NEGF Quantum Simulation of Field Emission Devices

ASME/JSME Thermal Engineering Conference
Honolulu, Hawaii

March 15, 2011

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This work is funded in part by an NSF IGERT

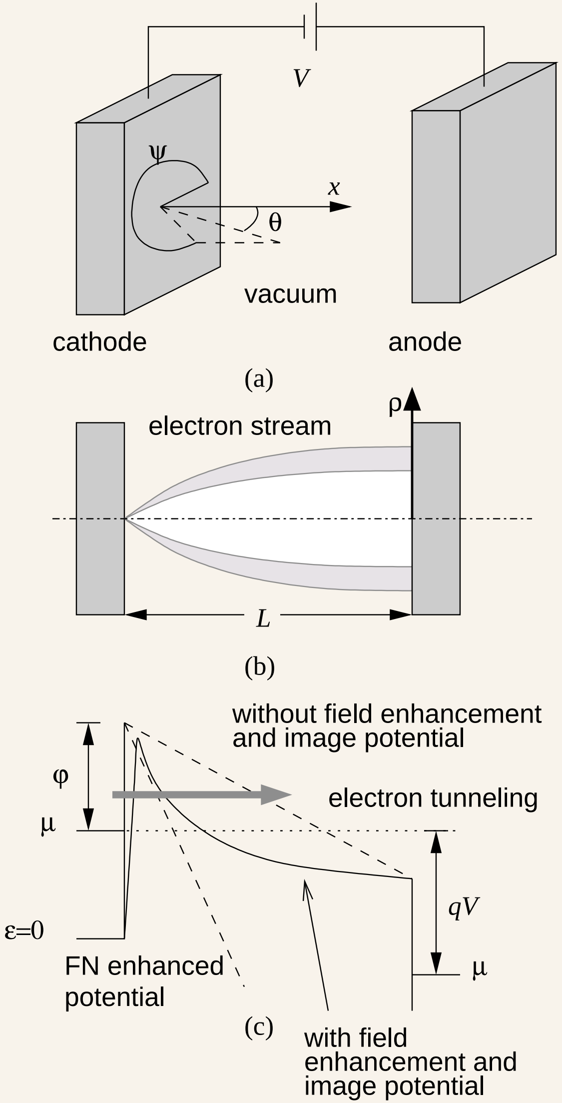
Fowler-Nordheim emission

- Derived from quantum mechanics using the WKB approximation

$$I = A_{\text{eff}} K_1 \frac{(\beta F)^2}{\phi} \exp\left(-\frac{K_2 \phi^{3/2}}{\beta F}\right)$$

- Limitations:
  - metals only
  - absolute zero degrees
    - Richardson's equation for thermionic emission
  - flat surfaces
    - geometric enhancement factor β artificially increases the local field
  - Local effects: adsorbates on surface, grain boundaries, non-uniform emission area, work function variations, ...
  - uncertainty in parameters
- Benefits: Data plotted in Fowler-Nordheim coordinates are often linear

