Electronic transport simulations for TE power factor in nanostructures

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General description of our group’s work

Theoretical investigations of:
- electronic
- thermal
- thermoelectric properties

in nanoscale materials and devices
Approach - Tools

**Electronic structure** (atomistic to continuum)
1) Tight-binding (sp$^3$d$^5$s$^*$)
2) Valence Force Fields
3) Force Constants
4) Effective mass approx.
5) Etc…

**Transport** (ballistic to diffusive)
1) Quantum mechanical (NEGF)
2) Semiclassical – L. Boltzmann
3) Monte Carlo
4) Landauer formalism

**Geometries** (1D-3D, non-uniform)
1) 3D geometry solvers
2) Nanocrystallines
3) Nanomeshes
4) Low-dimensional

- Graphene nanoribbon
- 3D geometry solvers
- Nanocrystallines
- Nanomeshes
- Low-dimensional geometries (1D-3D, non-uniform)
Motivation - Very high thermoelectric power factors

Very high PF:
2-phase materials: 15 mW/K²m⁻¹
3-phase materials: 22 mW/K²m⁻¹
(~7x compared to bulk Si)

Neophytou et al., Nanotechnology 2013,
Lorenzi et al, J. Electronic Materials 2014

Superlattices
Nanocrystalline materials
Multi-phase nanocomposites

Simultaneous improvement in $\sigma$ and $S$
Outline

- Non-Equilibrium Green’s Function (NEGF):
  - Method
  - Example 1: Influence of variations in SLs
  - Example 2: Filtering in 1D vs 2D
  - Example 3: Nanocomposites

- Monte Carlo semiclassical simulator development:
  - Method
  - Self-consistency
  - Scaling to large geometries
  - Inclusion of quantum effects

- Conclusions
Non-Equilibrium Green’s Function (NEGF)

- Device Green’s function:
  \[ G(E) = [(E + i0^+)I - H - \Sigma_1 - \Sigma_2]^{-1} \]

- Transmission:
  \[ T(E) = Trace(\Gamma_1 G \Gamma_2 G^+) \]

- TE coefficients:
  \[ I^{(j)} = \int_{-\infty}^{+\infty} \left( \frac{E - E_F}{k_B T} \right)^j T(E) \left( -\frac{\partial f}{\partial E} \right) dE \]

  \[ G = \left( \frac{2q^2}{h} \right) I^{(0)} \quad [1 / \Omega] \]

  \[ S = \left( -\frac{k_B}{q} \right) \frac{I^{(1)}}{I^{(0)}} \quad [V / K] \]

- Very powerful approach
- Can include scattering (decoherence)
- Can be computationally very expensive
- Captures the exact geometry and disorder
Example 1a: Variation study in superlattices

1. Variation in $V_B$ reduces PF
2. Variations in wells size, barrier width do not affect the PF
Example 1: Detrimental effect of tunneling

Quantum tunneling is detrimental to S and to the PF
Example 2: Filtering in 1D vs 2D

1D Superlattice

2D Superlattice

(1) Variation in energy of current is larger in 1D
(2) 1D Utilizes S of barriers and $\sigma$ of wells better
(3) 1D Utilizes energy filtering more effectively
Example 3: Nanocomposites – increase in $S$

Red spots: nano-inclusions (here they are barriers of $V_b=0.3\text{eV}$)
Blue region: channel

(1) Nano-inclusions improve $S$
(2) As the domain size decreases, the increase in $S$ is larger
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Monte Carlo method

- Electrons distributed in the channel according to the Fermi distribution and the Density of States
- Allowed to disperse under the influence of the potential
- Scattering by acoustic and optical phonons, ionized impurities, etc.
Thermoelectric coefficients from MC

1. Calculate the average energy of the current

   \[ S = \frac{-I_{\Delta T} \cdot \Delta V}{I_{\Delta V} \cdot \Delta T} \] for arbitrary \( \Delta V \) and \( \Delta T \)

2. \( S = \frac{\Delta V}{\Delta T} \) for \( I_{\Delta T} = I_{\Delta V} \)
Simulations of superlattices in MC

- Include all relevant scattering parameters (next Ionised Impurities)
Include self-consistent electrostatics

**ELECTROSTATICS**

- given $n \rightarrow U_{scf}$
- Poisson
- Iterate until convergence
- given $U_{scf} \rightarrow n$

**TRANSPORT**

- Obtain the actual potential profile for specific doping distributions
Extension to 2D

- Extend to larger geometries, where NEGF cannot reach
- Envision 100nm x 1000nm domains
- Nano-inclusions of various sizes
- Extend to nano-inclusions, grain boundaries dislocations, etc.

**Electron AND phonon transport**
Incorporate quantum tunneling

- Basic idea:
  - Solve 1D NEGF for simplified cases
  - Provide a probability of going through the barrier when an electron reaches a barrier in MC

Effect of tunneling through a barrier
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Conclusions
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- Techniques for electronic transport in nanocomposites
  - Quantum mechanical (NEGF)
  - Semiclassical Monte Carlo

- Extend to large geometries
- Perform realistic simulations
- Incorporate all important transport effects

Acknowledgements:

Mischa Thesberg, Hans Kosina (TU Vienna group), Dario Narducci (Univ. Milan-Bicocca)