ISBN: 978-3-95450-132-8 doi:10.18429/JACoW-IPAC2014-MOPRI026

COMPLETE SIMULATION OF LASER INDUCED FIELD EMISSION FROM NANOSTRUCTURES USING A DGTD, PIC AND FEM CODE *

A. Fallahi#, CFEL, Hamburg, Germany
R. Hobbs, Y. Yang, P. D. Keathley, M. E. Swanwick, and L. F. Velasquez-Garcia and K. K. Berggren MIT, Cambridge, USA
F. X. Kärtner CFEL, Hamburg, Germany and MIT, Cambridge, USA

Abstract

We present a general and efficient numerical algorithm for studying laser induced field emission from nanostructures. The method combines the Discontinuous Galerkin Time Domain (DGTD) method for solving the optical field profile, the Particle-In-Cell (PIC) method for capturing the electron dynamics and the Finite Element Method (FEM) for solving the static field distribution. The charge distribution is introduced to the time-domain method based on a modified Fowler-Nordheim field emission model, which accounts for the band-bending of the charge carriers at the emitter surface. This algorithm is capable of considering various effects in the emission process such as space-charge, Coulomb blockade and image charge. Simulation results are compared with experimental findings for optically driven electron emission from nanosharp Si-tips.

INTRODUCTION

Laser induced field emission from nanostructures is the focus of exciting research efforts geared towards applications such as the production of bright electron bunches for probing ultrafast dynamics on a molecular scale [1,2], the production of electron beams for coherent x-ray sources [3], and local probes on the nanometer scale. The main benefit of nanostructures over the usually used flat cathodes as a photoelectron source is the capability to produce ultrashort (<1ps) electron bunches with high transverse coherence. In this process, a laser pulse is locally enhanced at the region close to the tip apex, which triggers the photoemission process over a localized area. The tip is biased with a static voltage that lies below the threshold for field emission and extracts the emitted electrons away from the tip. Field emission from these tips has been actively studied in recent years and it has been found that the emission process is controllable on the sub-femtosecond timescale [4,5]. The initially ultrashort electron beam travels in the applied static voltage and broadens during propagation due to the differences in energy gain from the laser and the space-charge effects [6].

Studying the electron dynamics during field emission and the subsequent acceleration is challenging because of the encountered large range of length and time scales. Quantum tunneling happens on a sub-nanometer scale and subsequent acceleration occurs in the vicinity of both optical and static fields. These features call for developing efficient, robust and accurate algorithms which are able to capture all involved effects. In the following, we present a hybrid algorithm suitable for analysing the full-vector three-dimensional dynamics of the phenomenon.

METHODOLOGY

A method should be chosen for the simulation of the optical fields near the tips. Various methods have been developed for the simulation of the bunch evolution under a time-varying electromagnetic field. Some methods take advantage from an analytical formulation of the accelerating field, which lead to very fast computations but at the same time harsh restrictions in accuracy [7]. General methods such as FDTD/PIC and DGTD/PIC algorithms offer suitable platforms for pursuing a general study. Due to the existence of structures with different length scales, DGTD is more suitable for simulation of optical field propagation owing to its high order accuracy and handling of unstructured grids. Therefore, we select DGTD/PIC for the simulation of field propagation and particle motion.

To initialize a charge distribution to be accelerated in the propagating field, the Fowler-Nordheim emission model is used [8]. This model presents a widely accepted formulation for the field emission of the electrons from a surface under intense electric fields with its accuracy tested and verified through different experiments.

The conventional DGTD/PIC algorithm introduces equivalent charge $\rho(\boldsymbol{r})$ and current $\boldsymbol{J}(\boldsymbol{r})$ densities, and projects them into the computational grid [9]. This technique suffers from several restrictions which make it not suitable for problems involving ultrafast field variations and tiny charge distributions. First, in this technique the charge distribution should be modelled with smooth functions to avoid Gibbs type phenomena in field computations. Second, the algorithm is numerically unstable due to static charge and force build-up. Third and most importantly, the field solution is singular at the cell containing the charges. This problem makes the overall solution technique completely unstable, because the singular fields of the emitted charges introduce large errors when inserted to exponentially dependent Fowler-Nordheim current densities for the calculation of the emitted charge. To avoid all the aforementioned limitations, we have developed a particular DGTD/PIC implementation, in which the particle motion is influencing the propagating field through its radiation. In

*Work supported by CFEL-DESY, DARPA N66001-11-1-4192 and European Research Council (ERC) under grant 609920.
#arya.fallahi@cfel.de

ISBN: 978-3-95450-132-8 doi:10.18429/JACoW-IPAC2014-MOPRI026

other words, the radiated field of the particle is added to the propagating fields, in contrast to the traditional technique, where the part-icle distributions are added as current and charge densities. This method is named as field-based DGTD/PIC algorithm and its detailed description is presented in [10].

