# Simulation of Self Organized Electron Beams in Vacuum Microdiodes

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## **1 INTRODUCTION**

Vacuum electronics devices have been in continuous use for over a hundred years although their applications have varied (Barker et al, 2002); (Eichmeier and Thumm, 2008). As the name implies they are based on transporting electrons, or other charged particles, through a vacuum, often guided by electric and magnetic fields. Prior to the advent of the solid state transistor vacuum tubes were ubiquitous in electronics, but since then their use has become more specialized. In particular, vacuum electronic devices have been used for high power and high frequency applications where their superior performance characteristics have seen them keep the solid-state devices at bay.

The main drawback of vacuum electronic devices has been the complexity of their construction and the need to maintain a good vacuum for them to function properly. However, power efficiency and robustness are examples of their advantages. With the advent of modern fabrication techniques it is now possible to manufacture three dimensional microstructures in an inexpensive and reliable manner. An advantage of operating vacuum devices at the micro-scale is that the mean free path of electrons is of the same order as the characteristic dimension of the device itself even at atmospheric pressure. Thus the "vacuum" characteristics of the device are due to the small size rather than the low pressure. As a result of these developments the possibility arises for vacuum electronics devices to become an attractive option in many applications where they had been too costly before.

When modelling vacuum devices at this small scale it is important to take into account several physical effects that can, to a large degree be ignored in macro-scale devices, e.g. scattering and surface inhomogeneity. An important advantage is that the number of free electrons in such small systems is typically on the order of  $10^2$  to  $10^4$  and as a result it is practical to use a molecular dynamics method where the repulsive Coulomb interaction between every single free electron is taken into account. This means that discrete effects can be modelled with high fidelity –something that is not possible to the same extent with the particle-in-cell (PIC) methods that prevail in the plasma physics and vacuum electronics community.

Our previous work on a single emitter has shown that in the case of photoemission, when many electrons are released at the same time from a nanometric cathode, one may expect an oscillatory current through the device (Pedersen, 2010). Similar results have been obtained (de Lara et al., 2006), but with emitters larger than few millimeters. These oscillations are a result of the repulsive Coulomb forces between the electrons in the micro diode. A bunch of electrons just released from the cathode will be accelerated by the electric field across the

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Abstract: Simulation of vacuum micro-diodes can be done quite effectively using molecular dynamics methods. This results in much higher fidelity simulations than can be obtained using the particle-in-cell method (PIC), which is most common for plasma and particle beam simulations. In particular, this method is superior to the PIC method when treating systems where collisional effects are important. In this paper we present some results concerning electron beam structure in a vacuum micro-diode obtained using a molecular dynamics code developed at Reykjavík University.

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diode, but will also create an opposite electric field that may block the release of further electrons from the cathode temporarily. This novel beam bunching mechanism may be useful as a tunable oscillator operating in the THz domain. The frequency of the current at the anode is determined by the vacuum field and by the size of the emitter (Jonsson, 2013).

These unexpected results have motivated us to expand the study to investigate the effects of having an emitter area which is non-continuous, e.g. two circular emitters separated by a given distance or an arrangement of square emitters on the cathode. This is a preliminary step in studying several diodes working in parallel, which is required to increase the output power of a corresponding device. In this paper a brief outline on how the molecular dynamics approach has been used to model vacuum microdiodes will be given, as well as preliminary results regarding beam structure that emerges in the diode due to nonlinear Coulomb interaction between the particles in the electron beam released by two cathode areas. We will discuss both longitudinal (or temporal) and transverse structure in the beam due to these types of arrangements.

#### 2 SIMULATION APPROACH

The system under consideration consists of a parallel plate vacuum diode. The cathode is grounded, and the anode is at a potential,  $\Phi$ . The spacing between the anode and cathode is D. In the absence of any electrons in the gap between the cathode and anode the electric field is uniform and perpendicular to the electrodes and given by  $E_0 = \Phi/D$ . This is referred to as the vacuum field. Electrons originate at the cathode and are accelerated in the gap by the electric field. Once electrons are present in the gap they bring a new component of the electric field into existence due to their own charge (the spacecharge). In the event that the number of electrons in the gap becomes large enough the space-charge field can become a dominant factor in the beam dynamics, even to such an extent that it will inhibit further electrons from being emitted. This is known as the space-charge limited regime, and when operated under this condition the beam dynamics is highly nonlinear. In our model we assume that electrons are emitted from a cold cathode via photoemission, with negligible initial velocity.

In the simulation each time step is broken down into three sub-steps: Particle emission, particle advancement and absorption. A brief description will be given here, but a more complete description may be found in (Jonsson 2013).

#### 2.1 **Particle Emission**

At the beginning of each time step a random point on the emitter area is selected. If the electric field at that point is favourable in terms of pushing an electron into the diode gap an electron will be placed slightly above that point. If the field is unfavourable a failure of placement will be registered. While keeping time constant, this process is repeated, taking into account the electric field stemming from those electrons that have been placed in the system already. The iteration of this process is continued until 100 consecutive placement failures have been registered, at which time it is deemed that spacecharge limited emission has been reached.

