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# A two-temperature model of radiation damage in α-quartz

Carolyn L. Phillips[1], Rudolph Magyar[2], Paul S. Crozier[2]

[1]Applied Physics, University of Michigan

[2] Multiscale Material Modeling Department, Sandia National Laboratories

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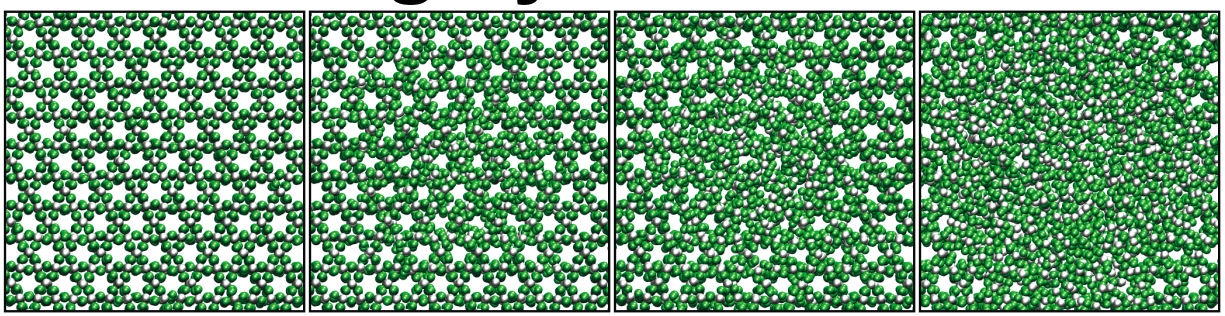
# Molecular Dynamics used to Model Material Responses

- Quantum MD
  - Includes electronic degrees of freedom
  - limited to small system sizes.
- Classical MD
  - simpler (pair-wise) interactions between point atoms
  - larger system

# Modeling Large Systems with "Coarse" Electronic Transport

- potentials adequate to capture non-equilibrium behavior
- energy losses due to inelastic scattering by electrons?



***Local material response is Temperature Dependent. The rate at which energy is transported can have a significant effect on the material response***

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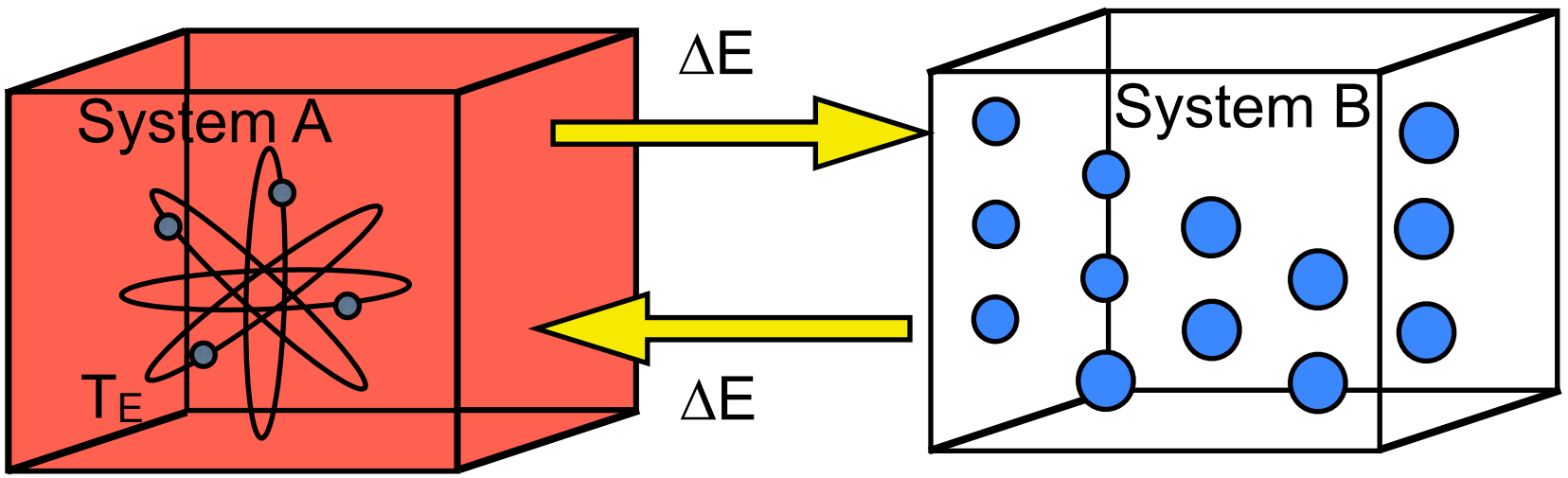
# What is a Two Temperature Model (TTM)?




