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NEGF QUANTUM SIMULATION OF FIELD EMISSION DEVICES

T.D. Musho

Interdisciplinary Program in
Materials Science
Vanderbilt University
Nashville, TN USA, 37235
terence.d.musho@vanderbilt.edu

S.M. Claiborne

Interdisciplinary Program in
Materials Science
Vanderbilt University
Nashville, TN USA, 37235
sarah-ann.m.claiborne@vanderbilt.edu

D.G. Walker*

Department of Mechanical Engineering
Vanderbilt University
Nashville, TN USA, 37235
greg.walker@vanderbilt.edu

ABSTRACT

Recent studies of wide band-gap diamond field emission devices have realized superior performance and lifetime. However, theoretical studies using standard Fowler-Nordheim (FN) theory do not fully capture the physics of diamond semiconductor emitters as a result of the fitting parameters inherent to the FN approximation. The following research computationally models wide band-gap field emission devices from a quantum point of view, using a novel non-equilibrium Green's function (NEGF) approach previously applied to modeling solid-state electronic devices. Findings from this research confirm non-linearities in the FN curve and provide alternative explanations to discrepancies between standard FN theory.

NOMENCLATURE

l Length (nm)
 A Area (cm^2)
 T Temperature (K)
 V Voltage (V)
 CB Conduction Band (eV)
 N_d Doping Concentration (cm^{-3})
 E_o Vacuum Level (eV)
 E_f Fermi Level (eV)
 I Current (A)
 E Electric Field (V/cm)
 ϕ Work Function (eV)
 β Field Enhancement Factor

A_{eff} Effective Area of Emission
 K_1 Fowler-Nordheim Constant ($AeVV^{-2}$)
 K_2 Fowler-Nordheim Constant ($eV^{-3/2}Vm^{-1}$)
 m_e Electron Mass (kg)
 m^* Effective Mass
 ϵ Relative Permittivity
 HFE High Field Emission Regime
 LFE LFE Field Emission Regime
 FN Fowler-Nordheim
 $NEGF$ Non-Equilibrium Green's Function

INTRODUCTION

Field emission devices (FED) have been studied and well described since the twenties when Fowler and Nordheim characterized the cold field emission of electrons from metal into vacuum. However, recent advances in semiconductor materials and semiconductor fabrication techniques have realized high field emission emitters. Fabrication techniques such as chemical vapor deposition have allowed arrays of emitters to be fabricated on the sub-micro level with the ability to control geometric aspect related to the performance. Recently, wide band-gap semiconductor emitter devices have been experimentally shown to increase emission performance both electronically and mechanically over metal type emitters [1]. Unfortunately, theoretical studies of such devices using standard Fowler-Nordheim (FN) theory doesn't completely capture the trends of semiconductor emitters as a result of the fitting parameters inherent in the FN approximation.

*Address all correspondence to this author.

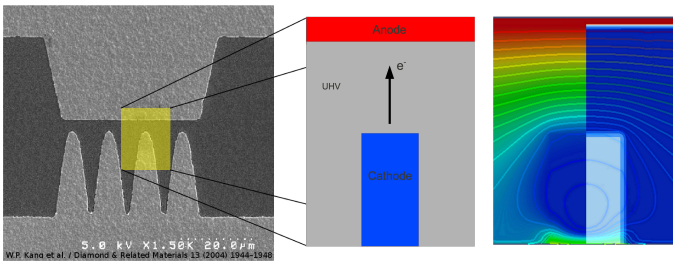


FIGURE 1: Illustration of the field effect device modeled. The domain is assumed to capture the performance of the tip region while simulating neighboring emitters through periodic boundary conditions. Image on far right is of the potential landscape calculated in the Hartree-Fock self-consistent loop of the NEGF formalism.

