ISBN: 978-3-95450-208-0 doi:10.18429/JACoW-IPAC2019-WEPTS069

THE EFFECTS OF STOCHASTIC SPACE CHARGE IN HIGH BRIGHTNESS PHOTOELECTRON BEAMLINES FOR ULTRAFAST ELECTRON DIFFRACTION

M. Gordon, Y. K. Kim, University of Chicago, Chicago, IL, USA
J. Maxson, Cornell University, Ithaca, NY, USA

Abstract

As we move to ultra-high brightness photocathodes and ultra-cold beams, we may become more sensitive to stochastic, point-to point effects such as disorder induced heating and the Boersch effect, given the failure of Debye screening. In this study, we explore the effects of stochastic scattering. Modern beam dynamics codes often approximate point to point interactions with a potential created by smoothing the charge over space, removing sensitivity to stochastic effects. This approximation is often used in beamline optimization, because it is much faster. We study the limits of validity of this approximation. In particular, we will simulate effects of stochastic space charge on a high brightness photoemission beamline, an ultrafast electron diffraction beamline with a photocathode temperature of 5 meV with a final beam energy of 225 keV. Emittance dilution in the transverse plane and transverse beam size relative to smooth space charge simulations will be presented.

INTRODUCTION

High brightness photoemission sources are a critical enabling technology for many applications, including synchrotron light sources like free electron lasers, high power accelerators like energy recovery linacs, and accelerator based electron sources for femtosecond electrton diffraction and microscopy. In each of these applications, the beam brightness is a critical figure of merit, and the maximum beam brightness is set by the photoemission source density and mean transverse energy (MTE), which is analogous to an effective photoemission beam temperature.

Great advances have been made in the reduction of photoemission MTE, with advanced cyrocooled photocathode sources anticipated to reach effective photoemission temperatures approaching $\sim$ 5 meV. At such small temperautres, Debye screening is ineffective for high extracted charge densities, and the traditional approximation of the space charge force arising from a continuous charge fluid fails. Particularly at low energies, direct point-to-point Coulomb repulsion between particles is anticipated to have a large impact on a beam. However, simulating a high density photoemission beam by exactly solving Maxwell's equations for a system with a large number of particles is CPU intensive and impractical in many cases. However, approximate methods have been developed which include point-to-point interactions for near neighbors, while treating long-range interactions via the mean field. These methods are attractive as the computation time scaling with the number of particles can be much faster than $O(N^2)$.

In this work, we investigate the role of stochastic point-to-point interactions in an ultrafast electron diffraction beamline with high density, low temperature photoemission conditions. Beam dynamics simulations were originally optimized including smooth space charge (calculated via the Poisson equation). Ultrafast electron diffraction (UED) is an ideal case study for the role of stochastic interactions, as the total number of electrons per bunch is often small ($10^5 - 10^7$) [1], but for example the short bunch lengths, long coherence lengths, and small spot sizes required to study atomic dynamics creates peak beam current densities comparable to those in FEL injectors. Thus we may model each individual electron in the bunch.

The UED beamline considered here is being commissioned at Cornell. The setup consists of a 225 kV DC gun followed by 2 solenoids and a normal conducting buncher Cavity [2]. The beamline layout is shown in Figure 1. In this gun, the photocathode is cryogenically cooled, and thus we assume a best case scenario in which the photoemission MTE = 5 meV (60 K). All simulations are performed with the space charge tracking code General Particle Tracer (GPT) [3]. In particular, we simulate the case which has been optimized for 10^5 electrons per bunch, and compare the evolution of the beam between the previously used smooth space charge calculation [2] with a modified Barnes Hut algorithm [4], detailed in the following section, which accounts for the stochastic nature of particle-particle interactions at small distances.

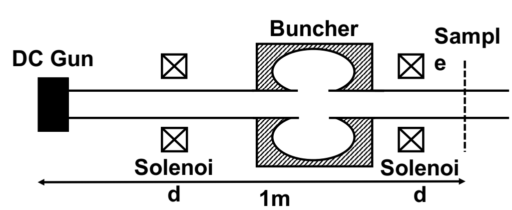


Figure 1: Layout of the cryogenically cooled photoemission gun and beamline used in the following simulations.

STOCHASTIC SPACE CHARGE ALGORITHM

To simulate the effects of stochastic space charge in this beamline, we use a modified Barnes-Hut algorithm in GPT which both calculates close range interactions and also includes the electron image charge at the cathode.

In the Barnes-Hut method, the effect of stochastic interactions in short range interactions are calculated exactly, while

ISBN: 978-3-95450-208-0 doi:10.18429/JACoW-IPAC2019-WEPTS069

long range interactions are approximated. This long range approximation is done through grouping bodies that are sufficiently nearby and representing them as a single particle at their center of mass with a total charge equal to the sum of the charge of the individual particles. A Barnes-Hut θ parameter of 0.3 was used for all simulations [4]. In order to avoid singularities in the electric field calculation, a smoothing radius is typically applied, which sets the minimum close-encounter distance between particles. Here the smoothing radius was chosen to be 10^{-10}m, 4 orders of magnitude under the average inter-particle spacing near the cathode (10^{-6} m), as it is found that multiple scattering generally regulates close encounters.

