Modeling of Electron Transport in Thin Films with Quantum and Scattering Effects

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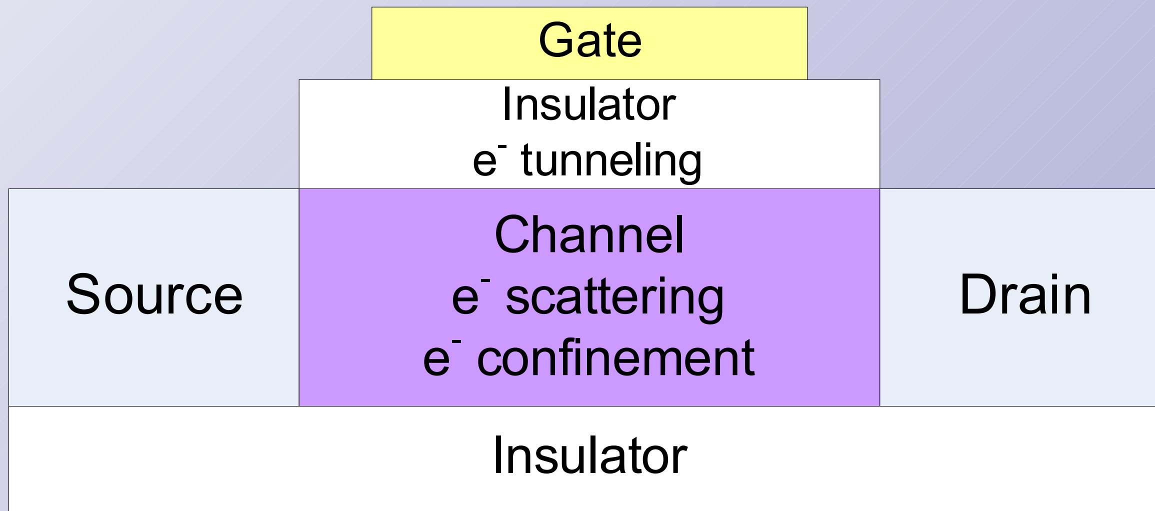
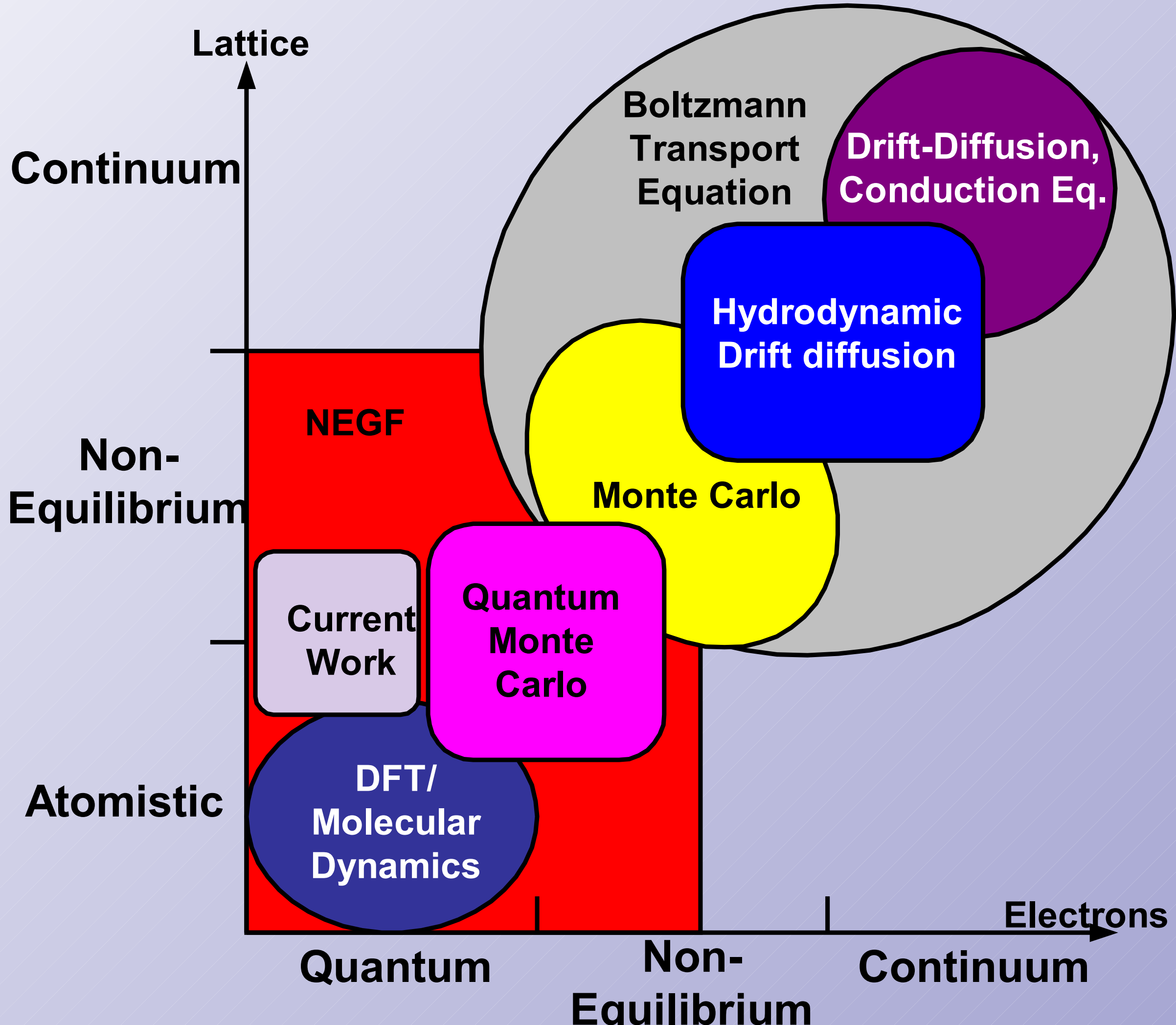
Motivation