ANALYSIS

Device Construction

Device construction studied in this research is based on nanoscale lateral field emission devices [1]. The nano tip dimensions that were studied ranged between 1-5nm. Figure 1 is a comparison of the experimental structure selected from the literature [1] and the device simulated in this study. The simulated structure focuses on modeling the tip of the device. It is well accepted that the end few nanometers near the radius of curvature is where majority of the field emission process is taking place. To simplify the discretization of the computational domain, the tip was made blunt so the boundary of the tip and the discretized cell edges align.

The device material selection for the emitter was crystalline [100] diamond material, which has been used extensively in the literature for its superior field emission properties [1, 2]. The medium between the emitter and collect was an ultra high vacuum (UHV). The collector material was a palladium metal. The materials were characterized by the effective mass, electronic conduction band (CB) and the relative permittivity. The conduction band of the diamond and palladium were determined based on assumed electron affinities in reference to the vacuum level. Table 1 outlines the parameters used in the model. The CB of the diamond emitter was determined based on the electron concentration as a result of lightly doped emitter ($N_d = 10^{14} \text{cm}^{-3}$).

NEGF Method

The formulation used in the this research is a non-equilibrium Green's function (NEGF) method. The NEGF formalism has several advantages for nanoscale studies because it is based on a quantum mechanical approach. Through a NEGF approach the problem is solved from a wave based point of view opposed to a particle based point of view allowing quantum effects such as tunneling to be captured without special treatment or quantum modifications.

The adaption of NEGF used from previous research [6, 7] of nanoscale thermoelectric materials was readily straight forward. The NEGF method in the context of electronic transport is a self-consistent field (SCF) approach in which Schrödinger's equation and Poisson's equation are solved self consistently. Schrödinger's equation solves the electron spatial probabilities while Poisson's equation maintains the many electron interaction. Care has been taken to use an Anderson mixing technique opposed to a simple mixing technique to reach a less computational intensive convergence. The NEGF formalism has been well documented over the years and is slightly out of the scope of this paper, but can be found in referenced microelectronic articles [8, 9].

Modifications have been made to the NEGF model to allow FED to be studied. The first modification from microelectric bilayer device models is the addition of a third material which captures the effects of the palladium plate. Second, the conduction band of the diamond was determined based on the reference of the Fermi level (0.1eV) and the vacuum level with the associated work function for each material. Additionally, the palladium CB was determined from the work function and vacuum level.

The code begins by constructing an effective mass Hamiltonian matrix that describes the band structure of the device. Particular emphasis is taken in describing the band structure of the emitter (crystalline diamond material) and the ultra-high vacuum (UHV) region. In addition to assembling the Hamiltonian, a spatially varying dielectric field is constructed that is described by the permittivity of the emitter and collector. The Hamiltonian description is used in the Green's function to calculate the space charge effects while the permittivity is used in Poisson's equation to calculate the potential. Lastly, the Green's function is assembled through a composite manner where broadening effect from the device contacts and the device channel are coupled together. The boundary condition at either contact are specified with a Fermi functions at a prescribed temperature, applied bias and in-scattering or broadening term. The remaining two boundaries on the lateral sides of the domain are assumed periodic and are handled through reflective boundary terms in the matrix.

The current voltage characteristics were determined by specifying a voltage bias between the emitter and collector and calculating the corresponding current transmission. The code calculates the transmission for a range of electron energies at a given sub-band energy. One can think of this as solving an elementary quantum barrier structure for a range of electron energies and barrier heights, with the added complexities of a two dimensional wave equation and a more complicated geometry. The integral of these transmission probabilities times the difference in Fermi functions at either contact times the quantum conductance give the current through the device. This approach of calculating the one electron ballistic current is often referred to as the Landaur formalism.

