



Thermal Properties of Yttrium Aluminum Garnet from Molecular Dynamics Simulations

ASME/JSME Thermal Engineering Conference
Honolulu, Hawaii

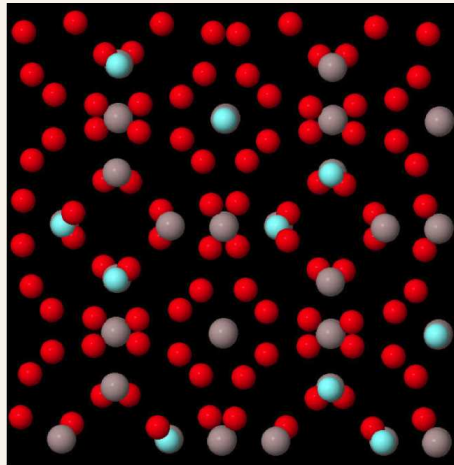
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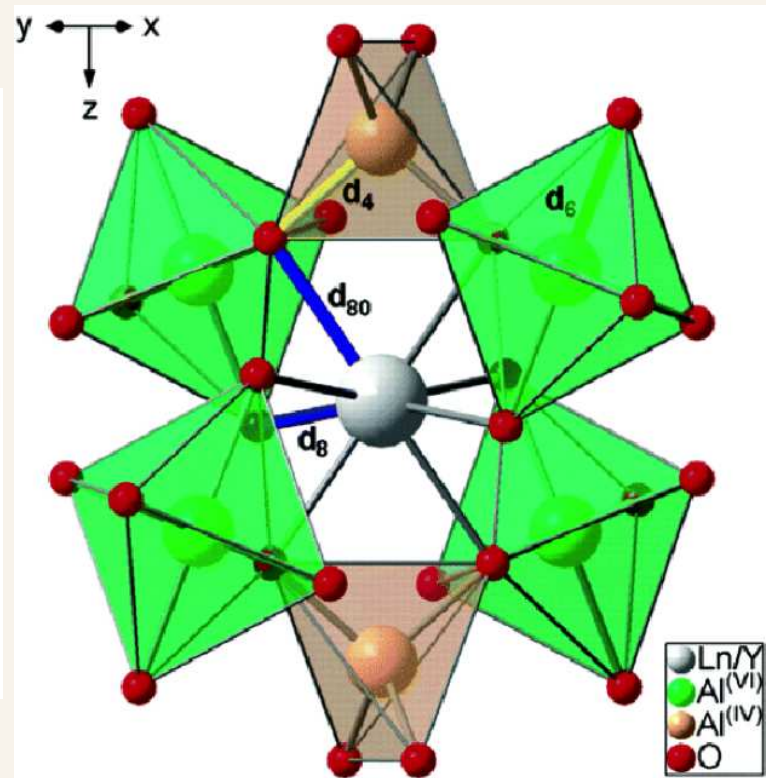
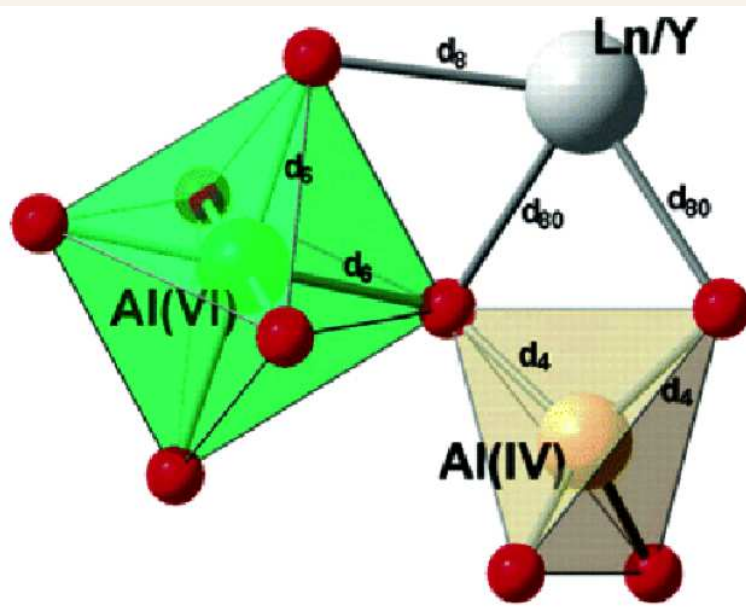
- YAG is interesting in general because of its applications
 - solid-state lighting
 - thermographic phosphor
 - thermal barrier coating
 - lasing medium
- YAG is particularly interesting to us because
 - radiation hardness
 - luminescence and transport are affected by substitutional species