- $L_{Device} \approx \lambda_{\text{de Broglie}} \Rightarrow$ quantum and scattering effects cannot be ignored.



- $L_{device} < \iota_r \Rightarrow$ assumption of minimal deviation from local equilibrium no-longer valid $\Rightarrow$ BTE moments cannot be applied to extreme non-equilibrium.
- Increased need for microelectronic device simulation models that incorporate both quantum and scattering effects without being computationally intensive.

Nanoscale Device Models



NEGF: Non-Equilibrium Green's function

Advantages of Non-Equilibrium Green's Function Method

- Incorporation of quantum interference effects such as tunneling and diffraction, not possible through the Boltzmann equation.
- Mathematically accurate approach to include rigorous scattering (electron-phonon scattering, surface scattering etc).
- Eliminates periodic boundary conditions as outgoing waves are planar.
- Multiscale formulation: Can be used to solve atomistic systems to mesoscopic systems.

Non-Equilibrium Green's Function Formalism

Original Schrödinger wave equation

$$\left(H+U\right)\psi_{\alpha}(r)=\varepsilon_{\alpha}\psi_{\alpha}(r)$$

Modified wave equation with self-energy terms

$$\left(H+U+\Sigma_{1}+\Sigma_{2}+\Sigma_{s}\right)\psi_{\alpha}(\vec{r})=\varepsilon_{\alpha}\psi_{\alpha}(\vec{r})$$

