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

Predictive Science and Engineering Design Cluster 2011

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Motivation and Applications

Electrical Conductivity in Metal Organic Frameworks

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

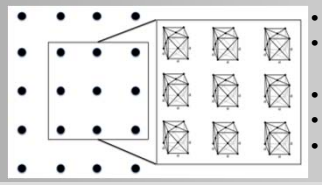
Electrically-Assisted Metal Forming

- 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

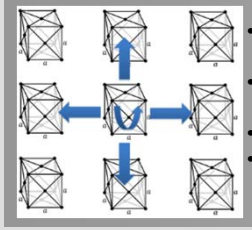
- Develop a simple and computationally inexpensive model that can simulate movement of electrons
- Design the framework so users can easily implement material defects and observe their implications
- Use model to bridge gap between atomistic and continuum scale models

Our Model

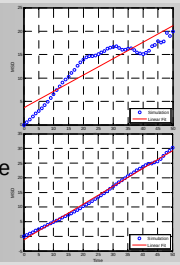


- Each site in lattice corresponds to unit cell of crystal
- Periodic boundary conditions allow a finite lattice size to represent infinitely-large material body
- Populate lattice with specified density of electrons
- Use random and field-driven motion to propel electrons
- Compute electron flux and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

Random Walk and Self-Diffusion of Electrons



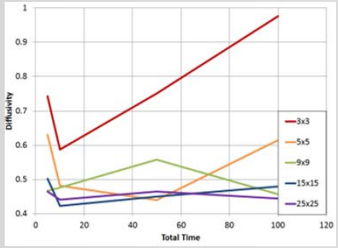
- Electrons have random, but equal, probability to move in any direction in the lattice space
- Random motion under zero applied field mimics 'self-diffusion' of particles through lattice
- Displacements of electrons are measured over time
- Self-Diffusivity is proportional to rate-of-change in mean-squared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



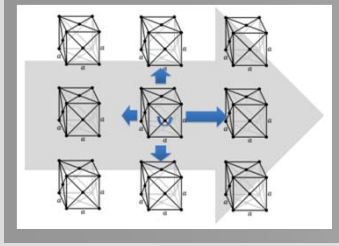
[Left-top]: Small lattice size (3x3 particles) shows unstable self-diffusivity (non-linear)

[Left-bottom]: Larger lattice (9x9 particles) shows stable, linear self-diffusivity

[Right]: Large lattices and long simulation times show most stable and convergent solution for diffusivity



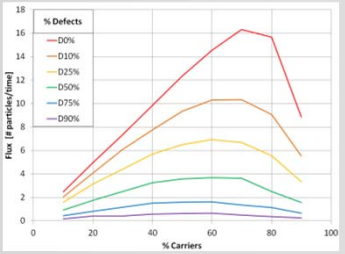
Conduction of Electrons under Applied Electric Field (with Random Material Defects)



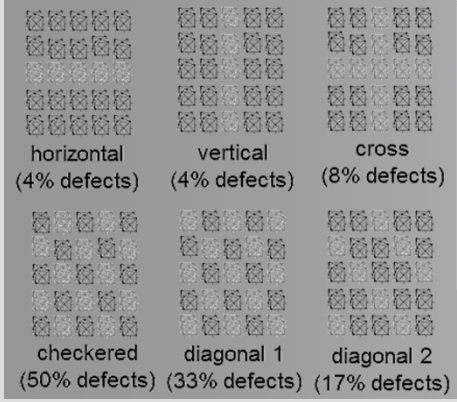
- Apply electric field by increasing probability of electron motion in a specified direction (ie. 'right')
- At defect sites, electrons regain random walk motion
- Measure flux of electrons through wall of lattice (wall is perpendicular to flow of electrons)
- Flux of electrons is proportional to conductivity

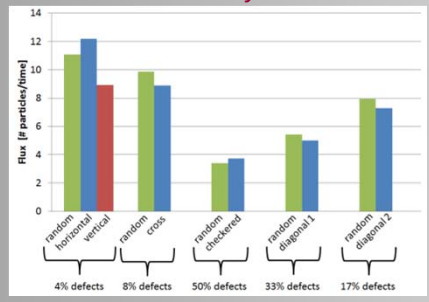
$$\mathbf{J} = -\frac{D}{RT} czF\mathbf{E} \quad \Rightarrow \quad \sigma = \frac{N_v e^2 D}{k_B T}$$

[Right]:
- Increasing % charge carriers (up to 50%) increases conductivity
- Increasing % defects decreases conductivity
- Maximum conductivity occurs between 50-75% charge carrier density



Influence of Random vs. Ordered Defects on Conductivity





[Right]: Various configurations of ordered defects and their corresponding defect density
[Top]: When comparing random and ordered defects, certain configurations of ordered defects (especially at low densities) can greatly influence overall 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