uniform systems, the very low emittance of the high work function cathode leads to a greater brightness than for the cathode with the low work function, even though the current for the latter is an order of magnitude larger. Due to the sensitivity of the emittance to the introduction of low work function patches, as seen in Fig. 7, the low work function minority checks decrease the brightness below the value for the low work function uniform cathode, Fig. 8(a). The much sensitivity of emittance to minority patch spacing [Fig. 8] compared to that of the current [Fig. 6] results in a decrease of the brightness with an increasing mean distance between the minority patches, Fig. 8(a). The existence of minority checks with higher work function generally reduces the brightness with an increasing number of minority patches, with the exception that a small number of such checks distributed over the surface may slightly increase the brightness beyond the value obtained for uniformly low work function emitter. Due to the decrease of emittance observed in Fig. 7(a), the brightness increases with the mean distance between the minority patches, Fig. 8(b).
IV. Conclusion

In this work, we examined the emittance and brightness from cathodes with a two-level work function, both periodically and randomly distributed. We found that the current increases slightly with the mean distance between the minority patches when they have the low work function, and it decreases slightly when they have the high work function. The emittance showed similar behavior but much more pronounced than the current. The higher sensitivity of the emittance compared to the current is in line with the previous work by Jensen et al. [14]. Consequently, the beam brightness is also sensitive, but with the opposite behavior, i.e., decreasing with the mean distance between the low-work-function patches when they were in the minority and increasing when the high-work-function patches were in the minority.

However, overall, the cathode’s emittance with nonuniform work function is greater than for the uniform case, and at the same time, the brightness decreases. The emittance results from the lateral motion of the particles due to both scattering and irregular distribution of space-charge over the cathode surface, i.e., nonuniform beam divergence. While in the homogeneous case the electron density profile in the vicinity of the cathode is nearly uniform (except at its boundaries), our work function variation leads to an inhomogeneous density profile, with zones of higher density emerging from the spots with low work function, which tend to diffuse into the zones of lower density emerging from the spots with high work function. These imbalanced lateral forces lead to an extra divergence of the beam and thus to an increased emittance.

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