Once the current voltage characteristics are known, the

TABLE 1: Material Parameters

Part	Material	Effective Mass, m^* []	Relative Permittivity, ϵ []	Work Function, ϕ [eV]
Emitter	Crystalline Diamond (001)	$0.54m_e$	5.5^\dagger	$4.6^{\dagger\dagger}$
Medium	Ultra High Vacuum (UHV)	m_e	1	-
Collector	Palladium	m_e	1	$5.4^{\dagger\dagger\dagger}$

TABLE 2: Material parameters for the NEGF computation. Work function values are referenced from a Fermi level of 0.1eV. (Sources: \dagger - [3], $\dagger\dagger$ - [4], $\dagger\dagger\dagger$ - [5])

Fowler-Nordheim (FN) relationship, Equation 1 can be applied. Where $K_1 = 1.541434 \times 10^{-6} AeVV^{-2}$ and $K_2 = 6.830888 \times 10^{-9} eV^{-3/2} Vm^{-1}$ are constants, ϕ is the work function, E is the electric field, A is the area, I is the current, and β is a geometric enhancement factor. The FN curve is a relationship that was derived to describe the emission performance of metal field emitters. The standard physical assumption to the Fowler-Nordheim equation can be found in several cited references [10]. These assumption however have been shown not to capture the emission of nanoscale field emission which is of interest in this research.

$$I = \frac{AK_1\beta^2E^2}{\phi} \exp \frac{K_2\phi^{3/2}}{\beta E} \quad (1)$$

Since the geometry of interest in this research has a small radius of curvature a field enhancement factor, β , is incorporated in the FN relation. It will be shown later that the FN relation will be a factor of both the area of emission and the field enhancement.

Analytic Model

An analytic model was devised that is based on the standard Fowler-Nordheim relationship of Equation 1. The model uses a finite volume method to determine the potential field between the emitter surface and the collector surface. The potential was calculated using a second order finite difference scheme paying particular attention to the geometry of the emitter (same square tip geometry model using NEGF). The model starts by solving the Laplace equation to determine the potential within the vacuum. Then the electric field near the surface was determined through Gauss's law which states that the electric field is proportional to the derivative of the potential. It is from this electric field at the surface of the emitter that a discretized Fowler-Nordheim approach can be applied which calculates the emission current for each discretized cell along the emitter surface. When calculating the current of each cell the field enhancement is assumed unity because they are effectively flat plate. Integration of discretized FN current is carried out for a range of applied potential in order to determine the overall IV characteristics. It is from these

IV characteristics Equation 2 is fit with incorporation of a field enhancement factor, β , and an effective area, A_{eff} as the free parameters. As will be shown in the following paragraph this approach is valid for determining the low current regime of field emission and gives some validity to the NEGF solution.

RESULTS

IV Characteristics

Initially, the IV characteristics were studied for a range of devices to determine if the correct trends were apparent. It is understood from other studies [1, 2, 4, 11] that field emission from semiconductor material is slightly different but you still see the classic turn on voltage or field as a metal field emitter. Indeed, as depicted in Figure 2 we see that as the field approaches $4 \cdot 10^7 V/cm$ we see the current density increase exponentially. Giving confidence that the NEGF code is modeling a field emission type behavior. This exponential increase in current is what provides the ability to plot the Fowler-Nordheim relation resulting in a linear fit which as we will see is not necessarily true for nanoscale emitters.

Nanoscale Fowler-Nordheim Curve

Kang [1] has shown experimentally from the FN curve of lateral field emission devices that the curve is comprised of two regions. He suggests the lower slope corresponds to the low emission current regime and the steeper slope corresponds to the high emission current regime [1]. He goes on to suggest the low current regime is a result of some emitters within the array having a more blunt tip resulting in a larger effective emission area acting in the low emission regime. While the remaining tips have a sharper tip acting in the high current regime. By analyzing a comparable $4nm$ nano tip emitter using NEGF a plot of the FN curve was derived which shows that the two regions are inherent to the physics and not a results of the bluntness.

