

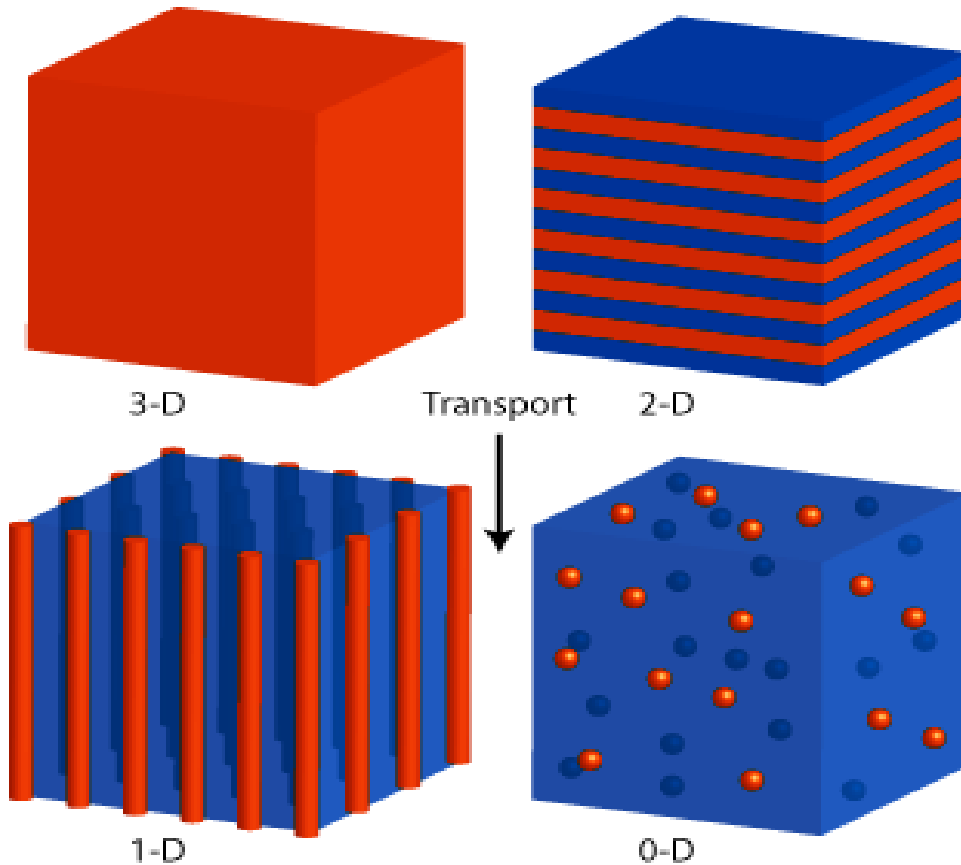
# Molecular Dynamics Simulation of Thermal Conductivity of Nanocrystalline Composite Films

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and

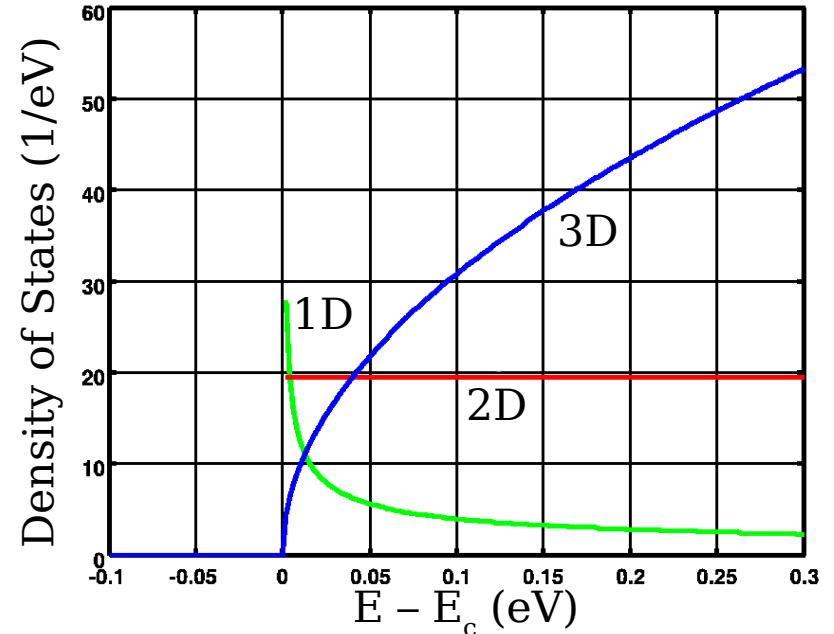
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# Motivation