To couple the radiated field of a moving particle to the propagating fields of the DGTD, we exploit the equivalence principle in electromagnetics. Suppose there are a number of charged particles residing in an element. For the region outside the element, this set of charge points can be replaced with a surrounding boundary S_f on which a particular magnetic and dielectric current is flowing. These currents are to be found from the radiated field according to

$$\boldsymbol{J}(\boldsymbol{r},t) \stackrel{\text{def}}{=} \hat{\boldsymbol{n}} \times \boldsymbol{H}(\boldsymbol{r},t),\ and\ \boldsymbol{M}(\boldsymbol{r},t) \stackrel{\text{def}}{=} -\hat{\boldsymbol{n}} \times \boldsymbol{E}(\boldsymbol{r},t) \qquad (1)$$

where $\boldsymbol{H}$ and $\boldsymbol{E}$ are the instantaneous radiated field of the charges inside the element. We consider S_f to be the boundary of one element. The fields inside the element according to the above currents will then be zero. The radiated fields are not affected by any boundary before reaching the element surfaces. Consequently, $\boldsymbol{H}$ and $\boldsymbol{E}$ can be derived from the Liénard-Wichert potential. After coupling to propagating fields, it will be reflected or transmitted by the boundaries around the charges.

The described procedure simulates the radiation of the charges while being accelerated under the influence of the strong laser field. However, there exists a Coulomb repulsion due to static forces between the electrons. In order to efficiently model these forces, advantage is taken from the domain tessellation for the DGTD implementation. The Coulomb forces vanish quickly with the distance from the charge point ($\sim r^{-2}$). Therefore, the dominant terms are due to the charges residing in the proximity of the observation point. Consequently, adding the Coulomb forces from the charges residing on the same element and the adjacent ones provide an appropriate estimation of the static space-charge forces.

In addition to all the above fields, the static field profile is playing a considerable role in the emission dynamics, making its computation indispensable for a complete analysis. For obtaining the static field at any point around the emitter the Poisson equation is solved using the FEM technique. Eventually, for both acceleration and field emission of electrons the static, optical and space-charge fields are superposed and inserted into the equation of motion and Fowler-Nordheim equation as the following:

$$\frac{\partial}{\partial t}(\gamma m_0 \boldsymbol{v}) = q\big(\boldsymbol{E} + \boldsymbol{E}_{SC} + \boldsymbol{E}_{DC} + \boldsymbol{v} \times (\boldsymbol{B} + \boldsymbol{B}_{SC})\big) \qquad (2)$$

and

$$\frac{\partial q}{\partial t} = A \frac{e^2 (E + E_{SC} + E_{DC})^2}{W t(y)} e^{-B v(y) \frac{W^{3/2}}{E + E_{SC} + E_{DC}}} \qquad (3)$$

where SC and DC subscripts refer to space-charge and static fields, W is the work function of the material, and A, B, $t(y)$ and $v(y)$ represent the standard Fowler-Nordheim constants and functions. For a semiconductor field emitter, the static field bends the electron and hole band diagram close to the emitter surface. This is the well-known band-bending effect occurring at the surface of biased semiconductors, practically shifting the chemical potential at the surface. To account for this effect a modified emission equation should be used in which the effect of the chemical potential on the emission process is considered. Note that in the conventional Fowler-Nordheim model for metals the chemical potential is assumed to be infinite. The modified equation reads as,

$$\frac{\partial q}{\partial t} = \frac{e^2 E^2 e^{-\frac{4\sqrt{2m}}{3\hbar e} v(y) \frac{W^{3/2}}{E}}}{16\pi^2 \hbar W t(y)} \left(1 - e^{-\frac{2\sqrt{2m}}{\hbar e} v(y) \frac{\mu\sqrt{W}}{E}} \frac{\hbar e E + 2\sqrt{2m}\, v(y) \mu \sqrt{W}}{\hbar e E}\right) \qquad (4)$$

The chemical potential μ is obtained using the depletion region approximation often used for predicting the performance of Schottkey diodes. Provided that the static field on the surface is E_{DC}, the width of the depletion region w is obtained from

$$E_{DC} = \frac{Ne}{\epsilon} w, \qquad (5)$$

with N the charge carrier density and ϵ the permittivity of the substrate. The amount of band bending is calculated via

$$\Delta V = \frac{Ne}{2\epsilon} w^2. \qquad (6)$$

The chemical potential at the surface is then written as $\mu_0 + \Delta V$, with μ_0 is the bulk chemical potential.

