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A HIGH-PRECISION EMISSION COMPUTATIONAL MODEL FOR ULTRACOLD ELECTRON SOURCES

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Abstract

The high-intensity, high-brightness and precision frontiers for charged particle beams are an increasingly important focus for study. Ultimately for electron beam applications, including FELs and microscopy, the quality of the source is the limiting factor in the final quality of the beam. It is imperative to understand and develop a new generation of sub-Kelvin electron sources, and the current state of PIC codes are not precise enough to adequately treat this ultracold regime. Our novel computational framework is capable of modelling electron field emission from nanoscale structures on a substrate, with the precision to handle the ultracold regime. This is accomplished by integrating a newly developed Poisson integral solver capable of treating highly curved surfaces and an innovative collisional N-body integrator to propagate the emitted electron with prescribed accuracy. The electrons are generated from a distribution that accounts for quantum confinement and material properties and propagated to the cathode surface. We will discuss the novel techniques that we have developed and implemented and show emission characteristics for several cathode designs.

INTRODUCTION

Broadly speaking, the current state of the art in low emittance electron sources fall into two categories: cold atom sources, and single nanotip emitters. In the former, atomic gasses are typically suspended in a magnetic trap, and optically cooled to sub-Kelvin temperatures. Emitted electrons exhibit the low temperatures of the source when photoionized near the threshold energy. The second category of emitter utilize an electric field enhancing sharp tip, which leads to highly localized emission. Such emitters have been shown to produce electrons with a normalized emittance only one order of magnitude above the quantum degeneracy limit [1], however such sources are limited to low emission currents. An array of nanometer sharp tip emitters (see Fig. 1) would lead to higher emission currents, and also allows for spatial patterning of the emitted beams.

Large arrays of nanotip emitters present a significant computational challenge. Specifically, they require both a precise description of physical processes on the scale of the sharp tip, which is highly curved and at $O(1\,\text{nm})$, and consideration of the interaction of the geometrically arranged array of emitters on a scale of $O(1\text{-}10\,\mu\text{m})$. Moreover, collisional particle dynamics become relevant for beams near the quantum degeneracy limit (the ultracold regime), so the relevant time scales of the simulation exhibit a similar, if not more significant range ($> 10^4$). Conventional simulation tools use particle-in-cell (PIC) and other finite-element methods (FEM), which involve a full three dimensional volume discretization. Additionally, these methods typically represent the charged particle beam as a continuous density or using macroparticles, which become increasingly inaccurate in the ultracold regime (as space-charge effects become more significant). In order to overcome those challenges, we are developing a high-precision emission (HiPE) computational model which includes particle-particle interactions directly and implements an adaptive, high-order boundary element method (BEM) to include the boundary conditions accurately and efficiently (Fig. 1c illustrates the decrease in surface element size near the sharp tip).

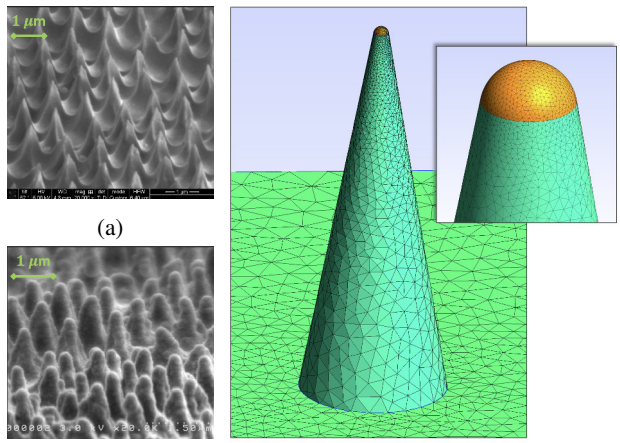

Figure 1: Images of nanotip array developed in collaboration with the engineering department. Shown are the fabricated Si nanotips (a), the tips after UNCD deposition (b), and the discretized boundary of a single nanotip model (c).

This model is being created using the Fortran based COSY Infinity, developed at MSU [2]. This gives HiPE access to a robust suite of beam physics routines and procedures (including map analysis/manipulation, and standard electromagnetic and optical accelerator components), and a language-level differential algebra (DA) implementation which HiPE utilizes on many levels. Nanotip boundary models are discretized using Gmsh [3], though any software capable of generating high-order surface discretizations could be used.

