Enhanced Molecular Dynamics for Simulating Thermal and Charge Transport Phenomena in Metals and Semiconductors

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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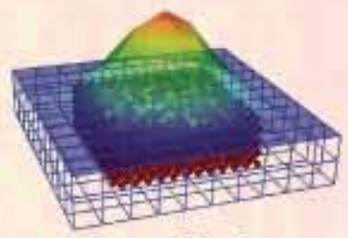
Project Summary

Problem: MD represents phonons and defects but not the electronic thermal & charge transport important in ICs, thermoelectrics, nanowire devices, etc.

Solution: Enhance MD with coupled and coincident FE-based hydrodynamic electron transport models.

Goal: To simulate electron-phonon exchange, Joule heating & thermopower effects on the nanodevice scale.

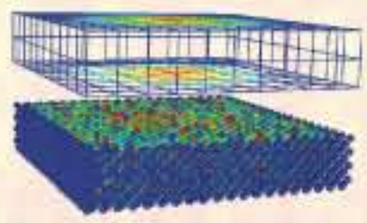
Significance: This project is extending a fundamental tool of material science & enabling a whole new class of predictive simulations, & nanoscale device design e.g. heat transport in defected metals under powered conditions



Pulse of energy superposed on a coupled FE/MD system

Algorithm

Replace empirical phonon transport with MD to add:
- Phonon-confinement
- Ballistic transport
- Defect & grain boundary scattering



FE mesh & MD lattice

(1) Two temperature model (TTM):

(2) Drift-diffusion model: driven by electrical potential (drift), & includes TTM effects (diffusion)

(3) Hydrodynamic model: high density of "hot" electrons, convection, & closest to Boltzmann transport

storage diffusion exchange source

electron: $\rho_e c_e \dot{T}_e = -k_e \nabla^2 T_e - g(T_e - T_p) + r_e$

phonon: $\rho_p c_p \dot{T}_p = -k_p \nabla^2 T_p - g(T_p - T_e)$

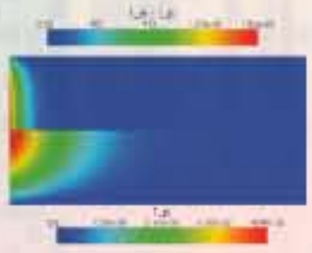
MD: $\begin{cases} m\dot{v} = f - \lambda \\ T_p = 1/3\kappa \langle mv^2 \rangle \end{cases}$

Timescales

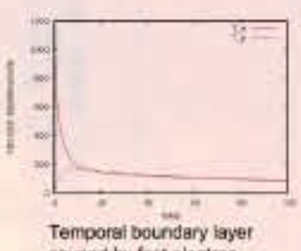
The TTM has three intrinsic timescales which are typically disparate & vary for different materials

Intrinsic timescales:

- **Phonon diffusion :** $\tau = \frac{L^2 c_p}{k_p}$
- **Electron diffusion** $\tau = \frac{L^2 c_e}{k_e}$
- **Electron -phonon exchange** $\tau = \frac{c_e c_p}{g(c_e + c_p)}$



Spatial boundary layer setup by injection of hot electrons (upper half) & diffusion of heat (lower half)



Temporal boundary layer caused by fast electron diffusion & electron-phonon exchange followed by slow phonon diffusion

Two new methods were developed to handle the disparate timescales & relative costs of FE vs. MD:
- Sub-cycling with explicit evolution of the electron transport (stability is still the limiting factor)
- Implicit integration of the electron transport (accuracy becomes the limiting factor)

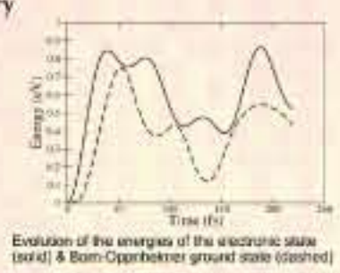
First Principles

Calculation of electon-phonon coupling

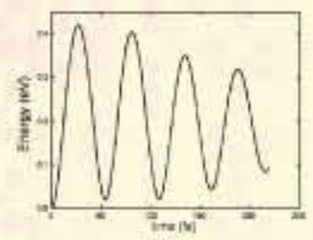
Unlike electron & phonon thermal conductivity & heat capacity, the electron-phonon coupling coefficient g is neither readily measured or calculated.