Electrons

Nuclei in a metallic crystal

- Rapid Heat Deposition (laser, radiation, etc.)
- Electrons and Nuclei are out-of-equilibrium
- Electrons Delocalized
- Heat transfer through the electronic subsystem is non-negligible

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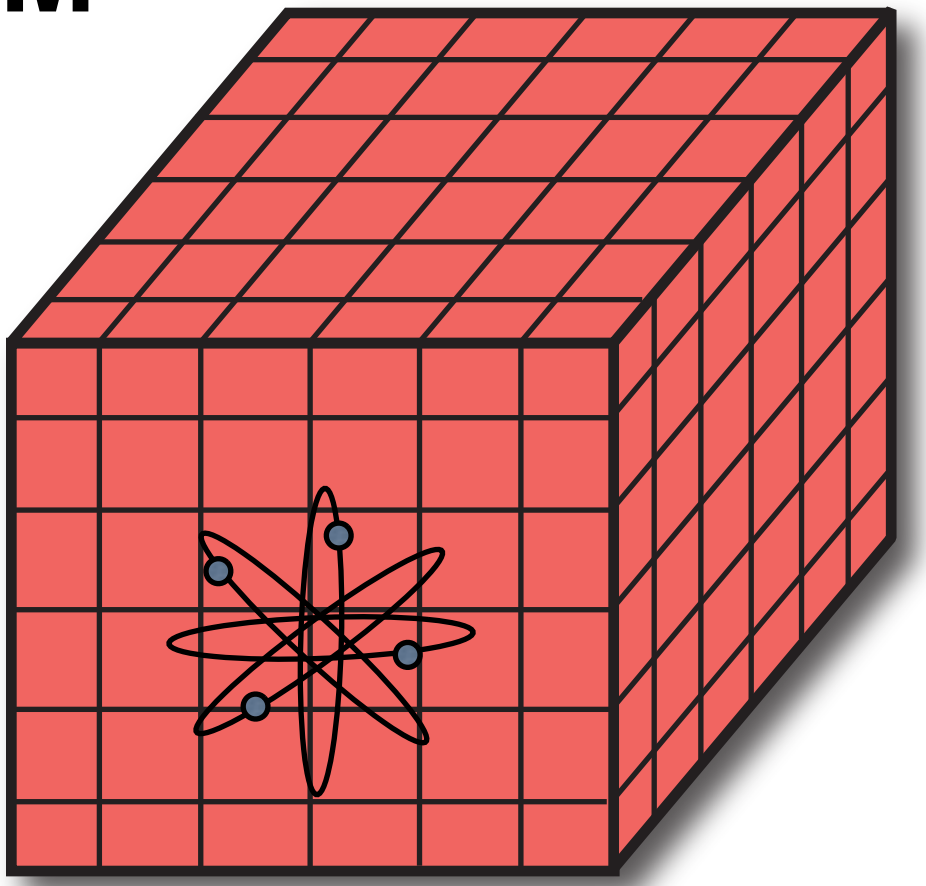