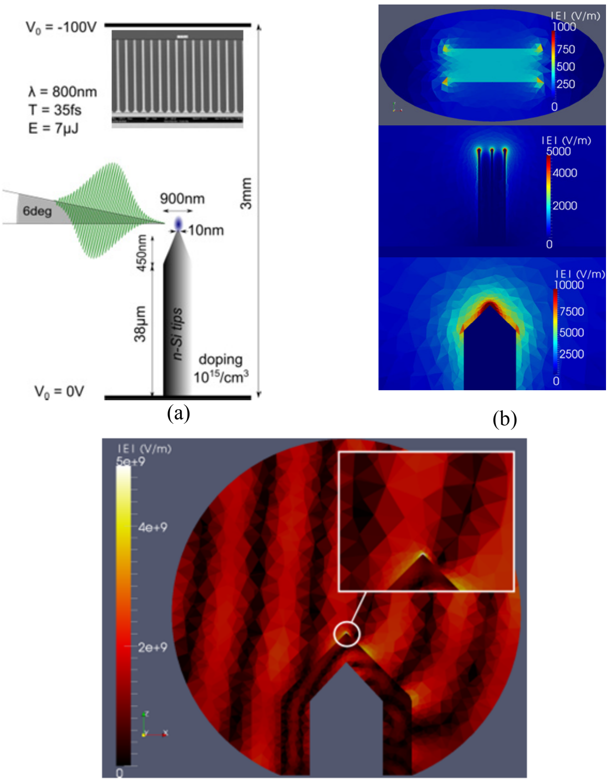
NUMERICAL RESULTS

The field-based DGTD/PIC technique is utilized for the analysis of laser induced field emission from n-doped silicon nano-tips [11]. The geometry of the problem is shown in Fig. 1a. A single silicon high aspect ratio nano-tip resides on a cathode plane. A 35 fs laser pulse with center wavelength at 800 nm and peak field amplitude E_0= 4.72 GV/m (pulse energy 7 μJ), illuminates the tip and causes field emission from the apex. The applied voltage between the two anode and cathode planes extracts the electrons over barrier created by space-charge and image-charge, thereby enhancing the emission efficiency of the device. Fig. 1b-c shows the obtained distributions for the static field and laser field. According to the FEM results, the static field is enhanced by about 60 times at the tip. The DGTD results showed that the optical field enhancement is only about 9.5. By changing the static voltage between the cathode and anode planes, we obtain the emitted charge as a function of the applied voltage which is compared against experimental measurements in Fig. 2. The experimental results are done for a large array of nano-tips as shown in Fig 1a. The deviations at low voltages are incurred by the space-charge effects due to the formation of an electron sheet above the emitters which virtually shields the laser and the static field. This effect is thoroughly discussed in [12].

The PIC technique enables the computation of position and energy of all particles (or macro-particles) emitted from the nano-tips. Hence, the developed software provides an excellent tool to study the characteristics of the produced electron bunch. Figure 3 shows the results for position and momentum distribution in three different directions 120 fs after the emission. According to the results, the initially small transverse size of the emitted charge (~50 nm) from a single emitter diverges quickly to

ISBN: 978-3-95450-132-8 doi:10.18429/JACoW-IPAC2014-MOPRI026

a larger beam size (~1μm) leading to the formation of an electron sheet above the nano-tip array.



(c)

Figure 1: (a) Geometry for field emission from a silicon nano-tip: A laser beam with 35 fs pulses obliquely illuminates a silicon nano-tip, emits electrons and simultaneously accelerates the emitted electrons. (b) The computed static field profile using a FEM Poisson solver for three tips. (c) The computed static field profile using the DGTD algorithm for one single tip.

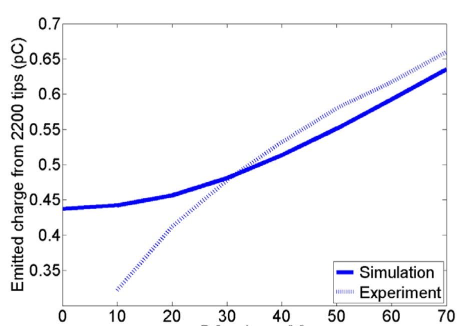


Figure 2: Emitted charge from 2200 tips versus the applied DC voltage obtained using the field-based DGTD/PIC and experimental measurements.

CONCLUSION

Simulation of the laser induced field emission from statically biased nanostructures is targeted. A hybrid code is developed based on the DGTD, PIC and FEM methods for the analysis of the field propagation, particle motion and static field profile, respectively. Combining the above three algorithms provides a powerful technique which captures all physics involved in the problem. By using a modified Fowler-Nordheim model for the field emission, the effect of static fields on the electron supply function is also included. The developed algorithm offers an excellent tool for characterizing and visualizing the emitted charge and its distribution in real and energy-momentum space from various nanostructures.