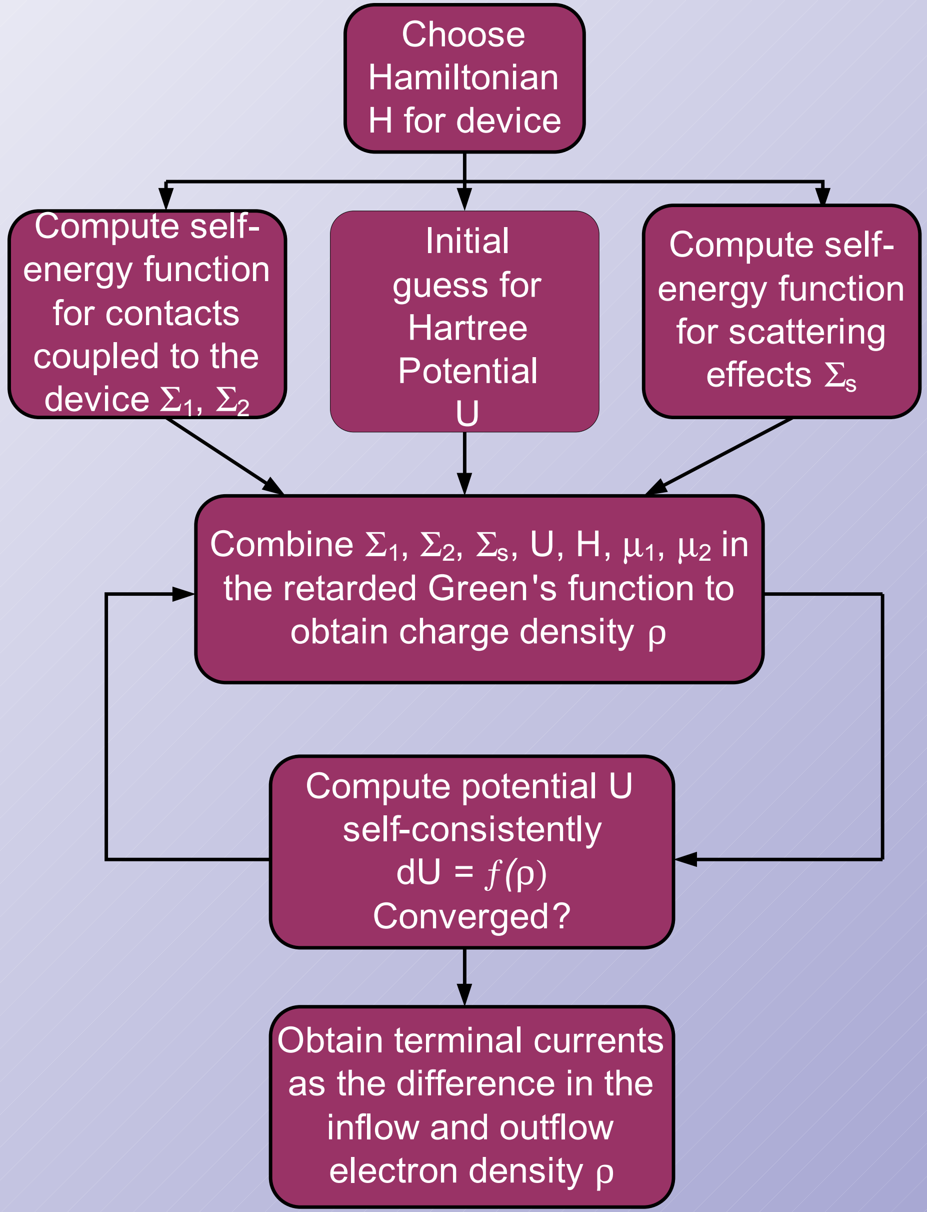
Green's function

$$G(E)=\left[\left(E-i0^{+}\right)I-H-\Sigma_{1}-\Sigma_{2}-\Sigma_{s}\right]^{-1}$$

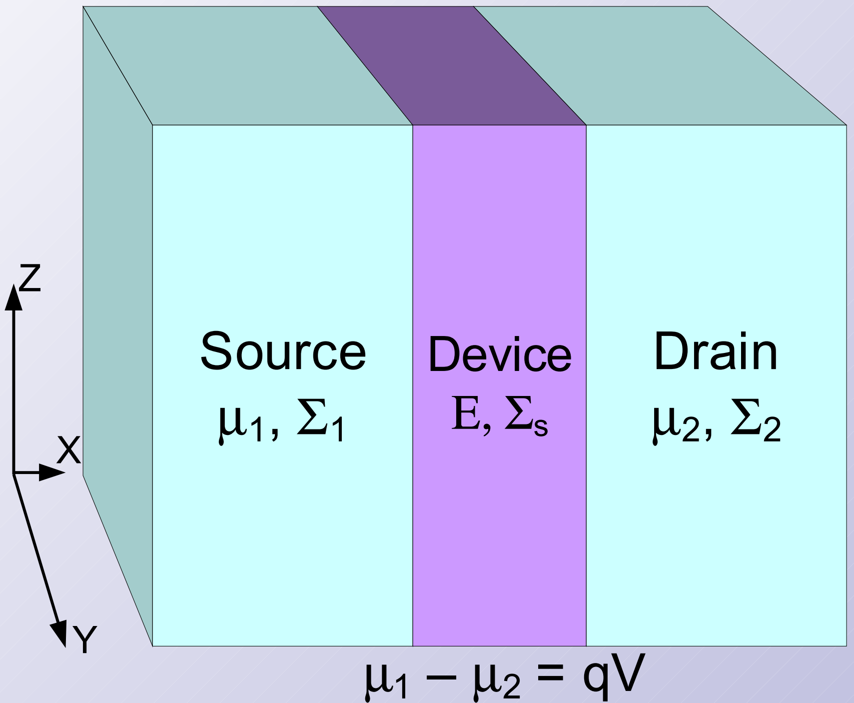
Device Current

$$I_{i}=\frac{-q}{\;}\int_{-\infty}^{+\infty}Trace\left[\Gamma_{i}A\right]f_{i}-Trace\left[\Gamma_{i}G^{n}\right]$$