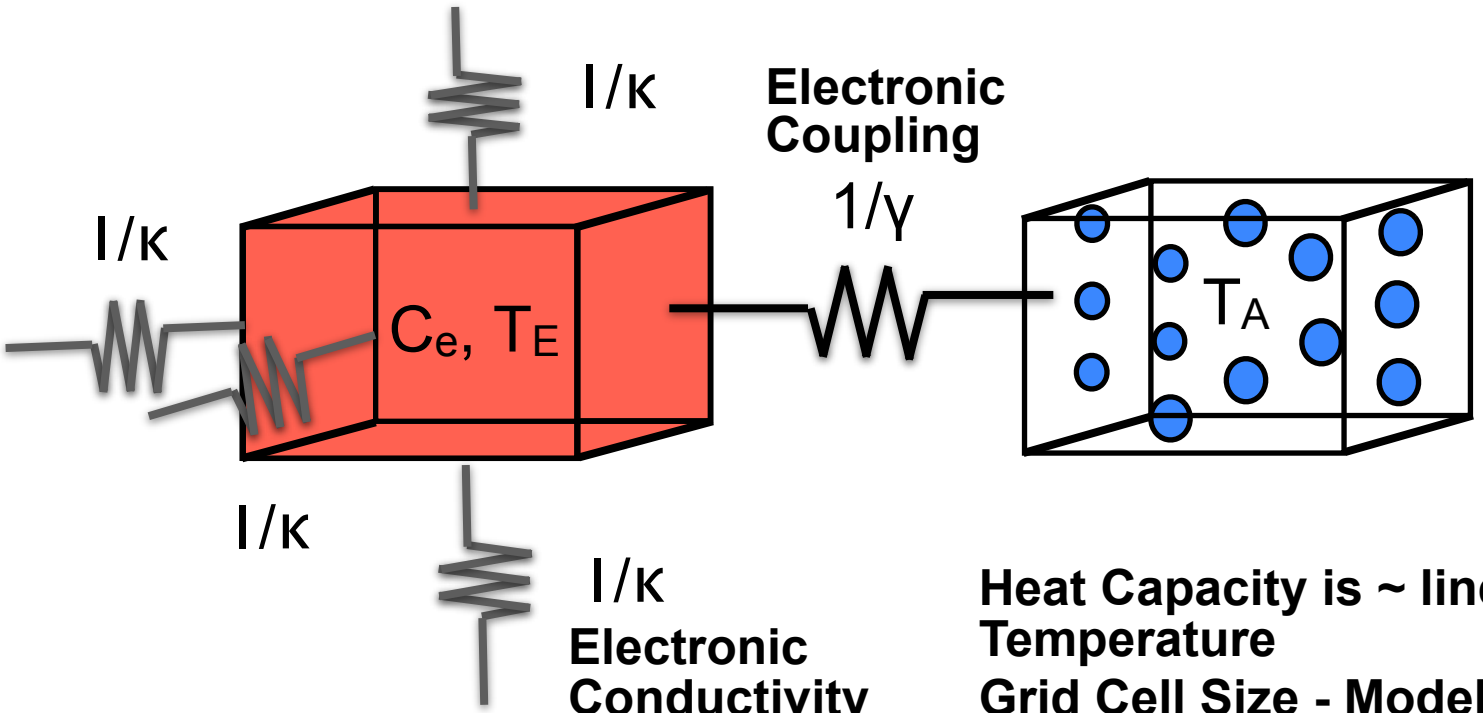
# History of TTM

- Caro & Victoria,1989
  - Fixed Constant Uniform $T_e$
- Rutherford & Duffy, 2007
  - Spatial and Temporal Variation in $T_e$
- Phillips & Crozier, 2009
  - Energy Conserving
  - Provided in LAMMPS