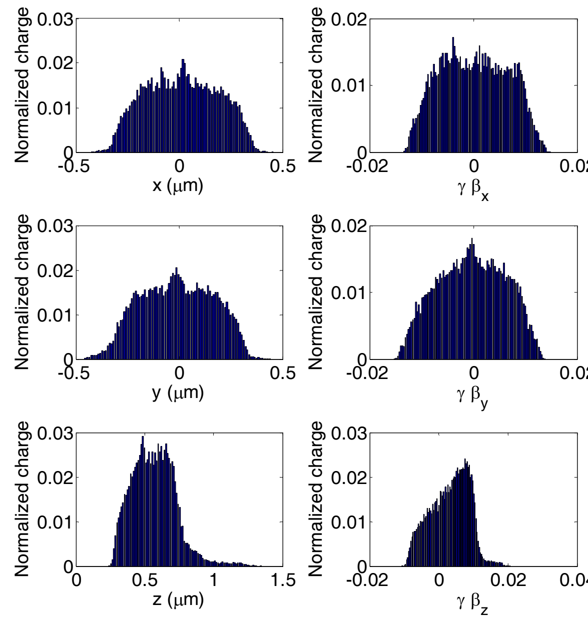


Figure 3: Position and momentum distribution of the electron bunch formed 120 fs after emission.

ACKNOWLEDGMENT

We would like to thank DESY HPC team for providing access and computation time at the HPC-center at DESY.

REFERENCES

[1] A.H. Zewail, "4D ultrafast electron diffraction, crystallography, and microscopy", *Annu. Rev. Phys. Chem.* **57**, 65 (2006).

[2] G. Sciaini and R.D. Miller, "Femtosecond electron diffraction: heralding the era of atomically resolved dynamics", *Reports on Progress in Physics* **74**, 096101 (2011).

[3] W. Graves, F. Kärtner, D. Moncton and P. Piot, "Intense superradiant x rays from a compact source using a nanocathode array and emittance exchange", *Phys. Rev. Lett.* **108**, 263904 (2012).

[4] P. Hommelhoff, Y. Sortais, A. Aghajani-Talesh and M.A. Kasevich, "Field emission tip as a nanometer source of free electron femtosecond pulses", *Phys. Rev. Lett.* **96**, 077401 (2006).

[5] P.D. Keathley, A. Sell, W.P. Putnam, S. Guerrera, L. Velásquez-García and F.X. Kärtner, "Strong-field photoemission from silicon field emitter arrays", *Annalen der Physik* **525**, 144 (2013).

ISBN: 978-3-95450-132-8 doi:10.18429/JACoW-IPAC2014-MOPRI026

[6] J. Hoffrogge, J-P. Stein, M. Krüger, M. Förster, J. Hammer, D. Ehberger, P. Baum and P. Hommelhoff, "A tip-based source of femtosecond electron pulses at 30keV", (2013), *arXiv preprint arXiv:1303.2383*
[7] L.J. Wong, A. Fallahi and F.X. Kärtner, "Compact electron acceleration and bunch compression in THz waveguides", *Optics Express* **21**, 9792 (2013).
[8] R.H. Fowler and L. Nordheim, "Electron emission in intense electric fields", *Proc. R. Soc. London, Ser. A,* 173 (1928).
[9] G. Jacobs and J. Hesthaven, "High-order nodal discontinuous Galerkin particle-in-cell method on unstructured grids", *Journal of Computational Physics* **214**, 96 (2006).
[10] A. Fallahi and F.X. Kärtner, "Field-based DGTD/PIC Technique for General and Stable Simulation of Interaction between Light and Electron Bunches", *submitted to J. Phys. B.*
[11] M. Swanwick, P. Keathley, F. Kartner and L. Velásquez-García, "Ultrafast photo-triggered field emission cathodes using massive, uniform arrays of nano-sharp high-aspect-ratio silicon structures", *Solid-State Sensors, Actuators and Microsystems (TRANSDUCERS & EUROSENSORS XXVII), 2013 Transducers & Eurosensors XXVII: The 17th International Conference on*: IEEE) p. 2680 (2013).
[12] P.D. Keathley, M.E. Swanwick, A. Fallahi, L.F. Velasquez-Garcia, and F. Kärtner, "Space Charge Effects in Strong-Field Emission From a Nanostructured Si Cathode", *CLEO: QELS_Fundamental Science*: Optical Society of America) p JW2A, 112 (2014).