Nonequilibrium Green's Function Method



Example of a Very-Small Scale Device Problem



2-D nanoresistor connected to source and drain contacts.

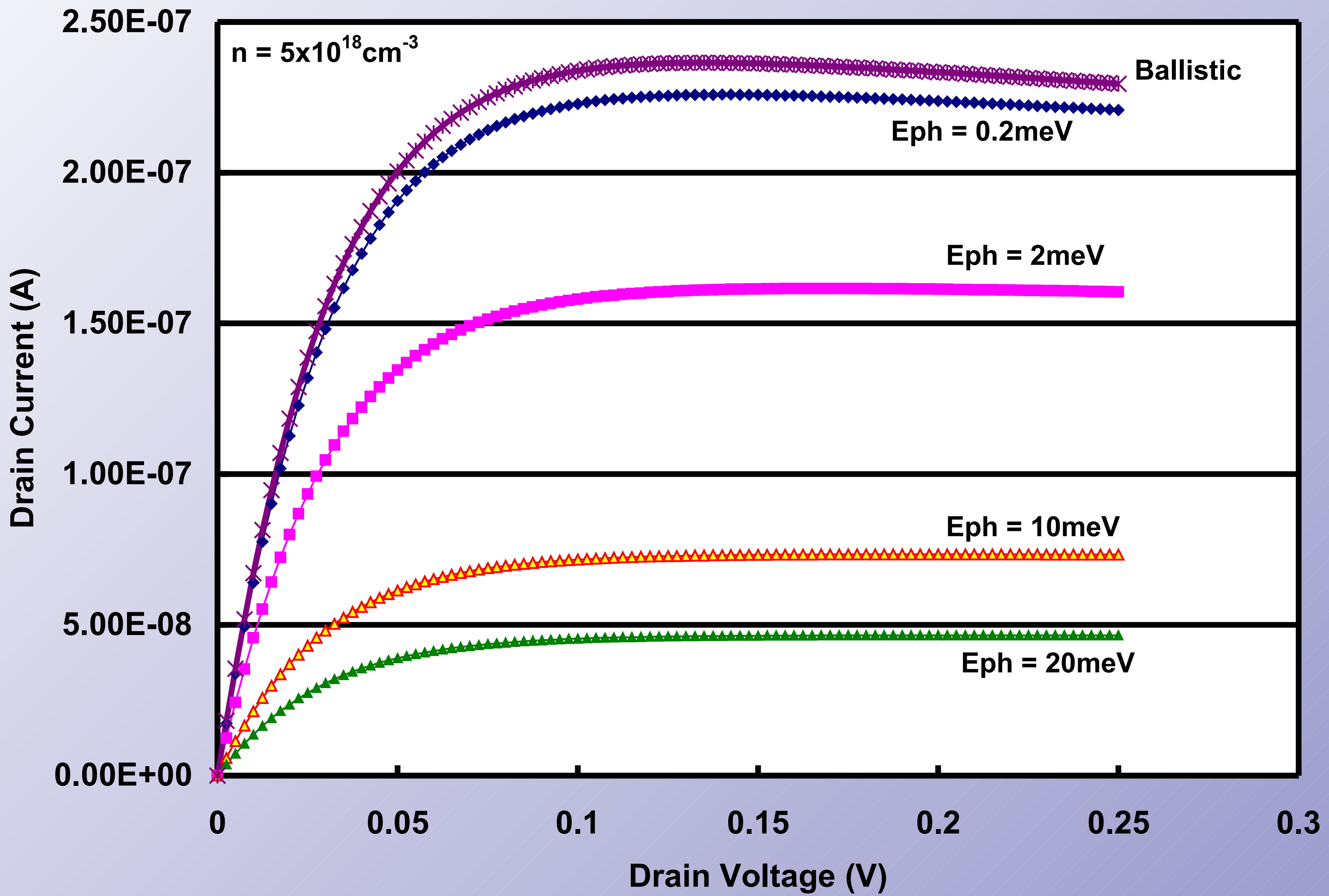
μ 1, μ 2 - source and drain chemical potentials.