- Low electrical conductivity means thermal transport is phonon dominated
- Some (experimental) thermal properties
 - thermal conductivity 10 – 14 W/mK
 - melting temperature 2213 K
 - Debye temperature $\theta_D = 750$ K
 - thermal expansion $7.0 \times 10^{-6} \text{K}^{-1}$ at 300 K
 - specific heat 600 kJ/kg K



- 160 atoms in unit cell
 - 24 Y
 - 40 Al
 - 96 O
- lattice constant is 12.01 Å



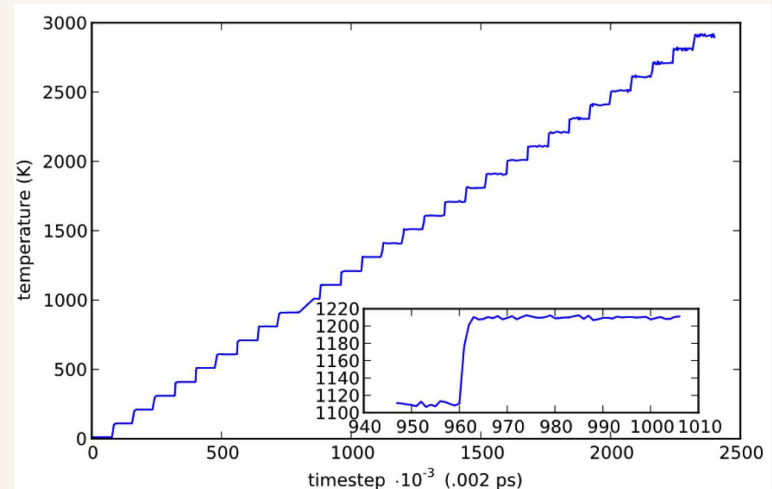
L. Dobrzycki, E. Bulska, D.A. Pawlak, Z. Frukacz and K. Wozniak, "Structure of YAG crystals doped/substituted with erbium and ytterbium," *Inorganic Chemistry*, 43(2), pp. 7656–7664, 2004. (Used with permission.)



- LAMMPS with custom potential
- Two-body potential
 - Coulomb electrostatics (Ewald summation)
 - Repulsive force
- Three-body potential
 - O–Al/Y–O, 109.5°
 - Al/Y–O–O, 109.5°

- Simulation parameters

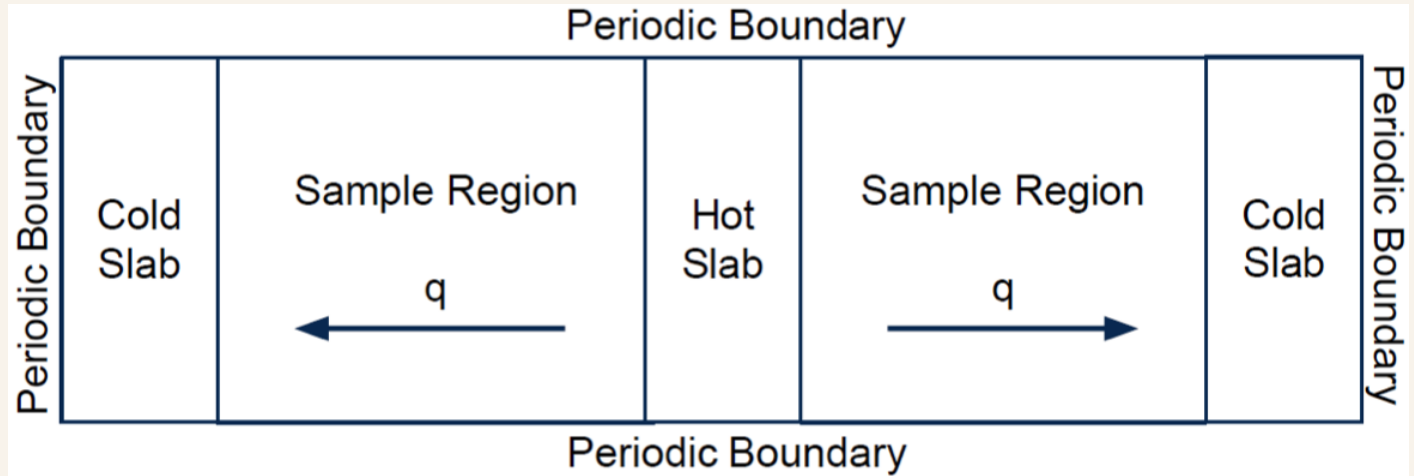
- 0.002 ps timestep
- 10^{-4} PPPM precision
- 7 Å cutoff
- periodic boundaries
- NPT ensemble; 1 ps damping
- each temperature equilibrated for 80,000 time steps (160 ps)



