First-Principles Phonon-Limited Resistivity of Metal Interconnects

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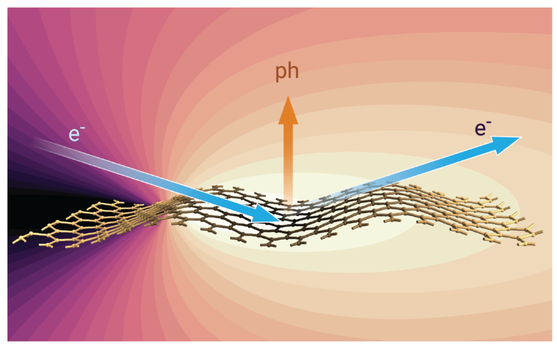
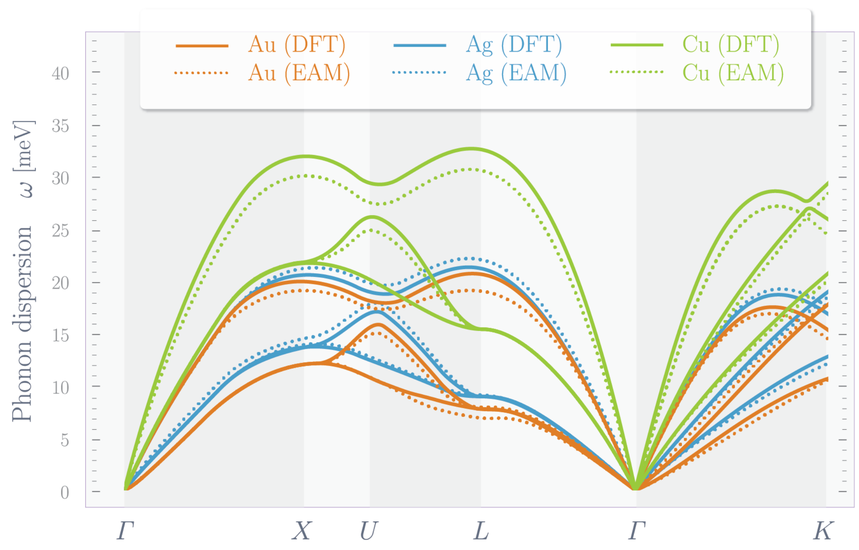
Abstract

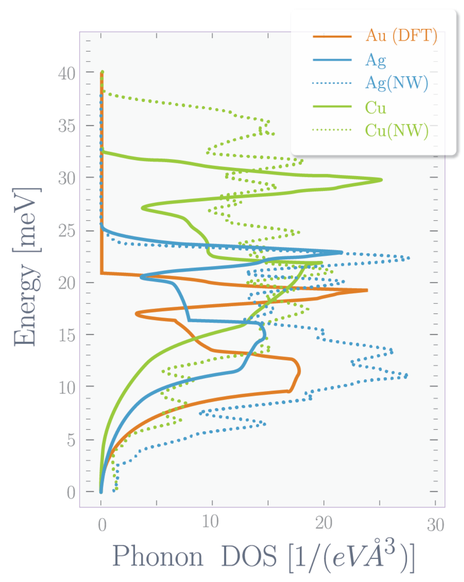
We present density functional theory calculations of the phonon-limited resistivity of three FCC metals (gold, silver and copper). We compare the resistivity of the bulk metals with that of narrow nanowires. We find resistivities in good agreement with experimental reference values for the bulk metals; specifically we find that gold has the highest resistivity followed by copper while silver is the most conductive. For nanowires of 1nm diameter, we find that the resistivity on average is more than doubled as compared to that of the bulk systems due to the increased electron-phonon coupling in the nanowires. In contrast to estimates from bulk mean-free-paths, we further show that Cu is far less conductive than Ag at room temperature when narrowed to the nanoscale. The examples illustrate several extensions to the Boltzmann Transport Equation (BTE) solver implemented in QuantumATK [1,2] that enables computationally efficient simulations of first-principles transport coefficients in linear response to an applied electric field, magnetic field or temperature gradient.