Figure 3 depicts three distinct regions where two of the regions correspond to the high and low current regimes as recognized in Kang's [1] experimental devices. The third region, labeled region one in Figure 3 is a result of electron saturation at

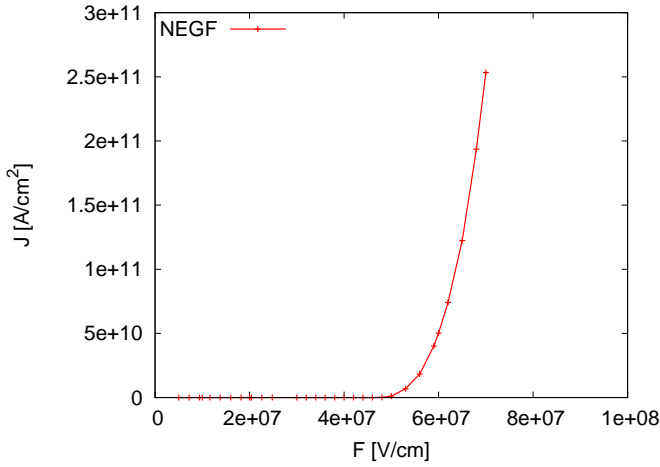


FIGURE 2: Plot of the current voltage characteristics of a 4nm diamond tip emitter. Modeling of an experimental diamond lateral nanotip emitter [1].

the tip. This saturation of the current is a result of a finite number of states near the surface of the tip. As these states become occupied and a large charge built up due to space charge effects, saturation of the current causes a decrease in emission current. It seems Kang did not increase the voltage high enough to see a saturation of the current in the FN curve.

The regions labeled two and three in Figure 3 are not as well understood at this time and require additional investigation. However, it can be certain that these high and low current regions of the FN curve are a function of the electron physics and not a function of two different tip geometries as pointed out by Kang [1]. It may be true that the slope of these lines are affected by the radius of curvature of the tips.

It was determined that in order to fit the FN curve to the Equation 1 an additional parameter termed the effective area, A_{eff} was required. This can be reasoned intuitively by arguing that the true area of emission at the tip is not known. The modified FN relation is as follows with an effective area parameter.

$$\ln\left(\frac{I}{E^2}\right) = \ln\left(\frac{A_{eff}AK_1\beta^2}{\phi}\right) - \frac{K_2\phi^{3/2}}{\beta E} \quad (2)$$

As is seen in Figure 3 and outlined in Table 4 both the field enhancement factor and the effective area of emission are function of the emission. Equation 2 was initially fit with just a field enhancement factor, β , however it didn't capture the trends of the curve. The trends suggest that as the applied field is increased the area of the emission increases and the geometric influence is decreased. Essentially, the area in which electrons are injected into the vacuum is getting larger.

TABLE 3: Material Parameters

Model	β	Effective Area, A_{eff}
HFE	0.814	1.874×10^{14}
LFE	5.98	8.324×10^{-1}
Analytic	30.2	9.644×10^{-5}

TABLE 4: Values of field enhancement factor, β , and effective area, A_{eff} , for a 4nm emitter. $A = 5.5 \times 10^{-7}cm$. These values correspond to Figure 3. HFE corresponds to the high field emission and LFE corresponds to the low field emission regime.

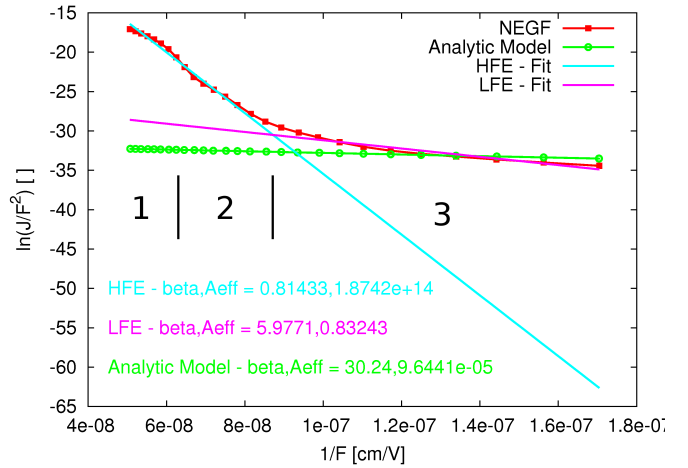


FIGURE 3: Plot of a 4nm tip diamond emission with a bias range from 0V to 9V. A high and low field emission regime exist that is apparent in experimental data as well as NEGF simulations.