Emission model

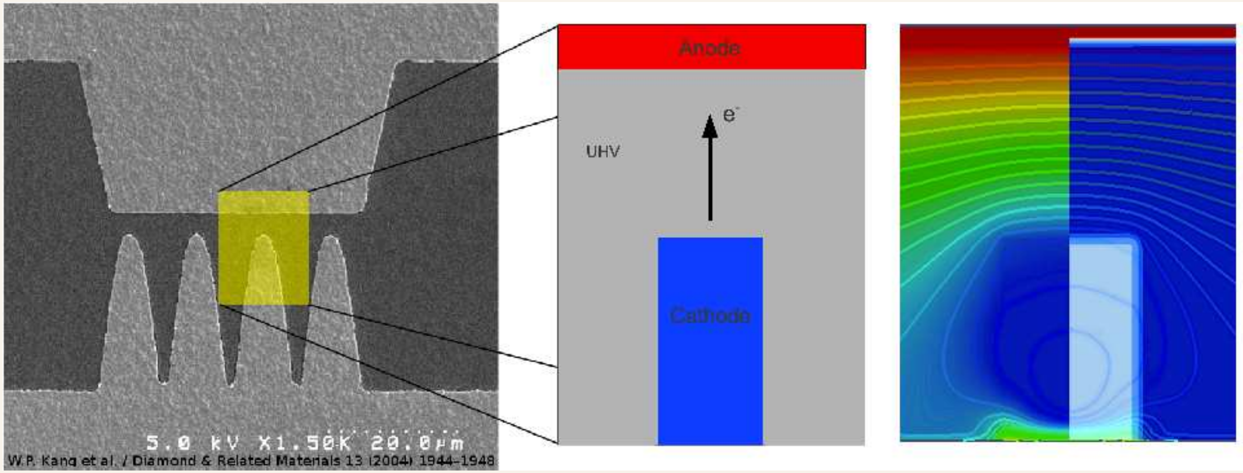


- Unenhanced potential (flat surface) is simply qV
- Enhanced FN potential is βqV
  - does not satisfy anode boundary condition
  - does not include image potential
  - does not have appropriate curvature
- more physical potentials have been developed to include local enhancement and image potential
- We will solve it numerically

Methodology

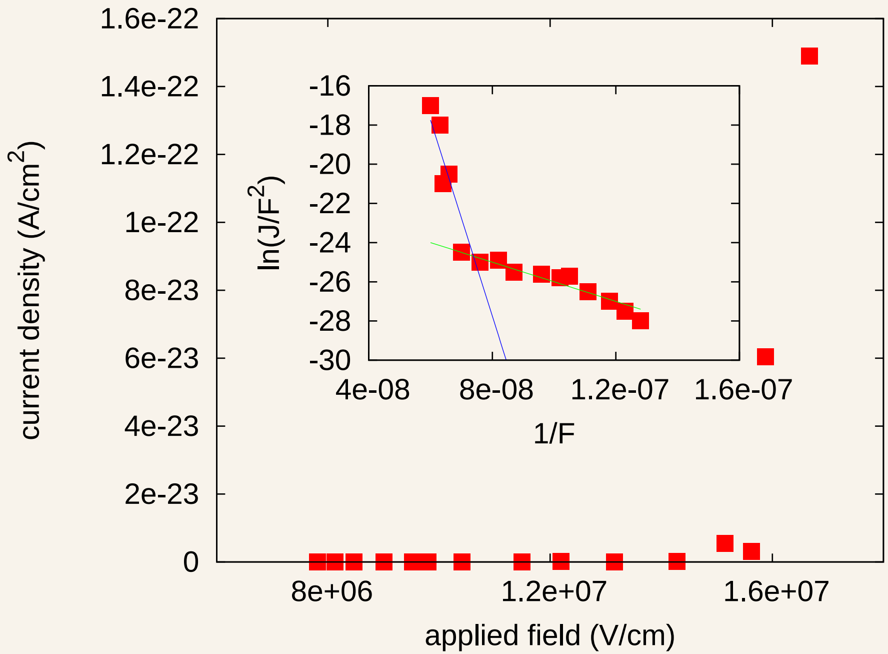
- Three mathematical models
  - Use non-equilibirum Green's function to determine ballistic electron transport
  - Discretized Fowler-Nordheim approach (no geometric enhancement)
  - Standard Fowler-Nordheim with geometric enhancement

- Device model



  - diamond emitter ($4\,\mathrm{nm}$ dimater), lightly doped ($N_d = 10^{14}\,\mathrm{cm}^3$); palladium anode; band in vacuum is determined by the work function