The emission can also be source limited, in which case the number of electrons per time step is limited to a predefined number, but that regime will not be discussed further in this paper. ATIONS

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#### **Particle Advancement** 2.2

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Once the space-charge limit has been reached, the force acting on each individual free electron in the system is calculated, taking into account both the external electric field and the Coulomb force from every single other free electron in the diode gap. Subsequently a velocity-Verlet method is used to calculate each electrons position at the end of the time step.

#### **Particle Absorption** 2.3

After calculating the final position of all the free electrons at the end of the time step, we determine which electrons have passed beyond the boundary of the diode and will be absorbed. The number of electrons absorbed at the anode per time step is used as a basis for calculating the time dependent current in the diode, which is obtained using a smoothed average of the absorption rate. Additionally the point of absorption is also registered.

#### 3 RESULTS

In our simulations we consider circular (disk) or square emitters on the cathode. The spacing between the cathode and anode is 500nm, and the electric potential is 2V. The time step used in the simulation is 0.25fs.

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### **3.1** Temporal Structure

We consider two circular emitters of radius 150 nm. We want to observe whether and how the Coulomb oscillations of the current are established in a device with two emitters working in parallel. We assume that in a realistic setup the two emitters may not be synchronized. Therefore we consider in the simulations a certain relative time delay, and the current begins to be drawn from one emitter before the other one. We set the time delay to one fourth of the period of the space charge induced oscillation, i.e. the current from the two circular emitters is initially 90° out of phase. Figures 1 and 2 show the temporal profile of the current at the anode for two different values of the spacing between the emitting disks. In Fig. 1 the distance between the centers of the disks is 305 nm, i.e. the disks are almost touching. In this case the onset of regular current oscillations starts after about 10 000 time steps. After this time the emission from the two disks on the cathode becomes synchronized and the current is qualitatively similar to that corresponding to a single disk. In Fig. 2 the distance between the centers of the disks is increased to 340 nm. In this case we see a much longer transient phase of fairly weak and chaotic oscillations. But, as time goes by the current from the two disks becomes synchronized and the amplitude of the oscillation grows to the same level as in Fig. 1. We have observed that the synchronization occurs even for larger spacing between the emitters, but only after a longer transient time.



Figure 1: Current at the absorber vs. time steps for two identical circular emitters, each one with radius of 150nm The distance between the centers of the disks is 305 nm, i.e. the disks are almost touching. The current is given arbitrary units and one time step is  $2.5 \times 10^{-16}$  s.



Figure 2: Current at the absorber vs. time steps for two identical circles (disks) with radius of 150 nm. The distance between the centers of the disks is 305 nm, i.e. the disks are almost touching. The current is given arbitrary units and one time step is  $2.5 \times 10^{-16}$  s.

## 3.2 Transverse Structure

We are interested in time-integrated charge absorption at the anode and its distribution perpendicular to the axis of beam propagation. This is the equivalent of what would be measured using the well-known experimental method of inserting a fluorescent screen into the path of an electron beam. Thus it is a useful method of comparison.



Figure 3: Two identical circles with radius of 150nm with centers separated by 305nm. Here the delay of 90°was introduced in the emission start between the two circular emitters.

We begin by looking at the same configuration as was used for investigation of the temporal structure, namely two emitting disks of radius 150nm with their centers separated by 340nm. Figure 3 shows the resulting pattern for absorption at the anode as well as that for emission at the cathode. We note that on the cathode, the current density is highest along the outer edges. This is in agreement with previous studies for two-dimensional space charge limited emission (Ragan-Kelley, 2009). We also note that at the anode, the beam takes on a circular cross section with a prominent halo. This is in agreement with the general characteristics of space charge dominated electron beams (Reiser, 2008). An interesting aspect is the bright line that dissects the circle on the upper part of Figure 3 (corresponding to the anode). This is along the line of the system and is due to interference of the current from the two emitters.



Figure 4: Two identical squares with side of 250nm each touching at the corners.

Next we conduct a similar investigation with slightly different configurations. First, we have two square emitters of side length 250nm touching at the corners, as depicted in Figure 4. Second a matrix of four identical squares with a side length of 250nm, touching at the corners as depicted in Figure 5. Once again we see that the beam pattern evolves into a circular form with a prominent halo. At the cathode the current is most intense at the outer edges of the emitter area. As before, we see that this is in character with expected beam behaviour. Similarly we also find that the charge density is greater along the lines of symmetry in the system.



Figure 5: Four identical squares with side of 250nm each touching at the corners.

## 4 CONCLUSIONS

We have developed a code for conducting high fidelity molecular dynamics simulations of vacuum microsystems with full representation of Coulomb forces. With this code we have been able to observe emergence of both temporal and spatial structure in the beam due to space charge forces. This holds some promise for the development of tuneable THz radiators and for the design of electron beamlets with a specified microstructure.

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