Surface States

As alluded to in the explanation of the current saturation in region one of Figure 2, the surface states and states within the tip control the emission properties. In the analytic treatment of field emission the local density of states (LDOS) or the total available states is often calculated using a simple scalar addition of states within the tip plus the states of the surface [12]. This theory has been applied to absorbents and other surface treatments to increase the emission performance. However, when dealing with semiconductor type material there are additional effects that change the band structure. One of the additional effects that will turn out to be critical in capturing is the band bending within the nano tip. The theory of band bending is well understood in the microelectronic community and is a result of the charge distribution in the device. This same theory of band bending is present in field emission and thus the self-consistent NEGF model is a good candidate to capture the physics.

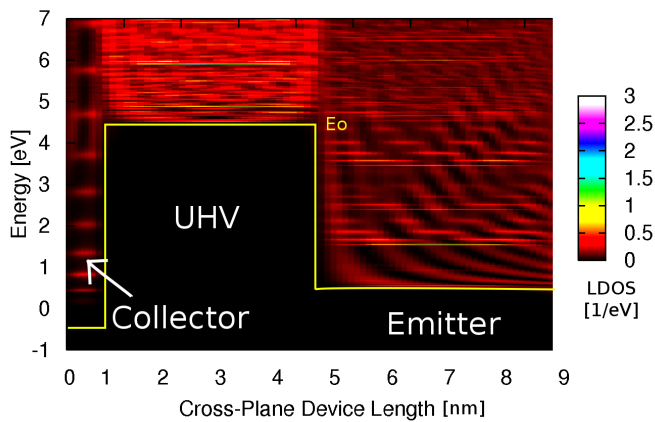


FIGURE 4: Plot of the local density of available states (LDOS) in a 4nm tip diamond emitter calculated from the NEGF code. The band bending modifies the LDOS within the emitter near the tip. The emitter is left facing from the right boundary.

In the absence of surface treatments we used the NEGF method to determine the local density of states of the actual structure. The LDOS is a result of the difference between the advancing and retarding Green's functions and is integrated over each sub-band level. The resulting plot for a 4nm tip device is shown in Figure 4 with the CB outlined in yellow. Band bending is apparent from the upward sweeping localized states near the tip. Another interesting artifact of quantum simulation is the wave like appearance of the density of states attributed to the wave nature of the fermions. It is also worth recognizing that the vacuum level is labeled in the plot and these states that lie below this level in the emitter are a result of tunneling electrons, which controls the field emitters performance.

Peak Emission Energy

The topic of where exactly the field emission electrons are emitted in the diamond emitters has been a on-going topic. Recent experimental research [13] has shown that a strong peak in the emission lies around the Fermi level for both an undoped "natural" diamond and a lightly doped diamond emitter. In accordance with these experimental results the NEGF supports results that suggest majority of the current is derived from the tunneling of electrons near the Fermi level (0.1eV). Figure 5 is a plot of the normalized current verse energy for both the emitter and collector under a 1V bias. There is a strong peak at 0.1eV suggesting that indeed the current is a result of tunneling electrons emitted from the diamond material near the Fermi level.

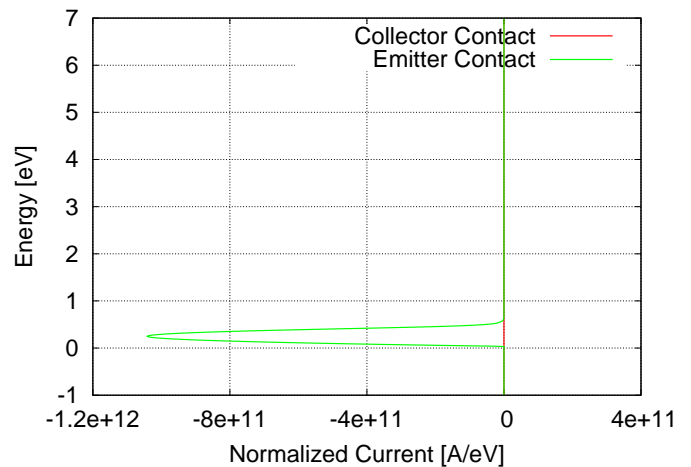


FIGURE 5: Plot of the normalized current shows that majority of the transmission current is a results of tunneling electrons near the conduction band edge of the diamond emitter. A bias of 9V is applied