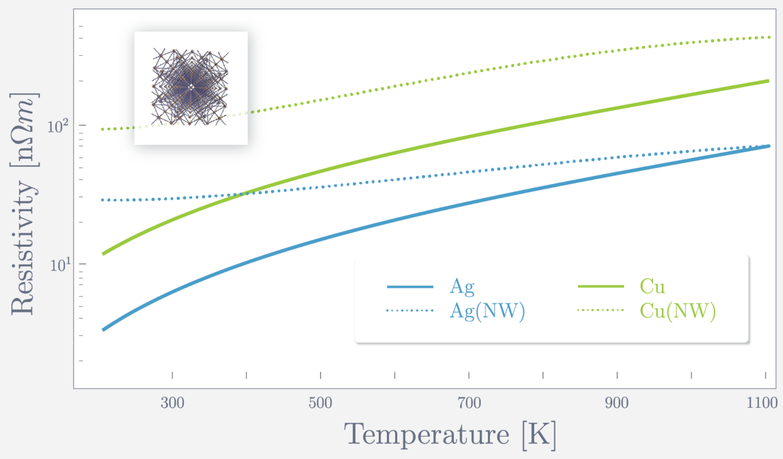
Concepts

- **Semiclassical Boltzmann transport**
  $\tau(\boldsymbol{k},\boldsymbol{q})$: life-time of quasi-particles
  $\mu(T,n)$: mobility at a given temperature and carrier density
- Motion of electrons when an electric field is applied.
  Key input in higher levet TCAD simulations.









Resistivity [nΩm]	DFT Simulation	Experiment
Au (Bulk)	27.0	20.5
Au (NW) [diameter: 1nm]	56.0	-
Ag (Bulk)	6.4	14.7
Ag (NW) [diameter: 1nm]	28.7	-
Cu (Bulk)	19.8	15.4
Cu (NW) [diameter: 1nm]	98.3	-

Table: First-principles resistivities at 300K compared with experimental values from ref. [13]. Au results from [10]. (NW: NanoWire)

QuantumATK Platform

QuantumATK is an integrated software suite for atomic-scale modeling. It combines the power of a (Python) scripting engine, with the ease-of-use provided by an intuitive GUI.

- NanoLab GUI:

- Simulation Engines:
  - DFT-LCAO → 10^3-10^4 atoms
  - DFT-PlaneWave → 10^2-10^3 atoms
  - Semi-Empirical → 10^5 atoms
  - ForceField → 10^5-10^7 atoms
  - NEGF, SGF device & surface simulations

Workflow for Phonon-Limited Resistivity Calculations

- **Phonons**
  - Choose a model (DFT, ForceField) for the vibrations.
  - Relax the structure and check the phonon bands.
- **Electronic Structure**
  - Choose a model (DFT, TB with distance-dependent hopping, etc.)
  - This does not have to (but can be) the same model as for the vibrational part.
  - The model should give a good description of the electronic bands and the e-ph coupling.
- **Hamiltonian Derivatives**
  - Select Number of repetitions.
  - Displacement distance.
- **Electron-Phonon Coupling**
  - Select the electronic bands that contribute carefully.
  - Select the k-points (Fermi-shift to study, k-points for band values within energy range, Monkhort-pack sampling for metals).
  - Select q-points (valleys for semiconductors, Monkhort-part sampling for metals).
- **Resistivity** - Choose a temperature
- **QuantumATK Output**
  - Mobility, Resistivity, Conductivity, Relaxation Rates, Seebeck coefficients, thermal conductivity, Hall coefficients, Hall conductivity

- Resources:

Tutorial: *Phonon-limited mobility in graphene using the Boltzmann transport equation* (https://docs.quantumatk.com/tutorials/mobility/mobility.html)
Webinar: *Simulating the phonon-limited electron mobility of materials* (https://www.synopsys.com/silicon/quantumatk/resources/on-demand-webinars.html)

References

[1] QuantumATK version P-2019.03, Synopsys QuantumATK (https://www.synopsys.com/silicon/quantumatk.html)
[2] T. Gunst, T. Markussen, K. Stokbro, M. Brandbyge, *"First principles method for electron-phonon coupling and electron mobility: Applications to two-dimensional materials"*, Phys. Rev. B, **93**, 035414, (2016).