A Simulation of the Dynamics of Electron Emission from Nanowires

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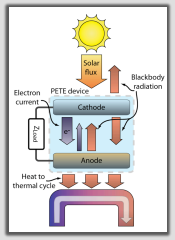
Abstract

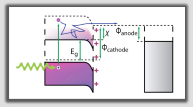
An hour's worth of the solar radiation striking the earth's surface would power the world for a year. The Photon-Enhanced Thermionic Emission (PETE) solar energy converter uses a hybrid photoemission and thermionic emission process to convert solar radiation into usable energy more efficiently than existing energy harvesting techniques. Unlike traditional photovoltaic cells, PETE can operate at high temperatures, allowing it to serve as an efficiency-boosting solar thermal topping cycle. Nanostructured materials can greatly enhance the efficiency of optoelectronic devices by maximizing both photon absorption and electron-surface collision frequency. Nanowires, in particular, add significantly to PETE's viability as a source of low-cost, renewable energy. In order to maximize PETE efficiency, we seek to better understand electron transport and emission in semiconductor nanowires. The probabilistic nature of the transport phenomenon lends itself well to stochastic simulation using Monte Carlo methods.

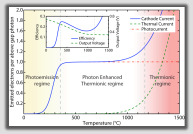
In this model, we characterize electron transport prior to recombination as a sequence of free flight segments punctuated by instantaneous scattering events, which alter the electron's trajectory and determine its final state (momentum) after scattering. Along with surface effects and band-to-band recombination, three primary bulk scattering mechanisms—phonon, ionized impurity, and carrier-carrier—are considered in our simulation of a GaAs nanowire.

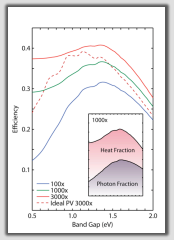
Photon-Enhanced Thermionic Emission (PETE)

A 21st century vacuum device



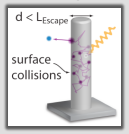


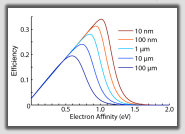




Why nanowires?

- ✧ Maximize photon absorption and electron emission
  - • Near-unity photoabsorption over wide spectral range
  - • 4X more electron-emissive surface collisions than thin film
- ✧ Long minority carrier lifetime (over 50μs ➔ 10^8 surface collisions)





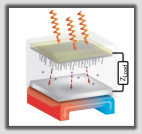
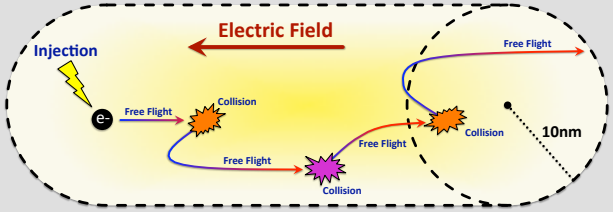
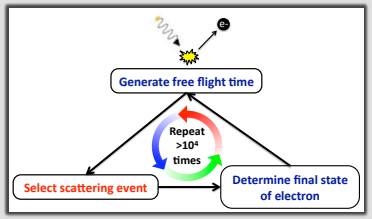
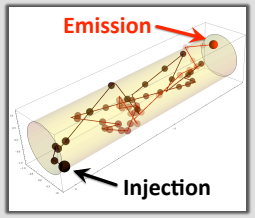


Image Credit: Abengoa Solar (CSP tower); Schwede, Bargatin, Riley, Hardin, Howe, Shen, Melosh (PETE diagrams)

The Monte Carlo Method

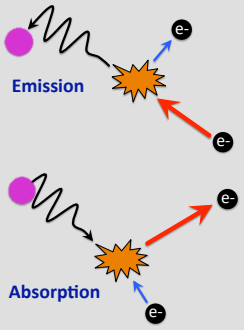


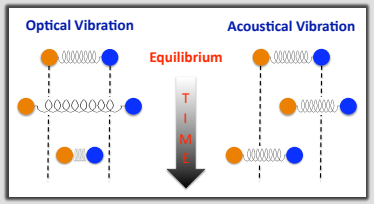


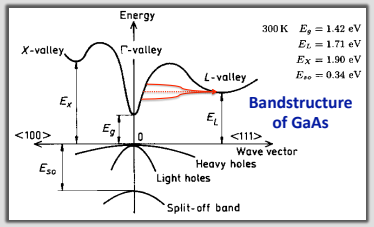


Scattering Mechanisms

Phonon







Ionized Impurity

Electron-Hole

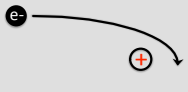
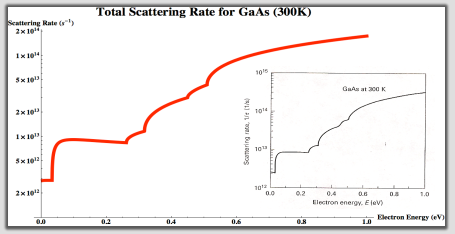


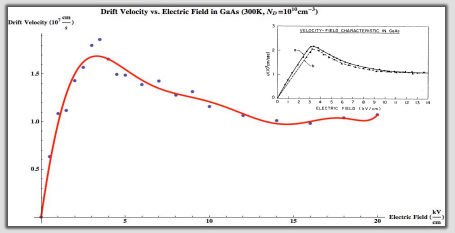
Image Credit: Ioffe Physical Technical Institute NSM Archive (GaAs bandstructure)

Testing the Simulation

Total Scattering Rate at 300K



Negative Differential Resistance (NDR)



Thermal Repopulation

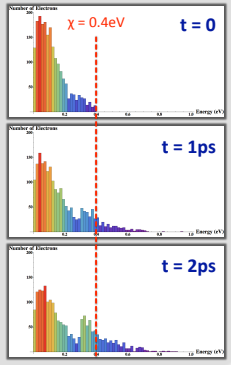
Procedure:

① Generate thermal distribution of electron energies

② Remove electrons with energies above the electron affinity (χ = 0.4eV)

③ Simulate 2000 electron trajectories for 2000 time steps (≈2ps)

④ Observe repopulation of higher electron energy levels due to inelastic scattering mechanisms



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