CONCLUSIONS

It was shown that NEGF method is a viable way to model field emission of nano tip field emitter and the experimental trends can be reproduced. Furthermore, it was determined that two independent parameters were required to fit the Fowler-Nordheim relation. Those two parameters were a field enhancement factor, β , and a effective area, A_{eff} . In comparison to Kang's [1] experimental data, the high current and low current regime were a result of the inherit physics and not the bluntness of experimental emitters as suggested. The effective area of emission was determined to increase considerably while geometric enhancement decreased when a large potential was applied. Further investigation of the sensitivity of the two current regimes as a function of emitter thickness is of interest.

REFERENCES

- [1] Kang, W., Davidson, J., Wisitsora-At, A., Wong, Y., Takalkar, R., Holmes, K., and Kerns, D., 2004. "Diamond vacuum field emission devices". *Diamond and Related Materials*, **13**(11-12), NOV-DEC, pp. 1944–1948.
- [2] Yamada, T., Hwang, D., Vinod, P., Makino, T., and Fujimori, N., 2005. "Characterization of field emission from nano-scale diamond tip arrays". *Japanese Journal of Applied Physics Part 2-Letters & Express Letters*, **44**(12-15), pp. L385–L387.
- [3] Kittel, C., 1986. *Introduction to Solid State Physics*, 6th ed. Wiley, New York.
- [4] Robertson, J., 1999. "Mechanics of electron field emission from diamond, diamond-like carbon and nanostruc-

- tered carbon”. *Journal of Vacuum Science and Technology B*, **17**(2), Mar., pp. 659–665.
- [5] Lide, D. R., 2007. *CRC Handbook of Chemistry and Physics, 88th Edition (Crc Handbook of Chemistry and Physics)*. CRC, June.
- [6] Bulusu, A., and Walker, D. G., 2007. “Modeling of thermoelectric properties of semiconductor thin films with quantum and scattering effects”. *Journal of Heat Transfer*, **129**(4), Apr., pp. 492–499.
- [7] Musho, T. D., and Walker, D. G., 2009. “Quantum transport properties in nanocrystalline composites for thermoelectric devices”. In ASME/Pacific Rim Technical Conference and Exhibition on Integration and Packaging of MEMS, NEMS and Electronic Systems, IPACK2009-89332.
- [8] Bulusu, A., and Walker, D. G., 2008. “One-dimensional thin-film phonon transport with generation”. *Microelectronics Journal*, **39**(7), July, pp. 950–956.
- [9] Datta, S., 2005. *Quantum Transport: Atom to Transistor*. Cambridge University Press, New York.
- [10] Forbes, R. G., 1999. “Refining the application of fowler-nordheim theory”. *Ultramicroscopy*, **79**(1-4), pp. 11 – 23.
- [11] Chen, J., Xu, N., Deng, S., She, J., and Chen, J., 2003. “Effects of the interface and surface nanostructures on field emission of amorphous diamond film”. *Journal of Vacuum Science & Technology B*, **21**(1), Jan-Feb, pp. 581–586.
- [12] Modinos, A., 1984. *Field, thermionic, and secondary electron emission spectroscopy*. Plenum Press.
- [13] Yamaguchi, H., Kudo, Y., Masuzawa, T., Kudo, M., Yamada, T., Takakuwa, Y., and Okano, K., 2008. “Combined x-ray photoelectron spectroscopy/ultraviolet photoelectron spectroscopy/field emission spectroscopy for characterization of electron-emission mechanism of diamond”. *Journal of Vacuum Science & Technology B*, **11**(3-4), pp. 127–139.