Double exponential



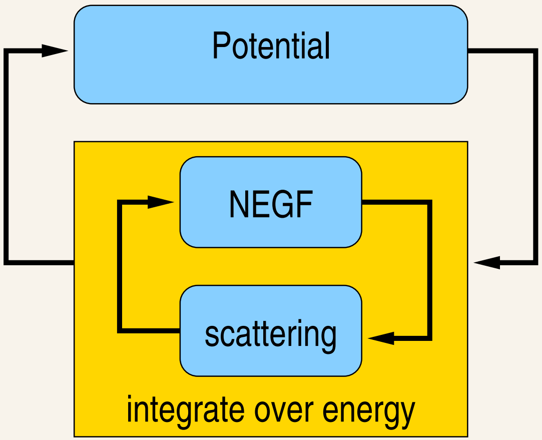
NEGF model

Governing equation $$[H+U]\Psi(\mathbf{r}) = \varepsilon_\alpha \Psi_\alpha(\mathbf{r})$$

Green's function $$[G(E)] = [(E+i0^+)I - H - \Sigma_1 - \Sigma_2 - \Sigma_S(E)]^{-1}$$

Density of States $$[A(E)] = 2\pi i([G(E)] - [G(E)]^+)$$

Density matrix $$[\rho] = \int_{-\infty}^{\infty} F_0(E-\mu)[A(E)]\,dE$$

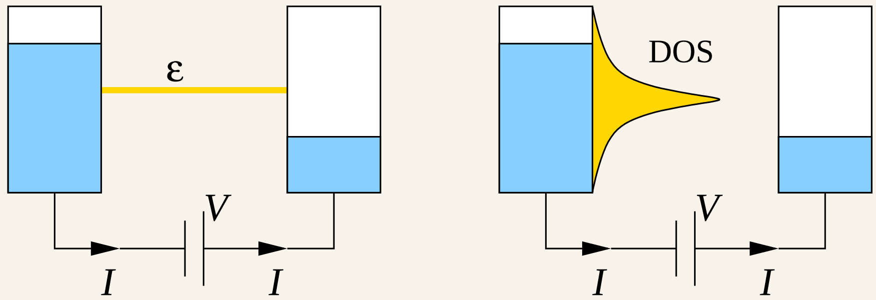


- Computational cost is in the inversion and in the integration
- integration loop is easily parallelizable

- Self-energy term $\Sigma_S(E)$ is derived from Fermi's golden rule, for example
- Transport is difference between incoming and outgoing quantities

More on NEGF

Isolated channel — Level broadening



- Broadening of energy density of states near source and drain contacts leads to restricted current flow.

- NEGF method does not require a statistical distribution of carriers within the device, so not restricted to near equilibrium.
- Can be used to solve extreme non-equilibrium problems

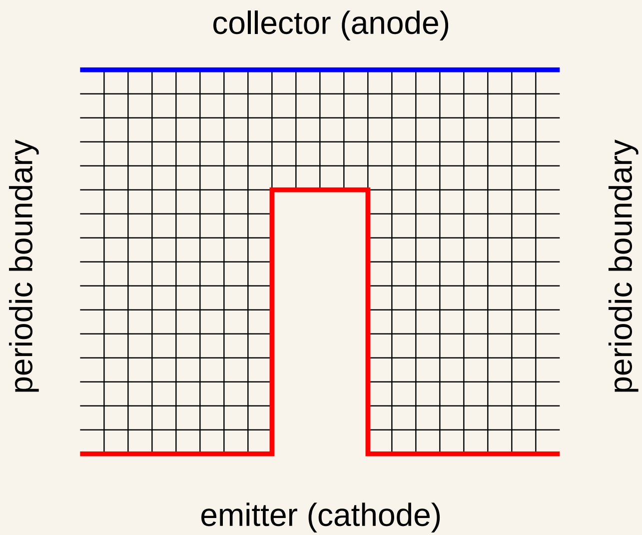
$$E_{2D} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{d_z}\right)^2$$

$$E_{1D} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2}{2m^*}\left(\frac{m\pi}{dy}\right)^2 + \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{d_z}\right)^2$$