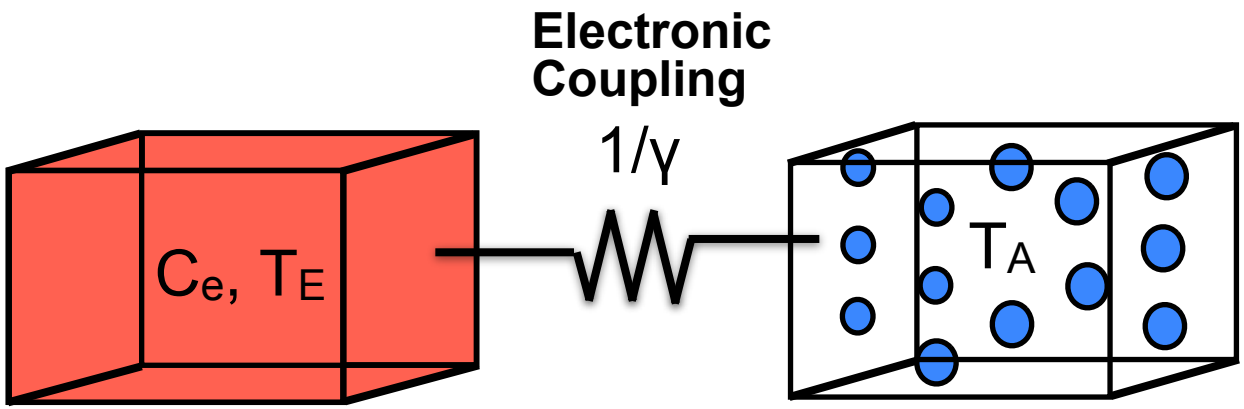
*Finite Element Mesh Coupled to atoms by inhomogeneous Langevin Thermostat*

# Standard Model - Metallic Gas




Heat Capacity is ~ linear with Temperature
Grid Cell Size - Model Parameter
Electronic Coupling is small
Electric Conductivity is high

# Insulator Model




**Heat Capacity is ~ Step function with Temperature**

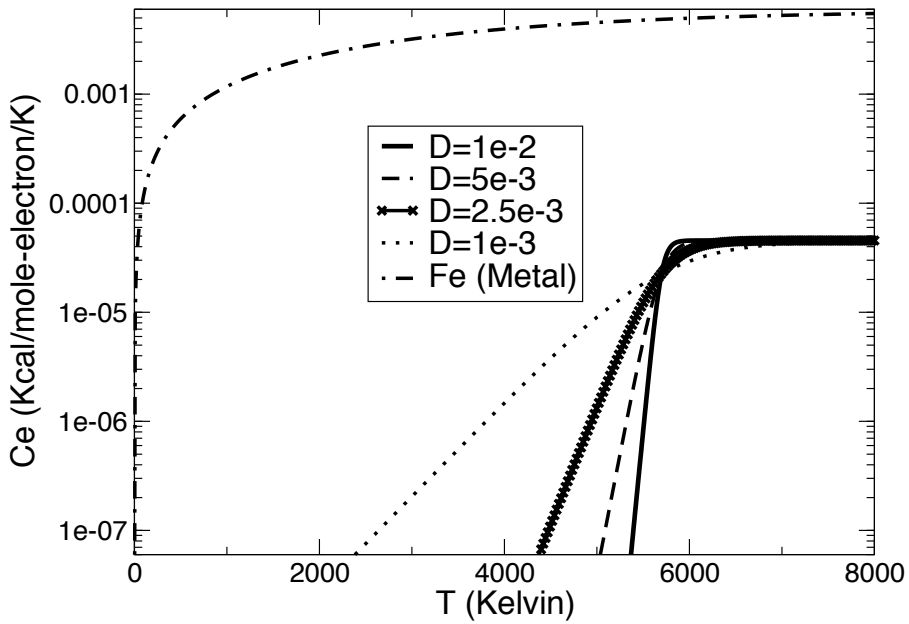
**Electronic Conductivity ~ Negligible**

