MODELING NANOMETER STRUCTURED LASER INDUCED FIELD EMISSION *

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Abstract

Laser induced field emission has become an enabling technology for building ultra-low emittance electron sources for particle accelerators, such as the X-ray free-electron laser (SwissFEL) under development at the Paul Scherrer Institut (PSI). One approach consists of a sharp pyramidal tip with lateral dimensions of a few nanometers, illuminated by a laser to increase the extracted electron current. Another approaches uses conventional cathodes. In both cases, there are structural details on the nanometer scale, that determine the interaction between the laser and the cathode and thus directly the quantum efficiency of the emitter. On the other hand, much of the tip geometry has a characteristic length scale on the order of a few micrometers. Thus, there is a factor of 200 or more between all the relevant length scales in the geometry. Such contrasts place an enormous burden onto any numerical scheme, particularly w.r.t. widely differing mesh element sizes. We demonstrate a 3-d full-wave finite element time domain (FETD) electromagnetic approach to understand the nano-optical interaction between structure and laser pulse. We analyze the complete 3-d geometry of a pyramidal field emission element and use dispersive material models for modeling metal in the optical region of the electromagnetic spectrum.

INTRODUCTION

X-ray free electron lasers (XFEL) deliver coherent and short-pulsed radiation with power and brightness increased by several orders of magnitude when compared to 3^{rd} generation synchrotron light sources, for a review e.g. [1]. The development at Paul Scherrer Institut (PSI) targets the realization of a XFEL (`fel.web.psi.ch`) with substantial reduction in size and cost of the facility. The most direct way to reduce length and therefore the size of an XFEL, is to develop electron sources that produce short electron bunches with ultra-low emittance and high brightness. Cathodes that utilize laser-induced field-emission are promising candidates [2, 3, 4, 5, 6]. The technical realization of such novel cathode technology is not only relevant for realizing the SwissFEL but for other technology application areas as well: e.g. namely for sources for electron microscopes and displays. Considerable effort has recently been invested into the development of novel cathode technology with nanometer-sized structural properties. There are 2 main architectures: (i) the needle cathode, i.e. one single sharpened tip [3, 4, 5] and (ii) field emitter arrays (FEA) which are arrangements of field emitters on a periodically spaced lattice [6, 7, 8, 9]. Most of this work has been on the experimental side and significantly less effort has been directed into theoretical models. Due to the large number of design choices, e.g. geometrical shapes, material systems, fabrication parameters etc. it has become increasingly difficult for experimental scientists fabricating such structures to select the right parameters. In order to accelerate the development of novel, innovative cathode technology, detailed 3-d and, eventually, self-consistent models are a prerequisite. Such models will support both the cathode designers and experimental physicists and their users. They may also be relevant for industrial applications for developing novel electron sources on tight budgets and strict time frames.

FORMULATION OF THE PROBLEM

We want to calculate the electric field distribution for the 3-d geometry of a field emitter array (FEA) element with pyramidal shape, Fig. 1. The pyramid is illuminated by an incoming laser pulse of central wavelength $\lambda = 532$ nm. The simulated shape is simplified w.r.t. the fabricated FEA pyramid, Fig. 1, in that we neglect the concave pyramidal side faces.

METHODS

We use a finite element time domain (FETD) method to calculate the electric field in 3-d space [10, 11]. The algorithm discretizes the electric field vector wave, aka. *curl-curl*, Eq. (1)

$$\nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} + \sigma \frac{\partial}{\partial t} \mathbf{E} + \frac{\partial^2}{\partial t^2} (\epsilon * \mathbf{E}) = -\frac{\partial}{\partial t} \mathbf{J} \quad (1)$$

in 3-d space and time using a tetrahedral mesh [12, 13] where $\mathbf{E}$ and $\mathbf{J}$ both depend on space $\mathbf{r}$ and time t. In particular, we assume: **(i)** isotropic, scalar materials; **(ii)** non-dispersive magnetic permeability μ; **(iii)** dispersive dielectric permittivity of the Drude [14] type, Eq. (2),

$$\epsilon_{\mathrm{Drude}}(\omega) = \epsilon_{\infty} - \frac{\omega_p^2}{\omega^2 - \imath \omega \gamma_p} \quad (2)$$

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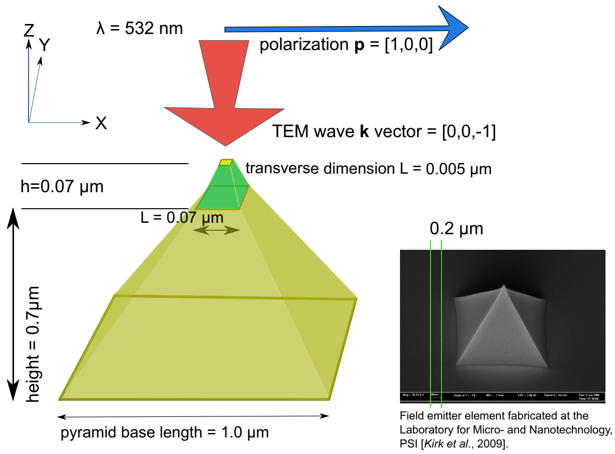

Figure 1: We show the 3-dimensional geometry of the pyramidal field emitter element and the parameters of the incoming transverse-electric-magnetic (TEM) wave. In the inset we show a scanning electron microscope (SEM) image of a field emitter array (FEA) element fabricated at the Laboratory for Micro- and Nano-Technology (LMN) at PSI [15]. We point at the challenges associated with electrodynamic modeling; in particular, we mention the wide span of characteristic length scales involved with the pyramidal tip: from micrometers at the base to transversal dimensions at the tip of approximately 5 nm. Thus, a factor of approximately 200 is to be dealt with in the geometrical discretization of the theoretical analysis.