Energy states along z-axis are quantized.

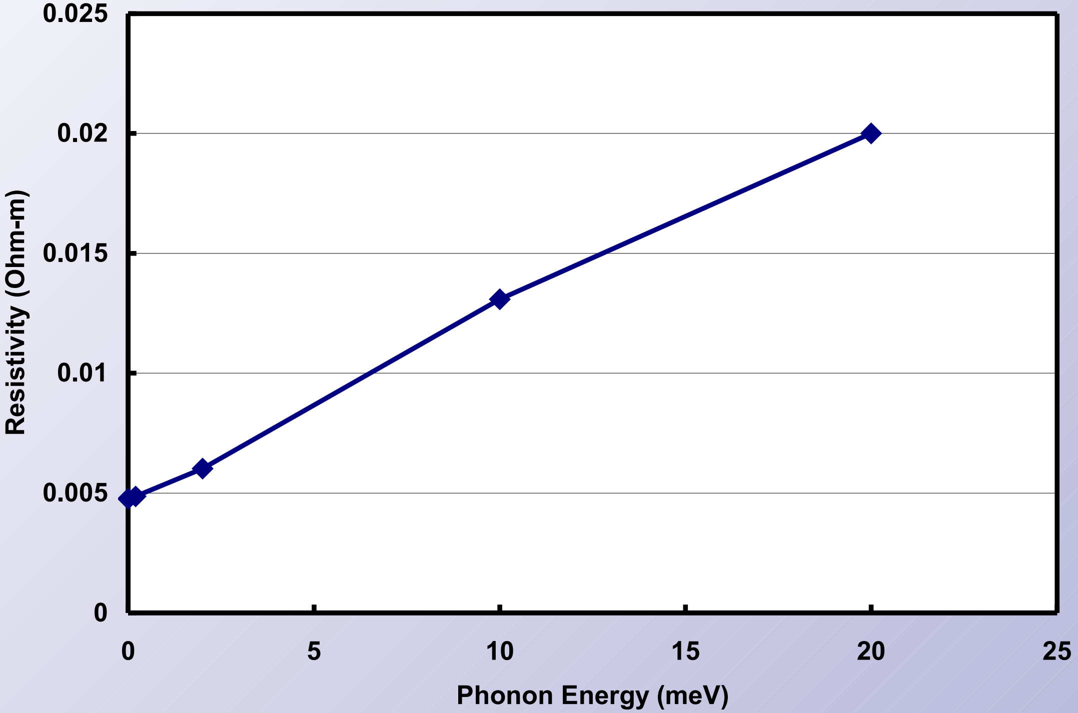
Electron-phonon scattering assumed to be independent of electron energy. e.g. $D_o = 0.1eV^2 \Rightarrow E_{ph} = 20meV$

$$\Sigma_s(E) = D_o G(E)$$

I-V Characteristics of Silicon Thin Films with Incoherent Near-Elastic Scattering