- Fermi functions are dependent on confined dispersions

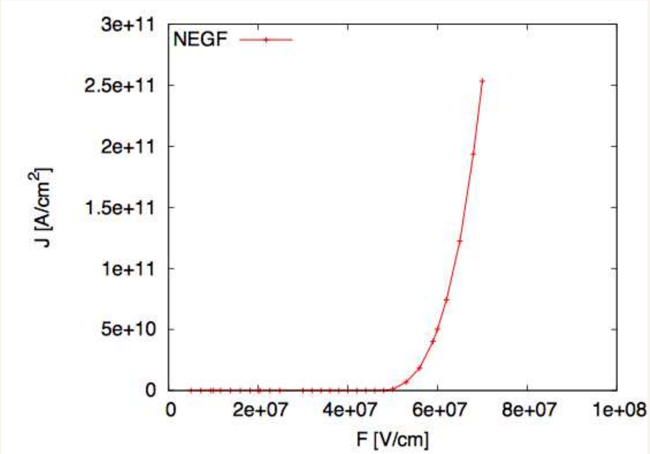
$$f_{2D}(E_{2D}) \quad f_{1D}(E_{1D})$$

Potential plus FN

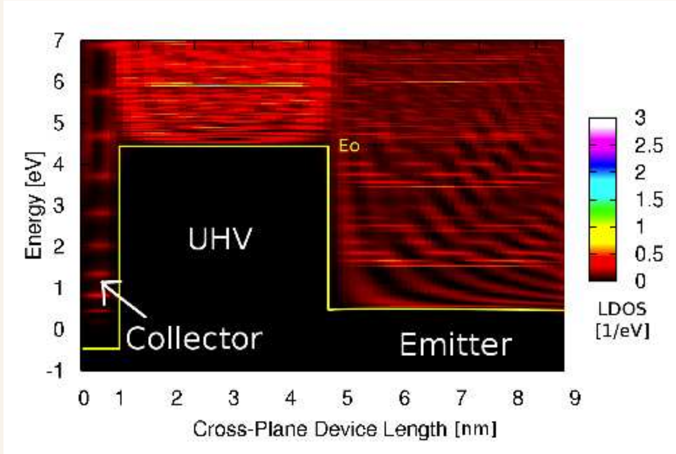


- At each element, Fowler-Nordheim is used without enhancement to estimate the local current.
- The contribution from every element on the tip is added to get the overall current

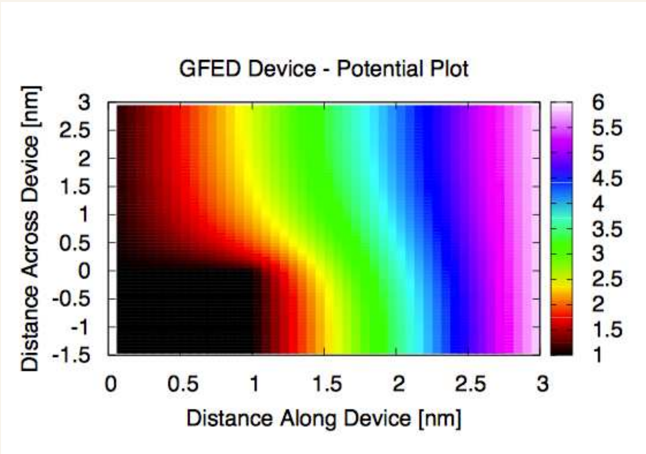
Results



(a)