CODE MODULES AND INTEGRATION

Accurate simulation of electron emission from a nanotip array cathode requires considering three fundamental processes (see Fig. 2). Electrons have some initial state within

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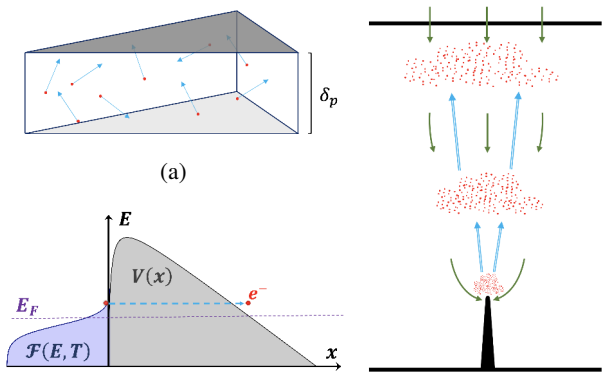

Figure 2: Red dots are electrons, and light blue arrows signify the direction of electron motion. Three fundamental processes in electron emission: electron distribution within a layer δ_p under a triangular surface element (a), electron tunneling through the surface potential barrier (b), and dynamics of electron beam in external electric fields (green arrows) (c).

the cathode, and during the emission process, relevant electrons undergo transport to the cathode surface boundary. At the surface, electrons are either reflected back to the bulk or transmitted through the surface boundary. Once emitted, electrons are propagated through space until they reach a sufficient distance that the interactions with the nanotip boundary is negligible.

HiPE is a dynamics code, and the propagation of time is implemented by breaking up the total time into discrete time steps of length τ. Currently, τ is a user-specified parameter that remains constant throughout the simulation. When the nanotip array is driven by field emission, electrons are generated, emitted, and propagated iteratively through each time step.

Initial Electron Distribution and Transport

The initial electron distribution is dependent on the geometric and material properties of the cathode. Using Fermi-Dirac statistics (which take into account the Pauli exclusion principle for Fermions) and assuming a distribution in thermodynamic equilibrium, the average number of electrons in a given energy state is given by the Fermi-Dirac function:

$$\mathcal{F}(E) = \frac{1}{\exp\left[\frac{E-\mu}{k_B T}\right] + 1}. \tag{1}$$

The density of states, $g(E)$, gives the allowed occupation levels for electrons, and can be calculated to include semiconductor properties and quantum confinement effects. The density of states for for a three-dimensional semiconductor (such as Si) is

$$g(E) = \frac{(2m^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E - E_c}, \tag{2}$$

where m^* is the electron effective mass, and E_c is the energy of the bottom of the conduction band. The average number of electrons per unit volume ($n(E)$) as a function of energy is given by the product of (1) and (2).

When the cathode surface is discretized (Fig. 1c), the area of each triangular element is saved. This area and the maximum distance an electron can travel within the cathode $\delta_p = \tau v_{max}$ form a volume (Fig. 2a) in which electrons are generated for the given time step. Here v_{max} is determined from the maximum electron energy given when $n(E)$ drops below a normalized value of 0.001. However, as shown in Fig. 2a, assuming an isotropic (equilibrium) distribution of electrons in the cathode, the majority of electrons sampled from $n(E)$ will not encounter the surface boundary during the time step τ. In fact, the probability that an electron initially at a depth of z_p will encounter the surface boundary,

$$P(E) = \frac{1}{2} - \sqrt{\frac{mz_p^2}{8E\tau^2}}, \tag{3}$$

is always less than 0.5. The total number of electrons that could possibly be emitted in one time step from a given depth is $N = \int_0^\infty P(E)n(E)\delta_p\tau\,\mathrm{d}E$.

Thus the N electron energies are sampled from $n(E)$, and their initial depth is sampled from (3) by treating z_p as the variable. The electron momentum vector is sampled from the angular distribution such that the electron does encounter the surface. In order to generalize and efficiently parallelize this procedure, electrons are generated and propagated to the surface of the two-dimensional right unit triangle. A parametric map $\mathcal{M}_o : \mathbb{R}^2 \to \mathbb{R}^3$ is formed from the unit right triangle to each triangular surface element (Fig. 1c). $\mathcal{M}_o$ is a polynomial map of order o formed using the DA framework in COSY, which yields both the points and the surface normals of the boundary element (Fig. 3).

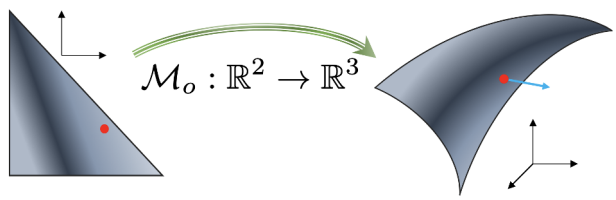

Figure 3: Parametric map $(u, v) \mapsto (x, y, z)$ for surface elements expresses both points (red) and surface normals (blue).