Quantity	LAMMPS	Chen*	experimental
melting temperature (K)	1900	2131	2213
thermal expansion (K^{-1})	7.8×10^{-6}		7.0×10^{-6}
lattice constant (Å) at 300 K	12.43	12.35	12.01
specific heat (kJ/kg K)	0.87		0.6

* J. Chen et al., 2007, Chin. Phys., 16(9):2779.

- Periodic boundaries are required because of long-range forces, so two “mirror” domains are simulated



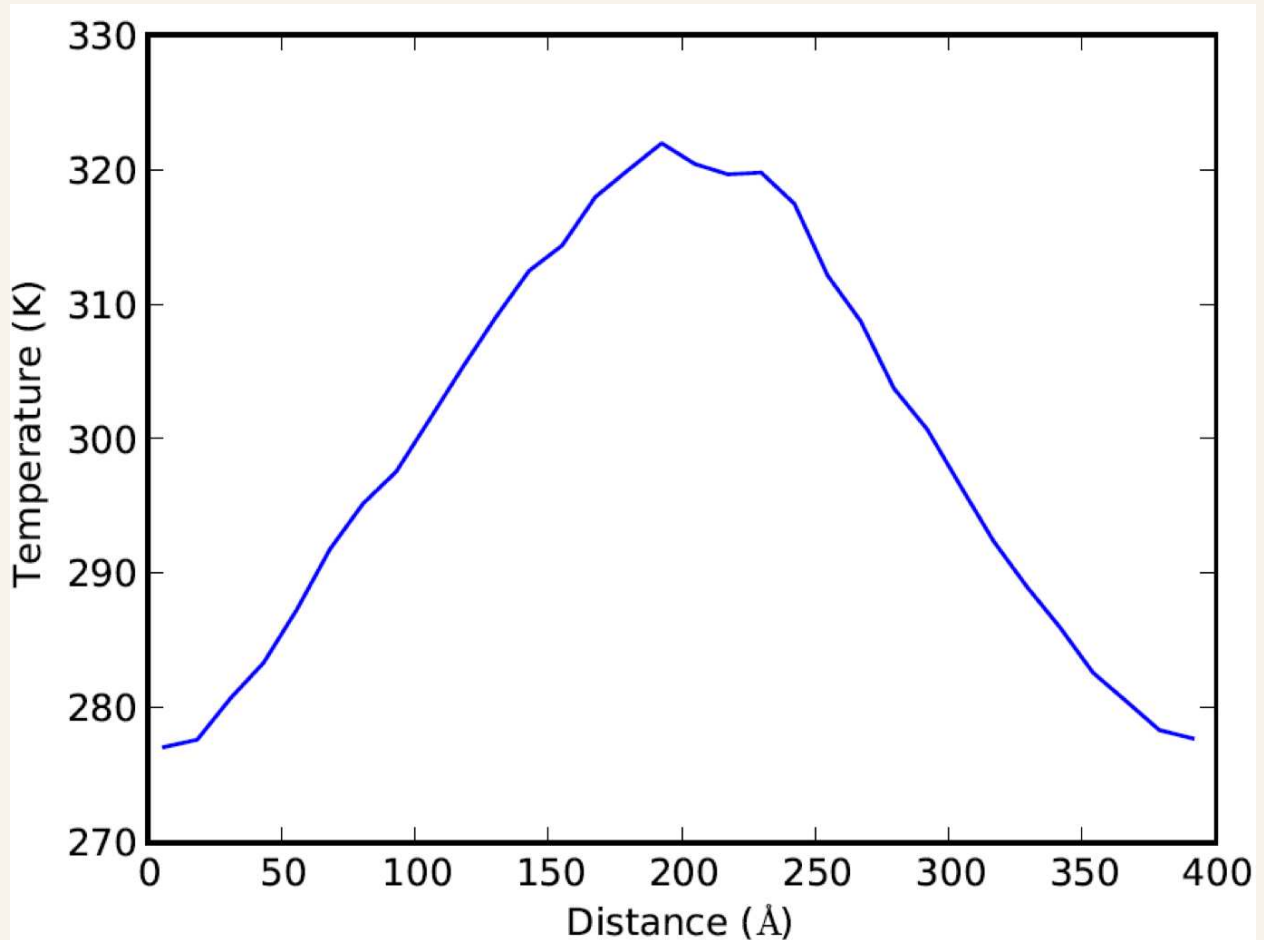
- Imposed bath temperature; amount of energy added computed.