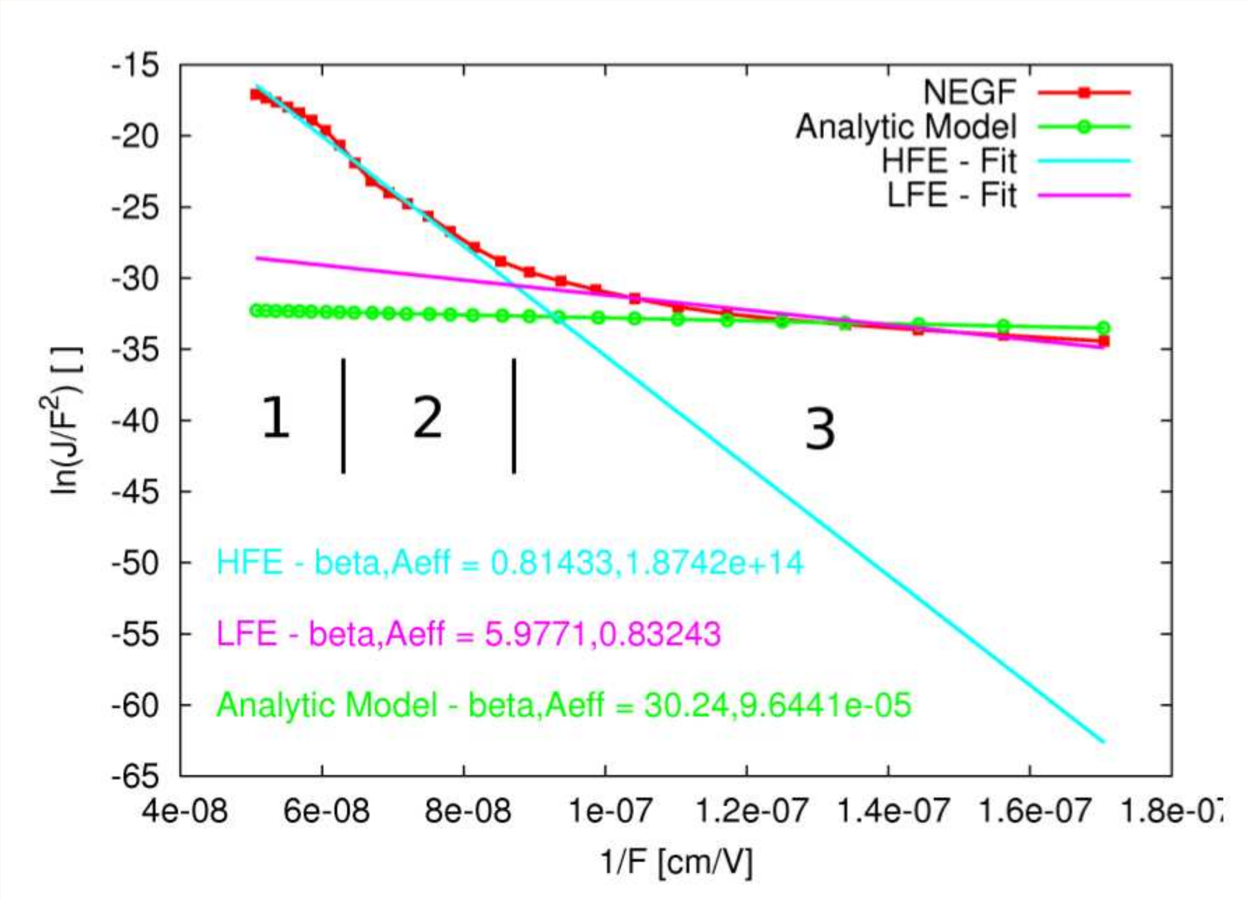
(b)



(c)

- (a) Current from FN model with enhancement
- (b) NEGF density of states
- (c) potential from discretized model

Results



- work function was held constant for all models

Summary

- Green's function approach naturally captures the double exponential, but we are not sure of the origin of this artifact.
- Green's function also possibly captures Child-Langmuir transport
- The discretized FN does not capture the total emission very well.
  - possibly due to grid independence (we can solve the potential with good accuracy, but can not capture the field easily).