**Grid Cell Size ~= Local Excitation Size**

**Electronic Coupling is High**

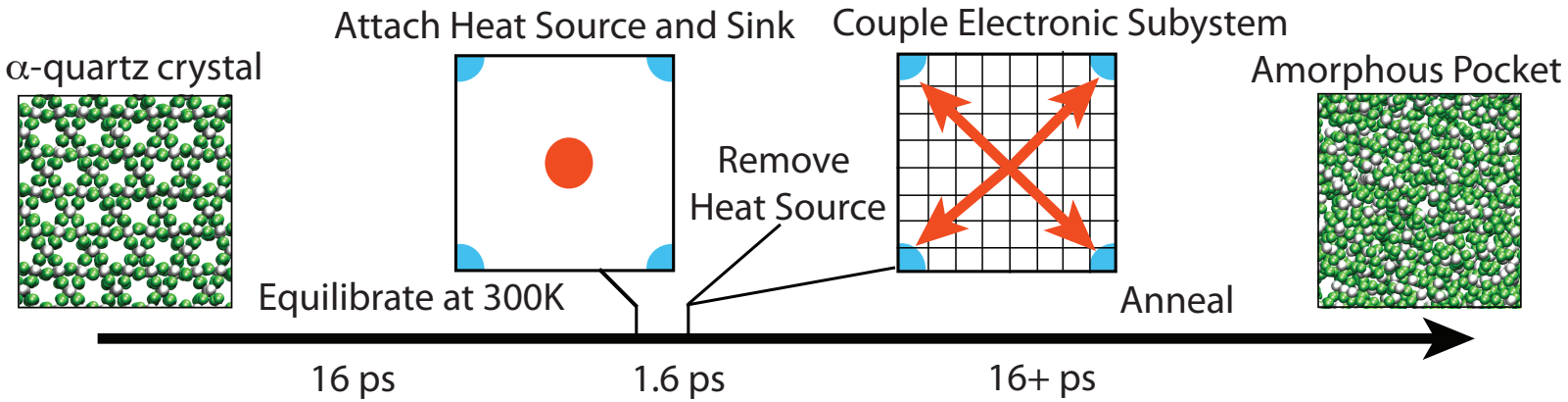
# Physics Parameters

- **Heat Capacity, $C_e$ - DFT calculation on 36 atom super cell**
- **Electron-ion coupling, $\Upsilon p = m/\tau$, $\tau$ = 20-200 fs.**
- **Excitation cell size - ?**
- **D, step softening parameter - ?**

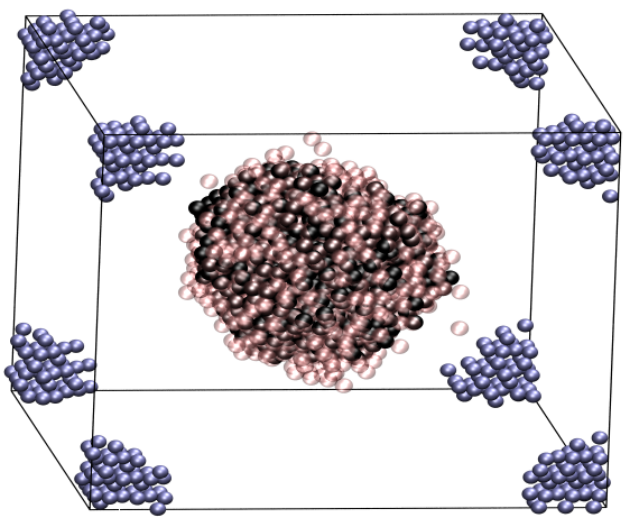



$$C_e(T) = \frac{C_{e,\infty}}{2} * (1 + \tanh(D * (T - T_{threshold})))$$

# Testing the Influence of Models




- **SiO2 modeled by BKS interaction potential**
- **65,000 atom system (20x20x19 primitive cells)**
- **14.3 keV deposited into spherical region**



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# Different models of electronic subsystem

- None
- "Short-Circuit"
- Insulator model
  - different size excitation cell
  - more or less tightly coupled
  - softened step function
- Metallic Model (Fe)
- "Hot" vs "Cold" Electronic Subsystem