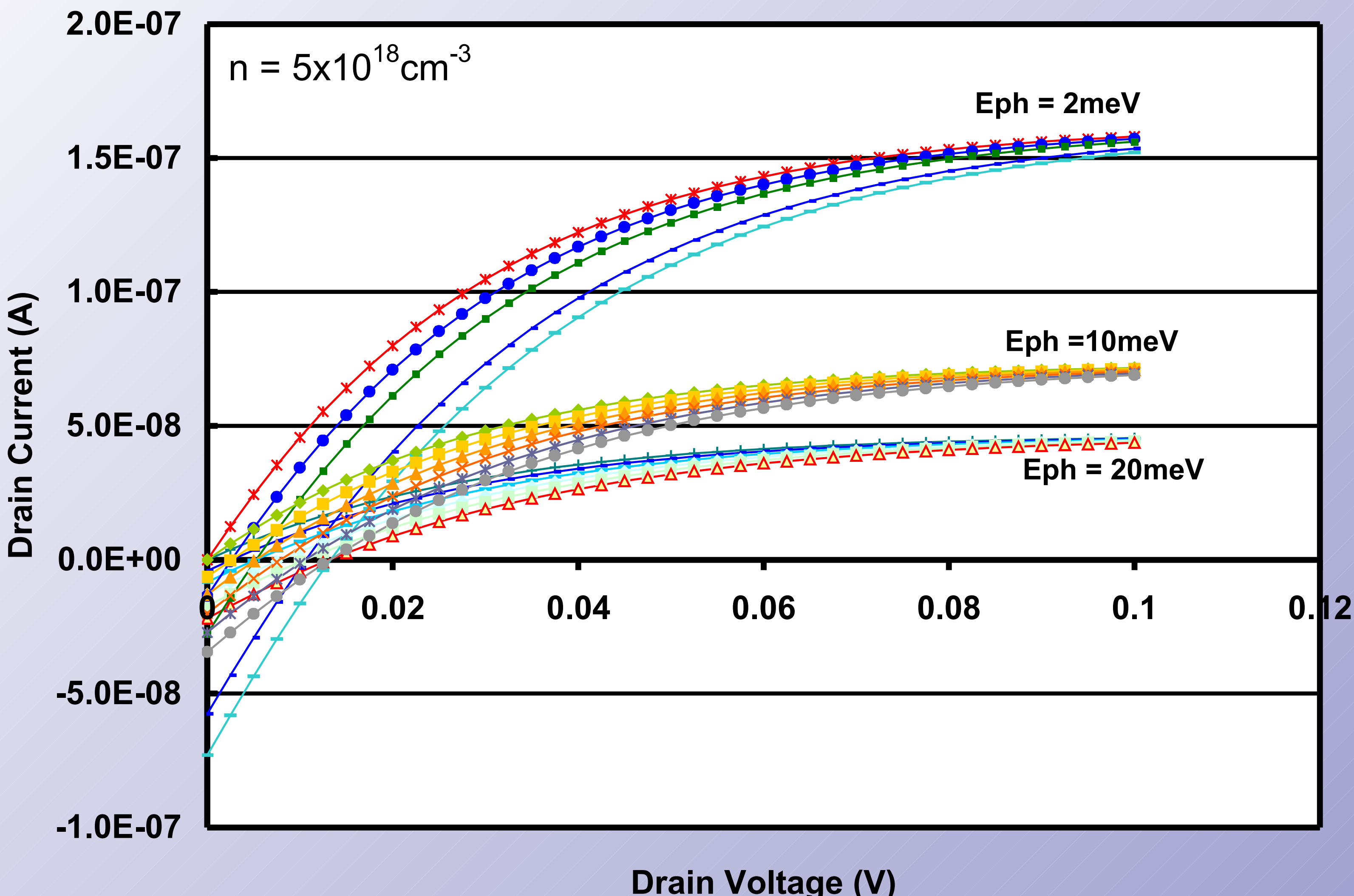
Effective Channel Resistivity with Incoherent Scattering



- **Continuous density of states from source and drain contacts spill over into the channel causing energy level broadening.**
- **Discrete energy states in narrow channel reduce the number of energy states available for the incoming electrons introducing resistance at the contacts.**