where $\epsilon_\infty = 1.0 \cdot \epsilon_0$ is the permittivity at infinite frequency, $\omega_p = 13.8 \cdot 10^{15}\ s^{-1}$ the pole frequency and $\gamma_p = 1.075 \cdot 10^{14}\ s^{-1}$ the inverse of the pole relaxation time, respectively. The *Drude* model usually works best towards the red and infra-red region of the spectrum [16] while towards the blue and ultra-violet (UV) region the addition of a *Lorentz* type model is required to provide sufficient accuracy; **(iv)** Ohmic current density $j_\Omega = \sigma \mathbf{E}$; and **(v)** impressed current density **J** or an incoming transverse electric magnetic (TEM) wave which are used to source the electromagnetic problem. In order to truncate the computational domain in a transparent manner we use the 1^{st} order absorbing boundary condition [12, 13]. Distinct advantages are associated with a tetrahedral mesh. First, a number of commercial and open-source mesh generators have been available for years, e.g. [17]. Second, the tetrahedral grid allows for a flexible, spatial discretization of geometries with a wide span of characteristic length scales through level of detail (LoD). We use 1^{st} order tangentially continuous vector finite elements (TVFE), aka. *Whitney* basis functions [12, 13], to approximate the electric field within the tetrahedral element. For assessing the accuracy of the numerical algorithm we have analyzed 2 analytically solvable physical problems: **(i)** the *Hertzian* dipole [18] radiating into free space and **(ii)** scattering of a plane (TEM) wave [19] at a sphere with diameter $d = 50$ nm whose dielectric permittivitiy in the optical range of the spectrum is of the *Drude* type with gold model parameters [14].

RESULTS AND DISCUSSION

In Fig. 2 we show the 3-d mesh which contains approximately $240'000$ tetrahedra. We have used a sinusoidal carrier at a center wavelength $\lambda = 532$ nm whose amplitude is modulated by a *Neumann* (derivative of the Gaussian) pulse with $\sigma = 1.64$ fs and shifted in time by 6 ns in order to guarantee a smooth excitation. We use the *Courant* criterion [20] from the finite difference time domain (FDTD) method to calculate the time step for stable integration

$$\Delta t = \frac{\Delta x}{\sqrt{3}\, c_0} \tag{3}$$

where c_0 is the speed of light in vacuum. Since the smallest edge in the mesh has a length $\Delta x = 0.28$ nm this requests a timestep $\Delta t = 0.55$ as. We could also have used the exact criterion given by *Jin* [13] which is however more complicated to evaluate. Usually, *Jin's* criterion requests a smaller time step and, thus, we choose the timestep $\Delta t = 0.1$ as to be on the safe side. In Fig. (2) we show a cut through

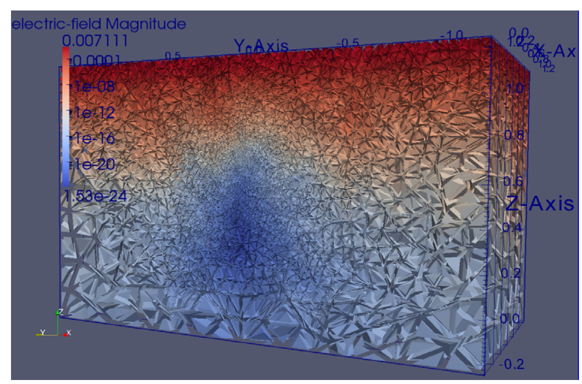

Figure 2: We show a cut through the tetrahedral mesh. The tetrahedra have been shrunk in order to visualize the differing characterisctic length scales in the mesh. The mesh contains approximately $240'000$ tetrahedra. In particular, the elements are much smaller around the tip region when compared to the base of the pyramid. The TEM wave illuminates the pyramid from above.

the computational domain along the yz plane. In particular, we mention the formation of a electromagnetic hot spot close to the tip of the pyramidal element, Fig. 3. This isolated zone of increased electric field corresponds to field enhancement which is caused by plasmonic resonances at sharp metal tips [14]. It is this very zone of increased electric field strength which is desired in order to increase current extracted by field emission.

SUMMARY AND CONCLUSIONS

We have demonstrated the ability to electromagnetically analyze, in 3-d space, a pyramidal shape used as an element in a field emitter array. We have modeled the metal

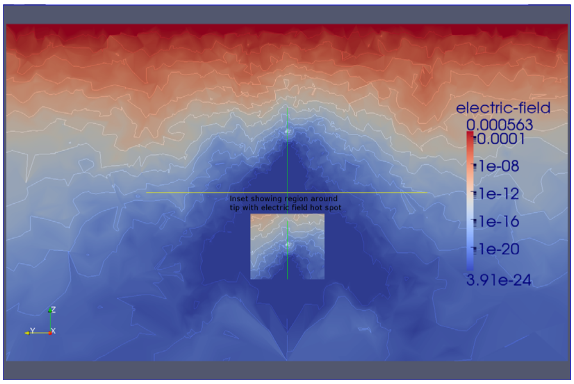

Figure 3: We show a cut through the computational domain and combine it with a contour plot of the electric field magnitude. We mention the formation of an electromagnetic hot spot close to the tip of the pyramidal element. This isolated zone of increased electric field corresponds to field enhancement which is caused by plasmonic resonances at sharp metal tips.

structure with the Drude model in the optical region of the spectrum and thus were able to show, qualitatively, an electromagnetic hot spot forming at the tip of the pyramid. The dimensions of the hot spot are correlated with the transverse dimension of the tip region. In order to further explore the extent and intensity of the zone of increased field strength we will need to build a mesh that is especially refined in the vicinity of the tip region in order to resolve the physics of plasmonic resonances.

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