Modeling Electrical Conductivity in Metallic Crystals using a Lattice-Site Model

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Motivation and Applications

Electrical Conductivity in Metal Organic Frameworks
- Metal Organic Frameworks are porous crystalline materials
- MOFs are well suited to adsorption and separation applications
- Electrically conductive MOFs can be used as novel sensing devices

Electrically-Assisted Metal Forming
- Electric current changes mechanical properties of metals
- Electrical effect occurs in addition to thermal effects (resistive heating)
- Effect is linked to resistivity and conductivity of material

Objectives
- Develop a simple and computationally inexpensive model that can simulate movement of electrons
- Design the framework so users can easily implement material defects and observe their implications
- Use model to bridge gap between atomistic and continuum scale models

Our Model
- Each site in lattice corresponds to unit cell of crystal
- Periodic boundary conditions allow a finite lattice size to represent infinitely-large material body
- Populate lattice with specified density of electrons
- Use random and field-driven motion to propel electrons
- Compute electron flux and conductivity over time

Random Walk and Self-Diffusion of Electrons
- Electrons have random, but equal, probability to move in any direction in the lattice space
- Random motion under zero applied field mimics ‘self-diffusion’ of particles through lattice
- Displacements of electrons are measured over time
- Self-Diffusivity is proportional to rate-of-change in mean-squared displacement of particles

Conduction of Electrons under Applied Electric Field (with Random Material Defects)
- Apply electric field by increasing probability of electron motion in a specified direction (ie. ‘right’)
- At defect sites, electrons regain random walk motion
- Measure flux of electrons through wall of lattice (wall is perpendicular to flow of electrons)
- Flux of electrons is proportional to conductivity

Influence of Random vs. Ordered Defects on Conductivity

Conclusions
- Our model provides a computationally inexpensive means of determining trends between charge carrier density, defect density, and defect structure in lattices
- Due to the nonlinearities and interactions in the model, the model is well suited for parameter optimization

Future Work
- Build material complexity into model framework:
  - Alloying, defect-interaction, electron occupancy
  - Lattice packing structure
- Further investigate structures of ordered defects:
  - Construct ‘grain boundaries’ in lattice model
- Apply model for design and optimization of conductive and metallic materials in electronic applications