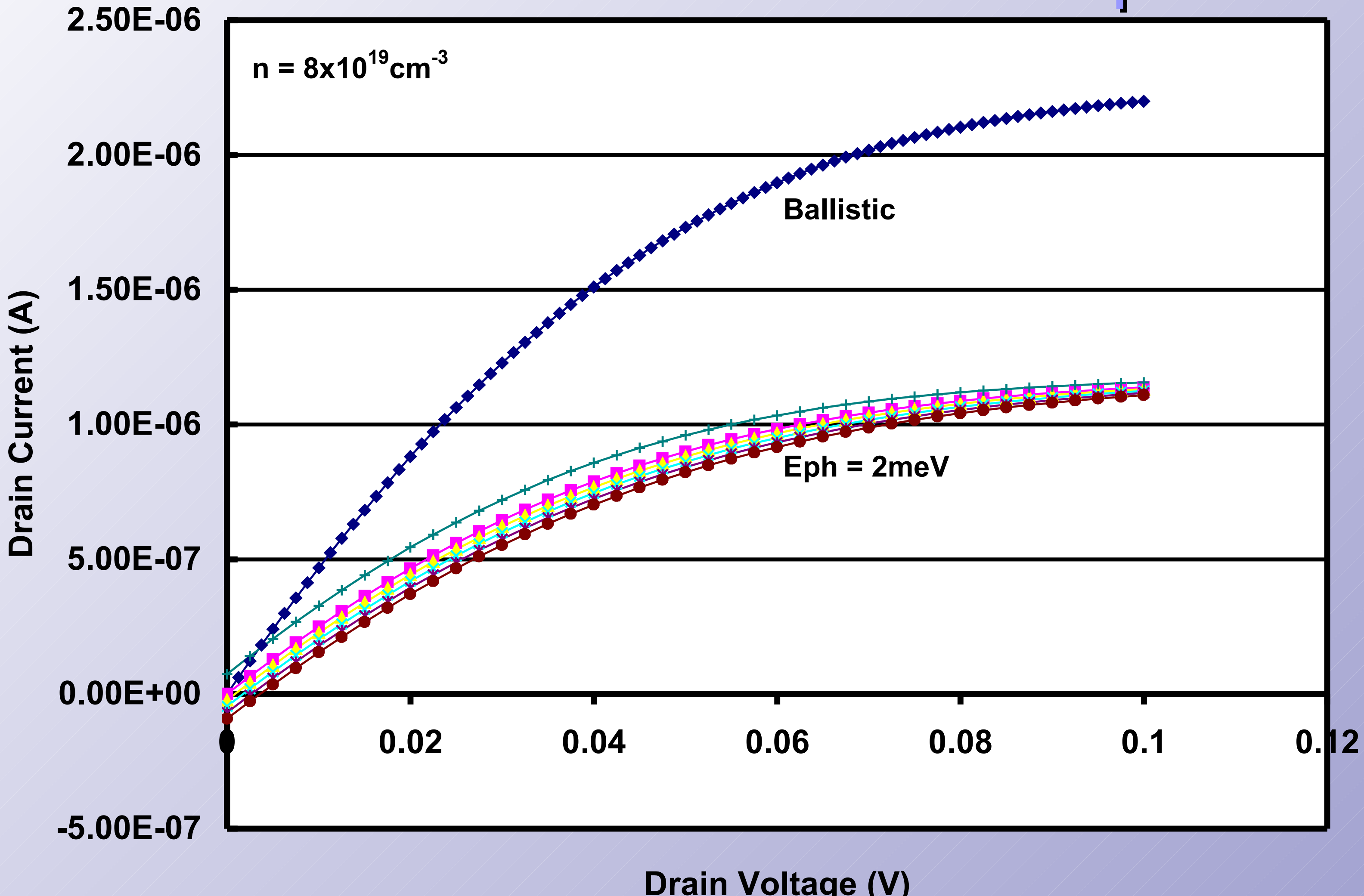
Increase in phonon energy from 0 to 20m eV for various resistors increases corresponding channel resistivity by a factor of 4.

Thermoelectric Properties of Silicon Thin Films



Predicted Seebeck coefficient value of 250μ V/K matches well with experiments. (Geballe, T. H. et.al, *Physical Review*, 98, 4, 1955).

Seebeck Coefficient for SiGe Superlattices



Calculated Seebeck value of 100 μ V/K matched well with experimentally measured values of 312μ V/K **(B.Yang et. al. Applied Physics Letters, 80, 10, 2002).**

Conclusions and Future Work

- The NEGF formalism successfully couples quantum effects with electron-phonon scattering.
- A 33% to 70% drop in channel current was noticed due to near-elastic electron-phonon scattering.
- Predicted Seebeck coefficient values are in good agreement with experiment for Silicon and SiGe superlattices.
- Extension of the present work to include energy-dependent electron-phonon scattering.