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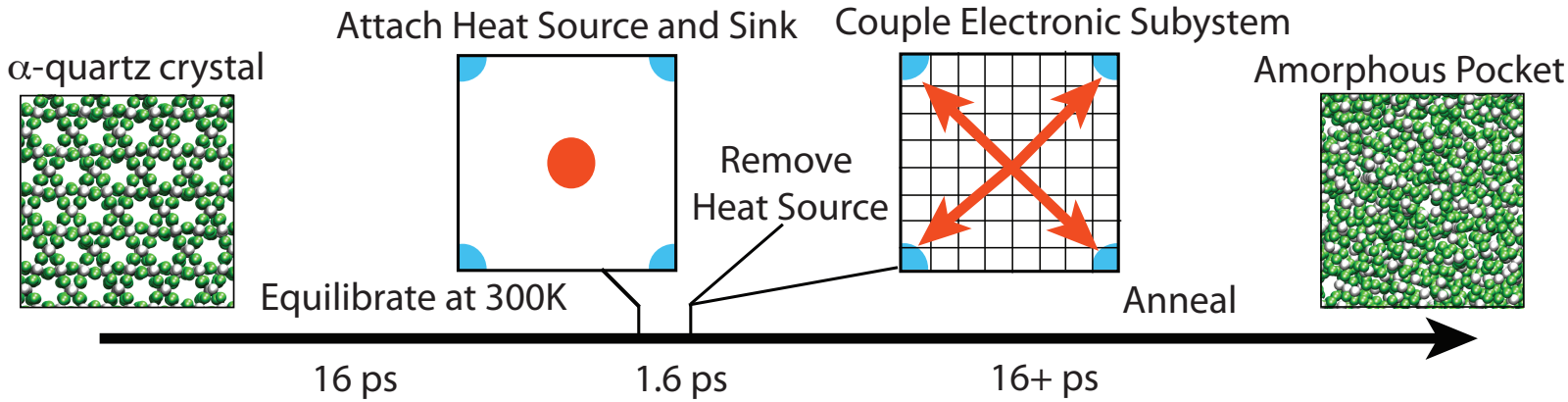
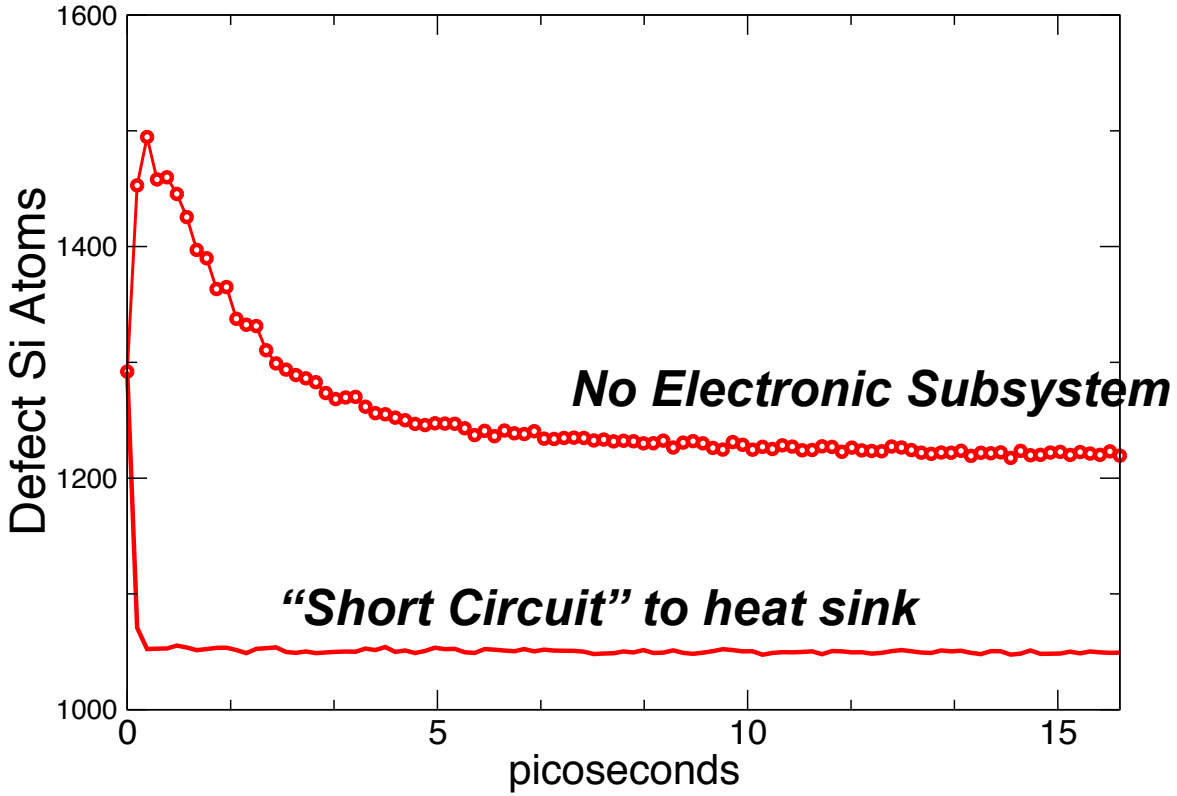