Electron Emission and Poisson Solver

At the cathode surface, electrons encounter a potential barrier, as shown in Fig. 2b, whose height is a function both of material properties and of the applied external electric fields. The transmission probability, as determined by the semi-classical 1D WKB method is

$$\mathrm{T}(E) = \exp\left[-\frac{2}{\hbar}\int\sqrt{2m(V(x) - E)}\,\mathrm{d}x\right], \tag{4}$$

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where the integral is taken over the classically forbidden region (ie. when $V > E$). The emission process is considered pseudo- one dimensionally, with constant transverse (parallel to the cathode surface) momentum, and with longitudinal momentum modified by the factor in (4). Thus (4) is calculated with $E = E_{\perp}$; the kinetic energy corresponding to the momentum component orthogonal to the surface.

The probability that an electron will be emitted is strongly dependent on the behavior of the electric potential near the cathode boundary. Figure 4 illustrates that the longitudinal electric field is highly nonlinear in the vicinity of the nanotip, leading to field enhancement factors as high as $\beta = O(100)$. The Poisson Integral Solver with Curved Surfaces (PISCS) [4] is a BEM specifically developed to solve the 3D Poisson boundary value problem when the boundary surface is highly curved. PISCS utilizes an adaptive high-order fast multipole method (FMM) [5] to perform all force computations with $O(N)$ operations.

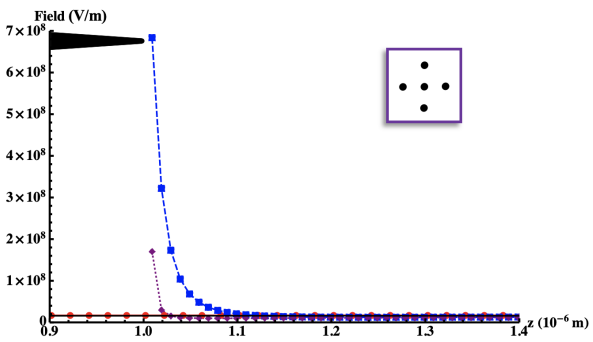

Figure 4: Electric field enhancement (longitudinal component) near the sharp tip. Plotted is the applied field (black), the field with no nanotip (red), the field with a single nanotip (blue), and the field for the center nanotip in an array arranged as in the inset with tip spacing equal to the nanotip height (purple).

PISCS is modified to return a functional form of the electric potential for evaluation of (4). The FMM expresses the multipole expansions of far sources in cartesian coordinates using COSY's DA framework, and the contribution of the near sources can be represented by a Taylor expansion (also formulated in the DA framework). The integral in (4) is then solved numerically using a fourth order Runge-Kutta method.

Propagation of Electrons Utilizing SIMO and PISCS

Computation of the electron dynamics near the nanotips is perfomed using the Simó integrator (SIMO) [6]. SIMO combines two main components: a variable order adaptive integrator implemented using DA, and use of Simó's theorem for automatic selection of optimal orders and time step size for a prescribed error tolerance. While near the cathode surface, emitted electrons cause a significant modification of the boundary potential. This process eventually leads to the formation of a "virtual cathode", which leads to an upper limit in the emission current. PISCS is used to rigorously include this effect, which will also have an impact on the dynamics of the newly emitted electron beam. The external electric field that the electrons "see" due to the boundary is expressed in a functional form using DA (similarly as described in the previous section), leading to more accurate dynamics throughout the simulation time step (τ).

Emitted electrons are tracked until they reach the evaluation surface (shown by the upper black line in Fig. 2c), which is the defined by the distance at which the effects of the nanotip(s) become negligible and the perceived field is simply the applied accelerating gradient. Saved at this point are the particle's position in phase space (6D), and the time that they crossed the evaluation surface. This particle file can then be converted and used as input for COSY, MADX, or similar to study the long term dynamics of the beam in the desired lattice.

CONCLUSION

Simulating electron emission from a nanotip array presents significant computational challenges. The orders of magnitude difference in the scale of relevant physical processes, both spatially and temporally, make accurate and efficient simulation a daunting task. HiPE is designed specifically to efficiently meet the accuracy standards necessary in the ultracold regime. This design includes an accurate, high-order surface parametrization, a particle-level model of electron emission, accurate computation of the electric potentials and fields factoring in the highly curved surface, and accurate beam dynamics near the cathode that takes into account all particle-particle collisions, including close encounters. PISCS, the FMM, SIMO and other scripts are available for download with documentation and examples from the Beam Physics Code Repository [7]. We expect to have a working version of HiPE with documentation and examples available in the coming months.

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