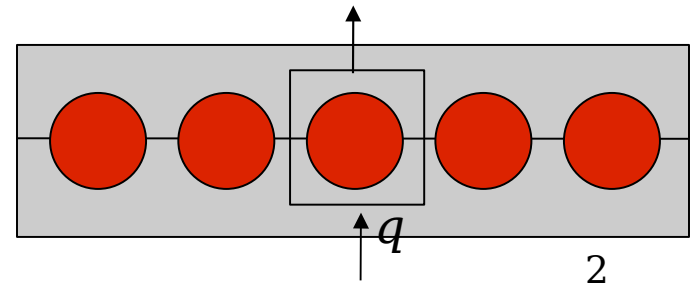
Nanostructured devices possess desirable characteristics for solid state energy conversion



[nel-8.case.edu/personal/research.html](http://nel-8.case.edu/personal/research.html)

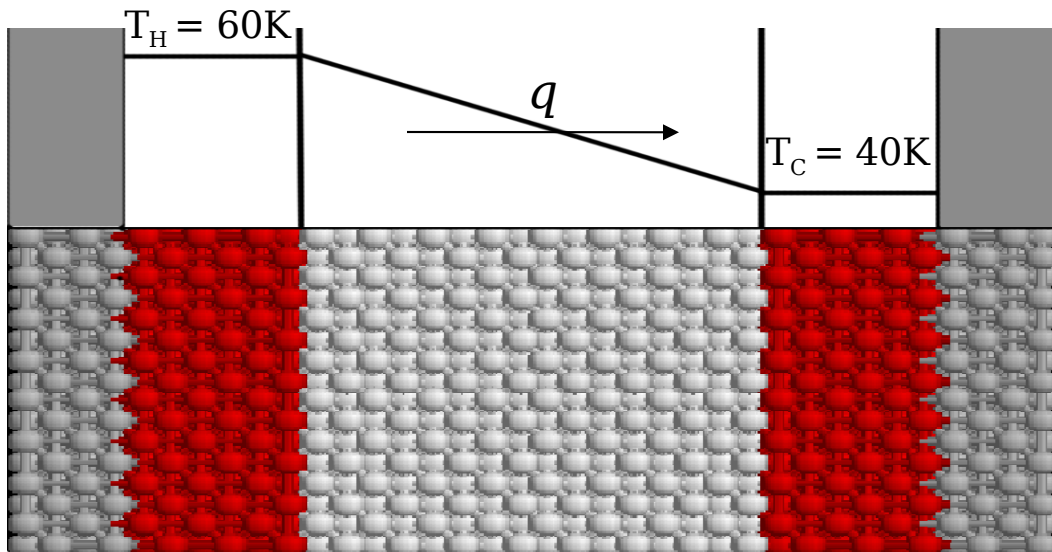


$$ZT = S^2 \sigma T / k$$



# Computational Model

- Using a Molecular Dynamics Code to calculate the effective thermal conductivity of a composite material
- Argon/Krypton FCC domain, wall and bath
- Boundary Conditions are constant temperature for boundaries orthogonal to transport and periodic parallel to transport
- Calculates flux between planes using approach outlined by Ikeshoji and Hafskjold, Molecular Physics (1994)