# Defects identified by a local bond order analysis

$$\alpha_j = q_8(i) \cdot q_8(j)$$

$$q_8(i) = \frac{1}{N_b(i)} \sum_{j=1}^{N_b(i)} Y_{8m}(\hat{r}_{ij})$$

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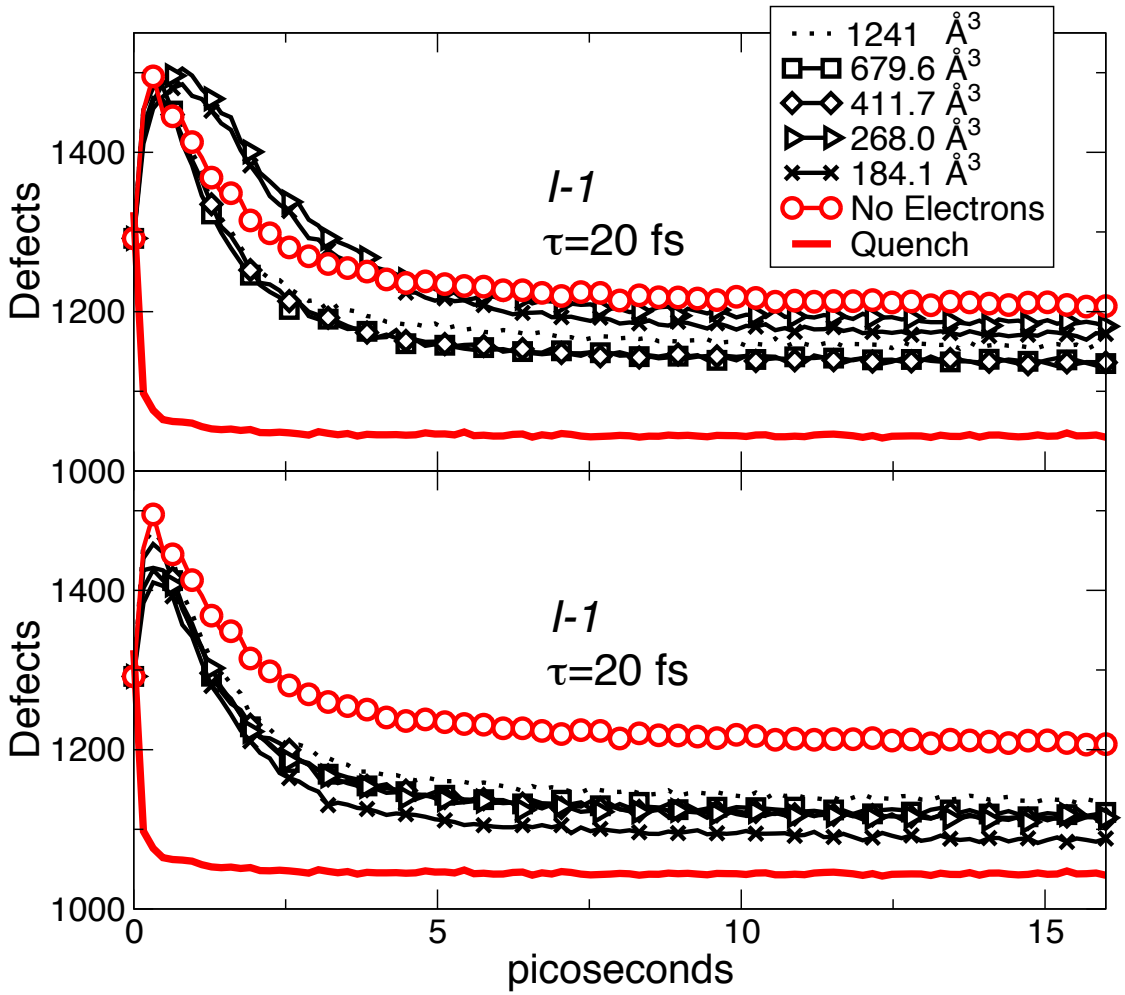
# Excitation cell size