The effect of the image charge was implemented into the algorithm in the following way. Each particle generates an image charge which is further shifted away from the real particle by a distance $2r_c$. The value for r_c is chosen as follows. The work function is defined as the minimum energy required to remove an electron to infinity from the surface of a metal. Using the method of image charges, the energy required to move a charge from infinity to a distance r_c from a cathode is:

$$U = qV = \frac{1}{4\pi\epsilon}\frac{q^2}{2r_c}$$

Setting this difference in energy equal to the work function, ϕ, an effective minimum distance from the cathode, r_c, can be found:

$$r_c = \frac{1}{8\pi\epsilon}\frac{q^2}{\phi}$$

For a work function of $\sim$ 1 eV, the corresponding r_c for the simulation is $\sim$ 1 nm. We use a value of 1.5 nm in the following simulations.

STOCHASTIC VS. SMOOTH: RMS COMPARISON

Figures 2 and 3 show the evolution of the rms transverse normalized emittance of the beam (which will be further referred to as simply the emittance), and the rms transverse size (spot size) of the beam, for the smooth and stochastic space charge algorithms respectively.

As seen in figure 2, the emittance of the beam in the stochastic simulation quickly becomes much larger than the smooth simulation. After the first solenoid, the values converge and remain similar until the beam focus. Emittance dilution at the beam focus is compared in Table 1.

As seen in figure 3, initially, the spot size of the beam using stochastic space charge grows faster than that from smooth space charge. This leads to an over focusing by the first solenoid in the beamline and an overall smaller spot size at the target. Spot sizes at the beam focus are compared in Table 1.

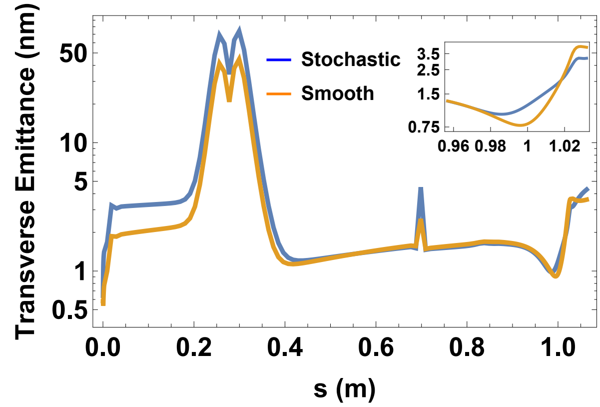


Figure 2: Transverse normalized rms emittance comparison for stochastic and smooth space charge simulations. Inset plot zooms in on emittance near beam focus.

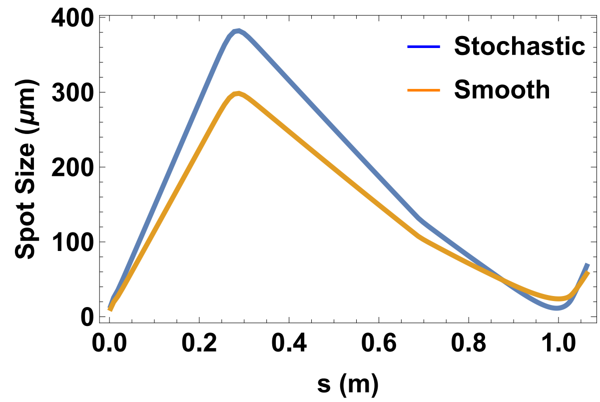


Figure 3: Transverse rms beam size comparison for stochastic and smooth space charge simulations

PHASE SPACE EVOLUTION COMPARISON

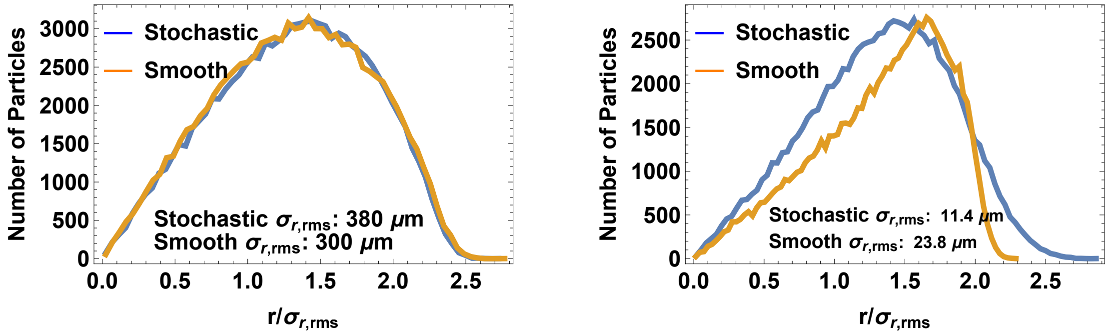
The rms quantities of a beam while useful for comparison do not fully characterize a beam. Another way to compare the smooth and stochastic simulations is to compare the phase spaces of the beams. Comparing the transverse radial distributions, one would expect a longer radial tail compared to the rms size of the beam for the stochastic simulation, representing particles kicked far from the beam center by large angle scattering.