Acknowledgements

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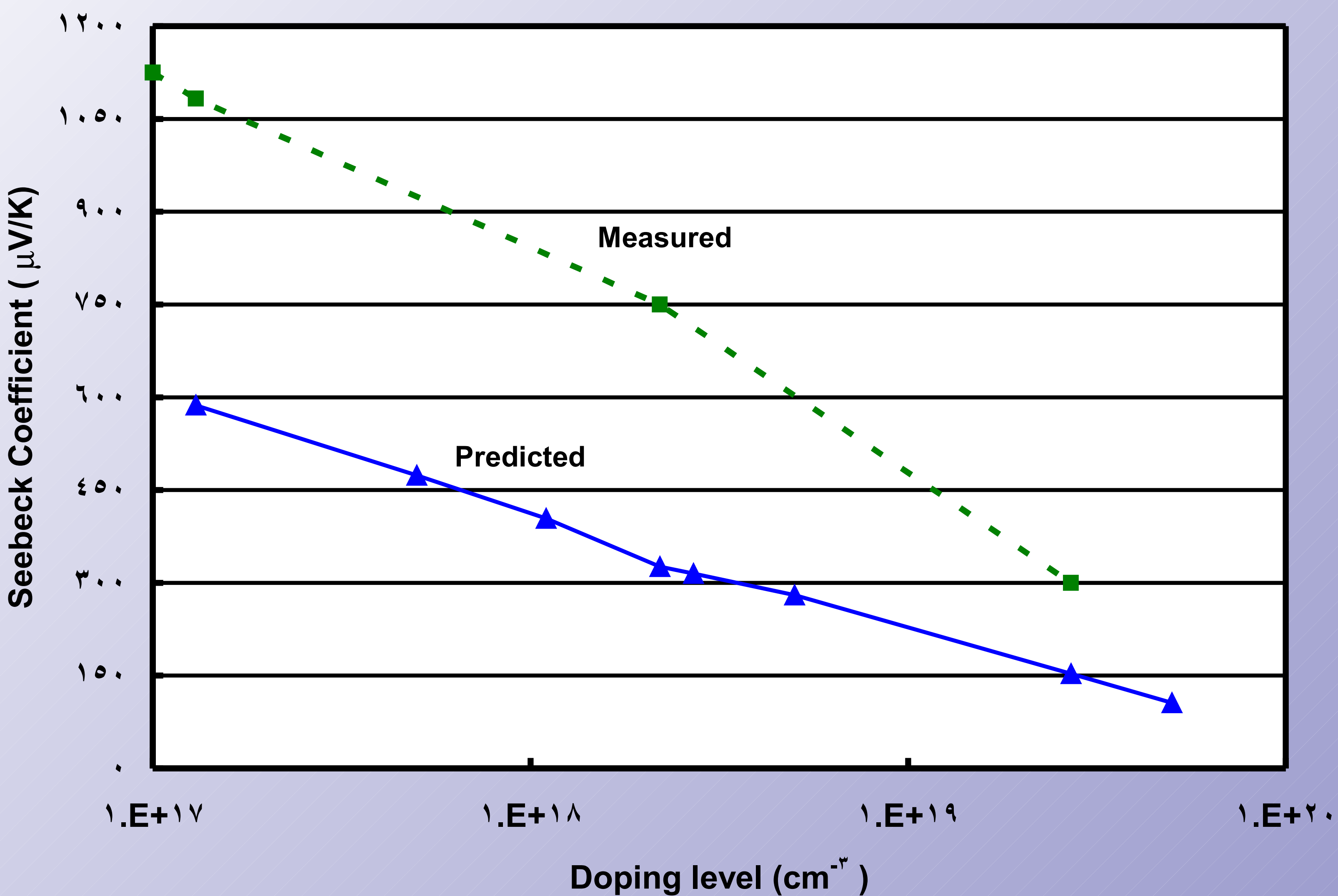
Seebeck Coefficient of Silicon Thin Films

(submitted to Journal of Applied Physics)



Non-Equilibrium Green's Function Formalism

Modified wave equation with self-energy terms

$$\left(H + U + \Sigma_1 + \Sigma_2 + \Sigma_s\right)\psi_\alpha(\vec{r}) = \varepsilon_\alpha \psi_\alpha(\vec{r})$$

Relation between lifetime of the eigen state and self energy

$$\frac{١}{\tau} = \frac{\gamma}{} = -\frac{٢\,\mathrm{Im}\,\Sigma}{}$$

Energy level broadening

$$\Gamma_{1,2,s} = i(\Sigma_{1,2,s} - \Sigma^{+}_{1,2,s}) \quad \Sigma_s(E) = D_o G(E)$$

Green's function

$$G(E) = \left[\left(E - i0^{+}\right)I - H - \Sigma_1 - \Sigma_2 - \Sigma_s\right]^{-1}$$

Spectral function

$$\frac{A(E)}{٢\pi} = D(E) = i\left(G(E) - G^{+}(E)\right) = \frac{\gamma}{\left(E - \varepsilon'\right)^{٢} + (\gamma / ٢)^{٢}}$$

Device Current

$$I_i = \frac{-q}{} \int_{-\infty}^{+\infty} Trace\left[\Gamma_i A\right] f_i - Trace\left[\Gamma_i G^{n}\right]$$