**Excitation Cell Size effect the system**

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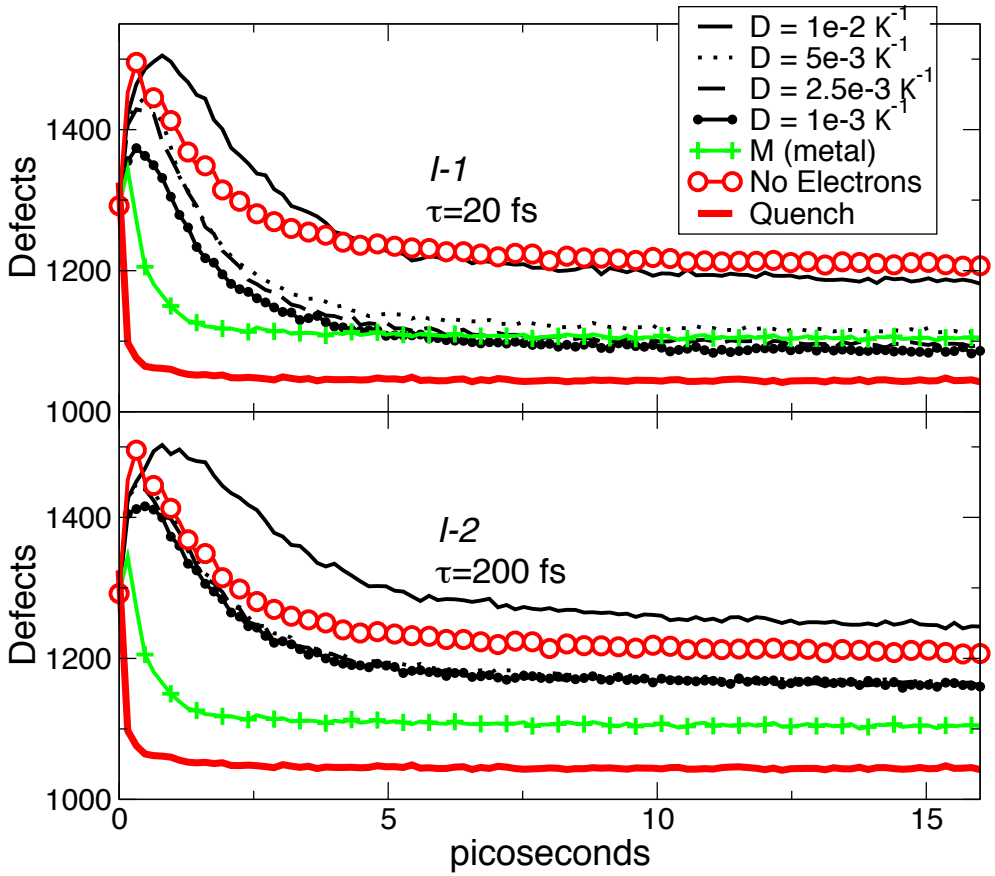
# Influence of D & τ

**Ranged from damage similar to a *metallic electronic subsystem* to *no electronic subsystem* at all.**

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# Conclusions

- **Important to include models of the modes of heat transport!**
- **The coarse model of the electronic subsystem is important.** ***An Insulator model acts very different from a Metal model.***
- **Refined physics parameters are needed.**

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