Thermal Conductivity Across Metal/Metal Oxide Interfaces

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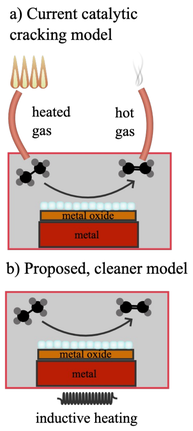
Motivation and Question



Catalytic cracking of ethane to ethylene currently requires a lot of unclean energy

⬇

Reduce energy by heating only the area where the reaction takes place

⬇

But how does heat travel through the **metal** and **metal oxide** layers to the reaction?

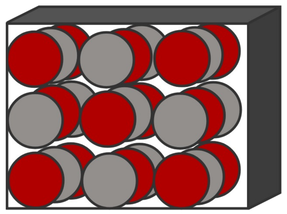
Two-Temperature Model

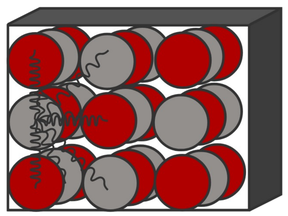
Thermal conductivity (κ) = how easily heat (kinetic energy) moves through a material

In **metals**, κ depends on both the atoms in the metal lattice *and* the electrons moving through it:

$$\kappa = \kappa_{lattice} + \kappa_{electrons}$$

The computational technique **Molecular Dynamics** (MD) can find $\kappa_{lattice}$ by tracking **lattice** movements

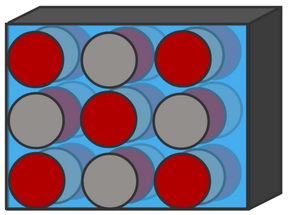




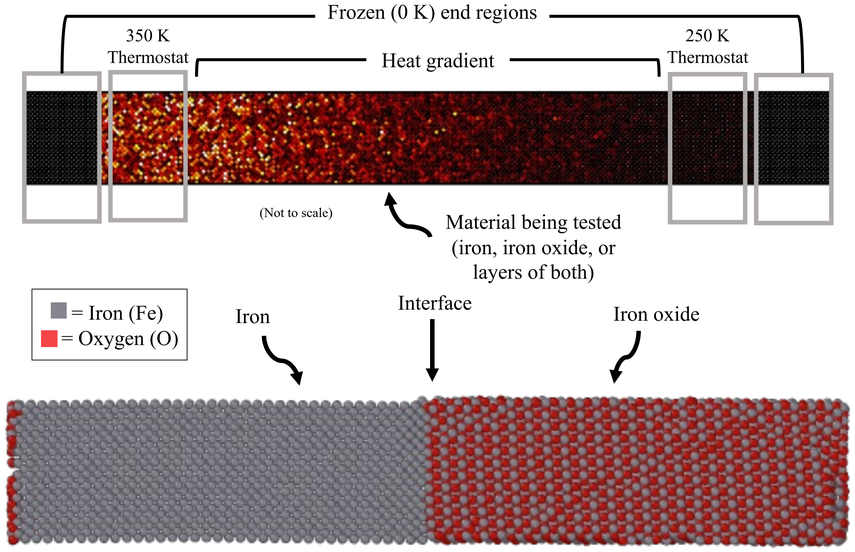
It repeatedly calculates the forces between atoms based on **interatomic potentials**, as if each atom were bouncing on a spring attached to its neighbors

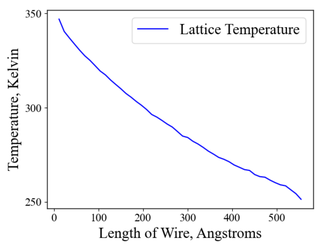
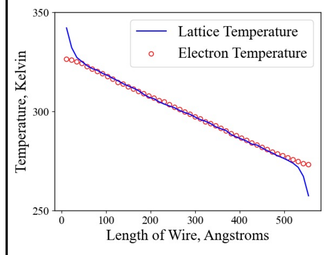
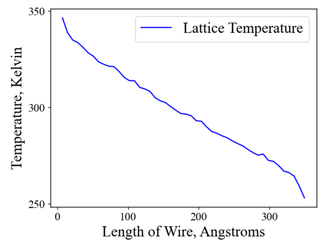
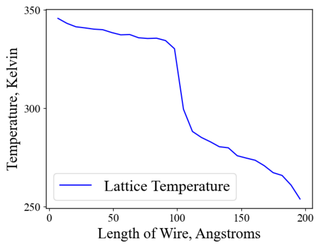
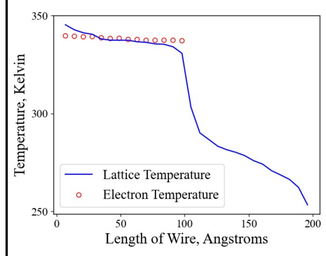
A **Two Temperature Model** (TTM) is an integrated multiphysics model that simulates electrons with an electron-like gas in an MD model

Electrons and lattice have different temperatures → TTM lets them exchange energy



Simulation Setups + Results



	MD Only	κ	MD + TTM
Fe		Experimental: $\kappa = 78.5 \pm 1.5$ W/m-K[a] **MD + TTM: $\kappa = 57 \pm 29$ W/m-K** MD Only: $\kappa_{lattice} = 12 \pm 7$ W/m-K	
FeO		Experimental: $\kappa = 8.6 \pm 0.2$ W/m-K[b] **MD Only: $\kappa = 10 \pm 3$ W/m-K**	Since FeO is ionic, it lacks conduction electrons! Therefore, it has negligible electronic contribution to thermal conductivity.
Fe/FeO		**MD + TTM: $\kappa = 1.1 \pm 0.5$ W/m-K** MD Only: $\kappa = 1.1 \pm 0.5$ W/m-K	

MD in Motion

Scan this code with your phone camera to see some of these simulations in motion!

Conclusions

- MD + TTM reduced the disparity between the calculated and experimental thermal conductivity of iron by 67%
- MD and MD + TTM both predicted a low thermal conductivity across a small Fe/FeO interface
- **This system can now be modified to test other metal/insulator systems**

Future Directions

- Improvement of Fe/FeO modeling through new FeO interatomic potential data updated for calculating thermal conductivity and larger simulations on the order of 10^5 or 10^6 atoms
- Testing of a proposed Ni/C/NiO system for catalytic cracking

Acknowledgements + References

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References:

[a] Williams, R. K. et al. (1981). *Journal of Applied Physics.*

[b] Takeda, M. et al. (2009). *Materials Transactions*.

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