Three methods were explored:
- An integral over electron-phonon coupling coefficients obtained to first order from perturbation
- Using Green-Kubo relations and the density-density correlations
- Time-dependent Density Functional Theory (TDDFT) simulation of the transient relaxation of electron energy to the ion cores

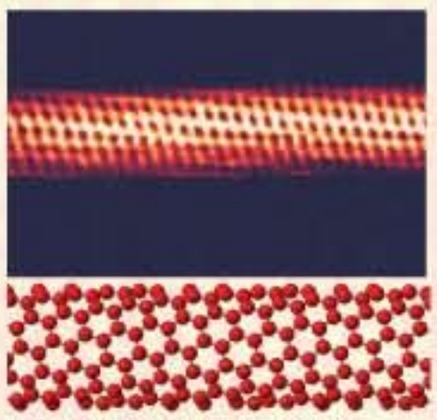
We are primarily using TDDFT, since unlike the first two methods TDDFT is not based on perturbation theory



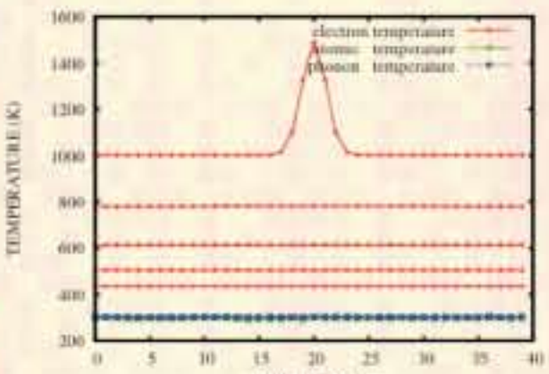
Evolution of the energies of the electronic state (solid) & Born-Oppenheimer ground state (dashed)



Difference energy, showing mean relaxation over time



Carbon nanotube (CNT) image [TU Delft] & lattice



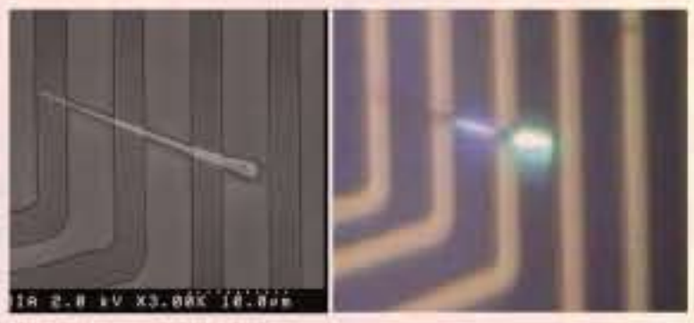
CNT response to an initial Gaussian pulse

MD/FE Simulations

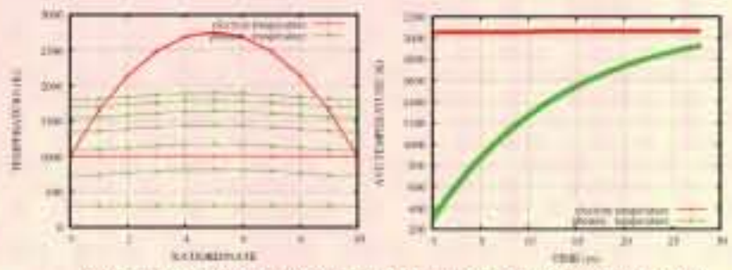
of laser & Joule heating

We now have the capability to simulate of non-equilibrium processes like the relaxation after laser heating & quasi-steady Joule heating.

We are leveraging Ed Webb's work on a related LDRD: Developing a thermal microscopy platform for in-situ thermal/thermoelectric structure-property studies of individual nanotubes and nanowires



GaN nanowire under power and showing photoluminescense (right) [A. Talin, SNL]



Joule heating of a Cu nanowire showing fast response of the electron system and slower equilibration of the phonon system

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
SAND 2008-4594 P CreativeArts 90429.1.W.8.08

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