Figure 4a shows the radial distributions for the smooth and stochastic simulations in the first solenoid, at the peak of the spot size distribution. There is no significant difference in the distribution shapes, but the rms spot sizes differ significantly. The shapes of the distributions remain constant until after the second solenoid. Figure 4b shows the radial distributions for the smooth and stochastic simulations at the beam's focus. The long tail on the stochastic distribution is likely indicative of large angle scattering expected from stochastic scattering. Figure 5 shows the phase space distribution for a) smooth and b) stochastic space charge at the respective beam focus.

ISBN: 978-3-95450-208-0 doi:10.18429/JACoW-IPAC2019-WEPTS069

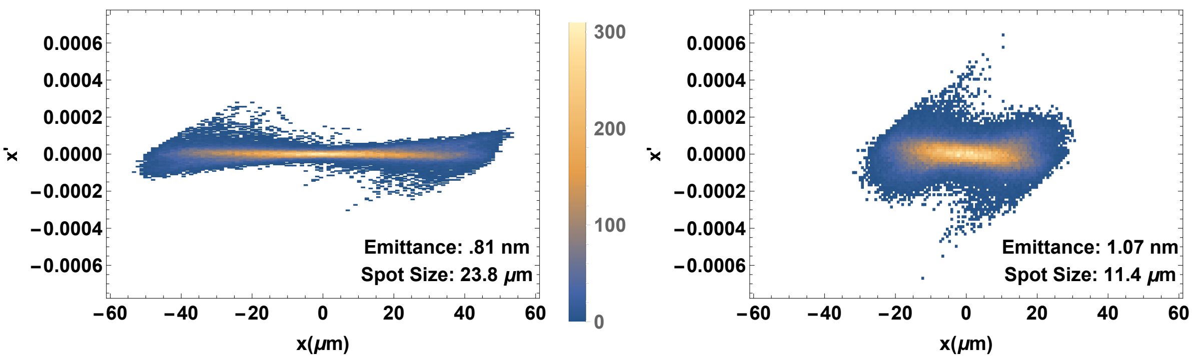
Table 1: Summary of the rms Results at the Beam Focus for Stochastic and Smooth Space Charge Simulations

Simulation	Position of Beam Focus(m)	Emittance(nm)	Spot Size(μm)
Stochastic	0.995	1.07	11.4
Smooth	1.001	0.81	23.8



(a) (b)

Figure 4: Transverse radial distribution of particles at a) the first solenoid b) the beam focus for smooth and stochastic space charge. The radii were normalized by the spot size of the simulation to distill shape information.



(a) (b)

Figure 5: Phase space distribution for a) smooth and b) stochastic space charge at the beam focus.

CONCLUSION

A UED beamline with a photocathode temperature of 5 meV with a final beam energy of 225keV and 10^5 electrons in a bunch was simulated using a stochastic space charge algorithm. Table 1 contains the results for emittance dilution and spot size differences at the beam focus compared to the smooth space charge approximation. It was observed that large angle scattering did not have an impact on the radial distribution shape during the beam's initial acceleration. However the smooth space charge algorithm underestimated the spot size of the beam by 20% at the first solenoid. During the final focusing of the beam, the stochastic nature of space charge is seen to play an important role, as large angle scattering is seen to significantly alter the beams radial distribution. In our next steps, we plan to extend our analysis with more diagnostics such as core emittance and apply this analysis to more beamlines to see if it is possible to make more general statements about the effects of stochastic space charge in modern UED beamlines.

ACKNOWLEDGMENT

We wish to thank Colwyn Gulliford for the use of his beamline optimization and particle distribution generator.

This work was supported by the Center for Bright Beams, NSF PHY-1549132.

REFERENCES

[1] Germán Sciaini and R. J. Wayne Miller, "Femtosecond electron diffraction: heralding the era of atomically resolved dynamics", *Reports on Progress in Physics*, vol. 74, no. 9, p. 096101, Aug. 2011.

[2] Colwyn Gulliford, Adam Bartnik, and Ivan Bazarov, "Multi-objective optimizations of a novel cryocooled dc gun based ultrafast electron diffraction beam line", *Physical Review Accelerators and Beams*, vol. 19, no. 9, p. 093402, 2016.

[3] Pulsar Website for GPT. `http://www.pulsar.nl/gpt/`

[4] Josh Barnes and Piet Hut, "A hierarchical O(N log N) force-calculation algorithm", *Nature*, vol. 324, no. 6096, pp. 446-449, 1986.