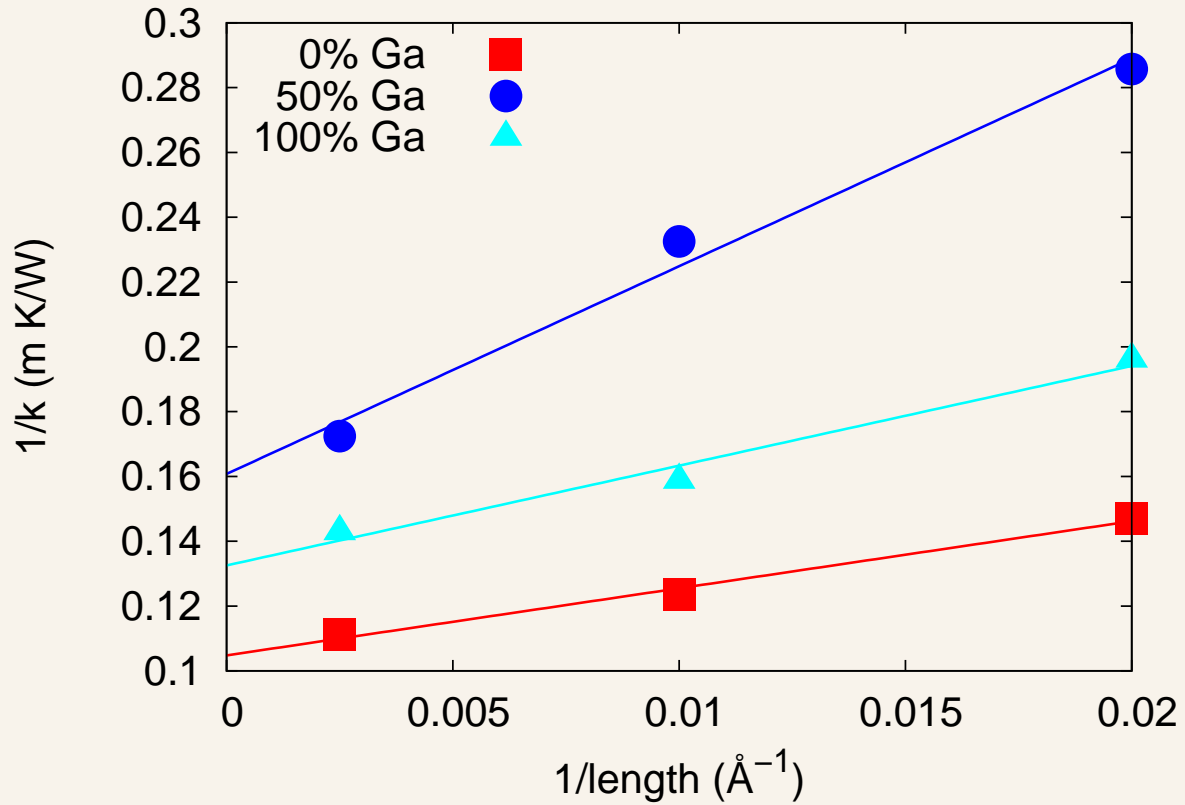
$$k = -\frac{q \, dx}{A \, dT}$$

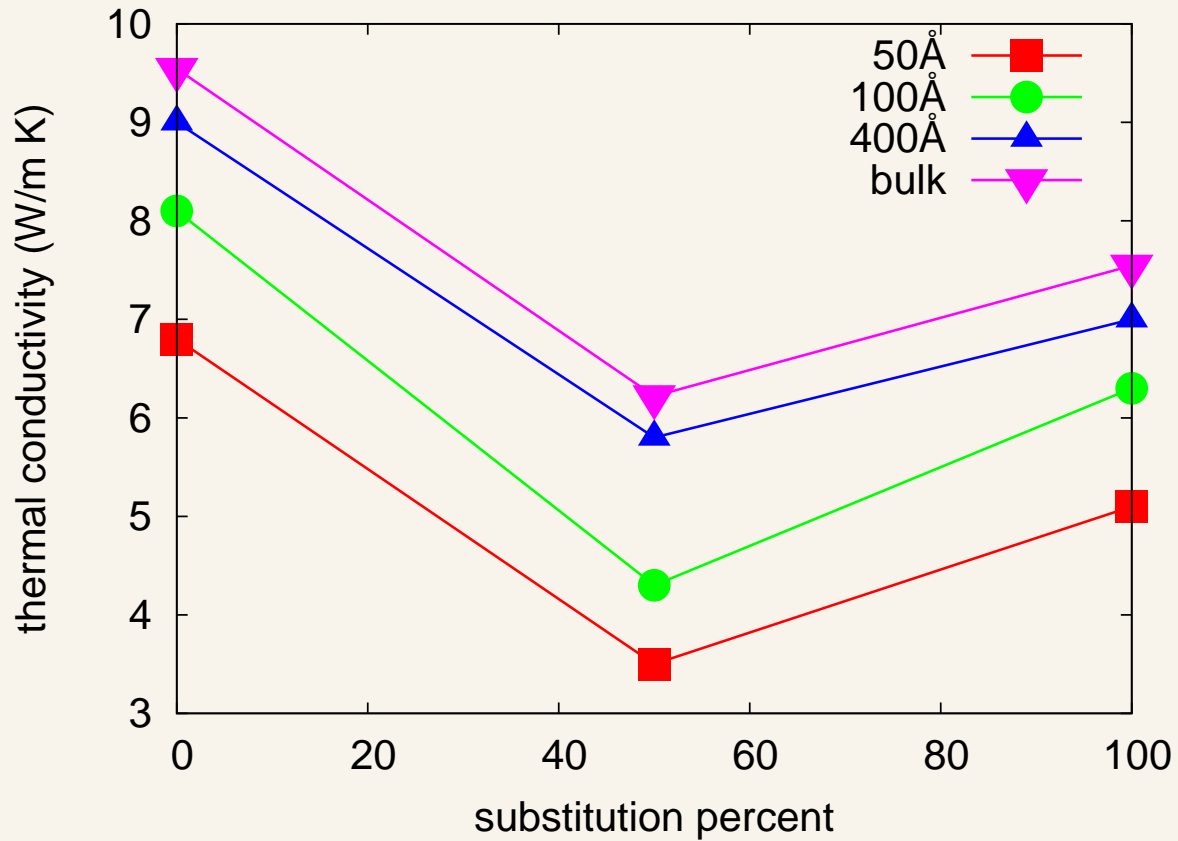


- Simulation settings
 - 0.001 ps timestep
 - 4 Å exponential cutoff; 7 Å Coulombic cutoff
 - 10^{-5} PPPM precision
- Simulation parameters
 - NVE integrator
 - Aluminum substitutions: 0%, 50%, 100%
 - Average temperature: 300 K; $\Delta T = 40$ K
 - Lengths: 4, 8, 16, and 32 unit cells (height and width are 1 unit cell each)

- Typical average temperature distribution from all data after equilibration









- Simulations showed decent agreement with several thermal properties (experimental and other equivalent model)
- More data (other substitution percentages) are needed for further confidence.
- The interatomic potential for the gallium substitution was not altered because no potential exists for this configuration. Density functional calculations can be used to determine potential parameters.
- In the process of performing equilibrium analysis to validate further the foregoing results