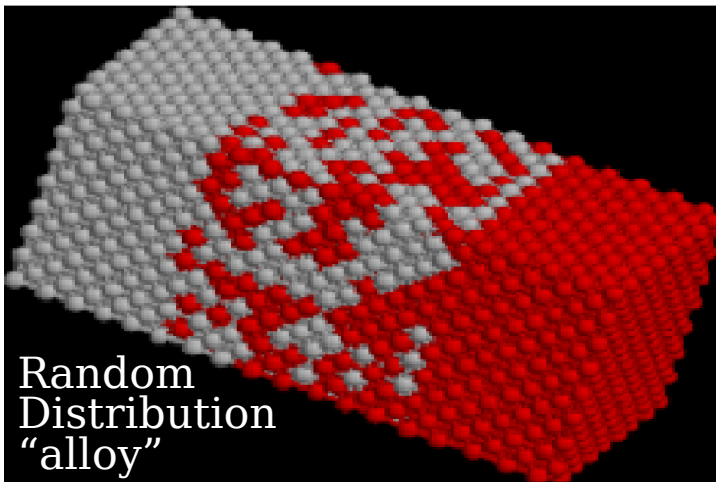
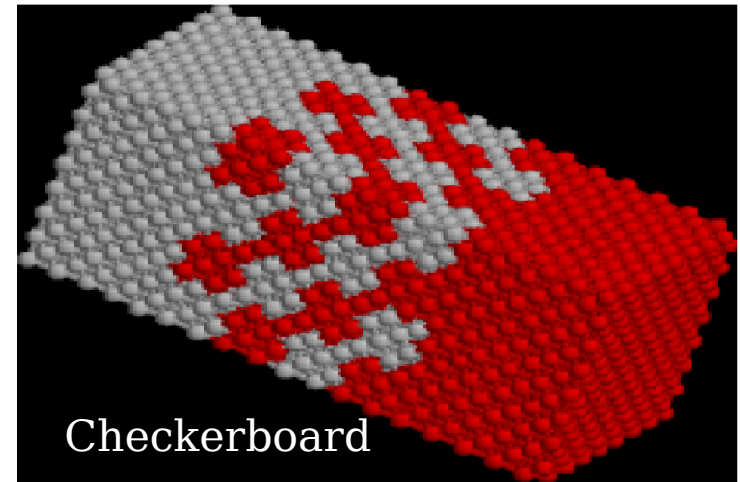
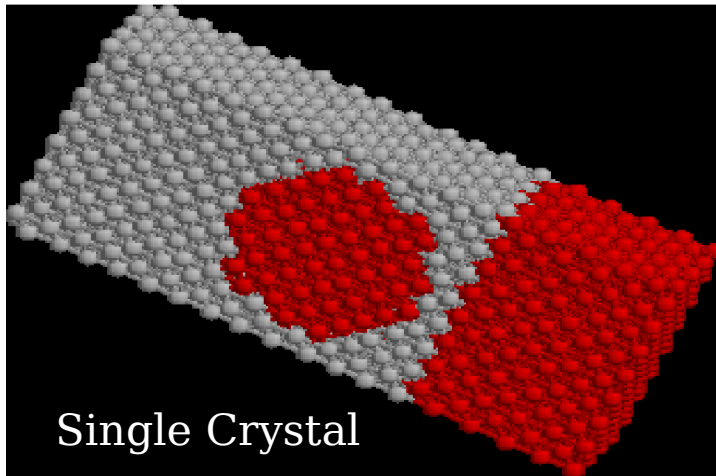


$$V(r_{ij}) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

$$q = -kA \frac{\Delta T}{L}$$

Material	Parameter	Value
Kr	$\epsilon$ (J)	2.25E-21
	$\sigma$ (m)	3.65E-10
	$a$ (m)	5.69E-10
	$r_{cutoff}$ (m)	9.49E-10
Ar	$m$ (kg)	1.35E-25
	$\epsilon$ (J)	1.67E-21
	$\sigma$ (m)	3.40E-10
	$a$ (m)	5.30E-10
	$r_{cutoff}$ (m)	8.84E-10
	$m$ (kg)	6.63E-26

# Simulations

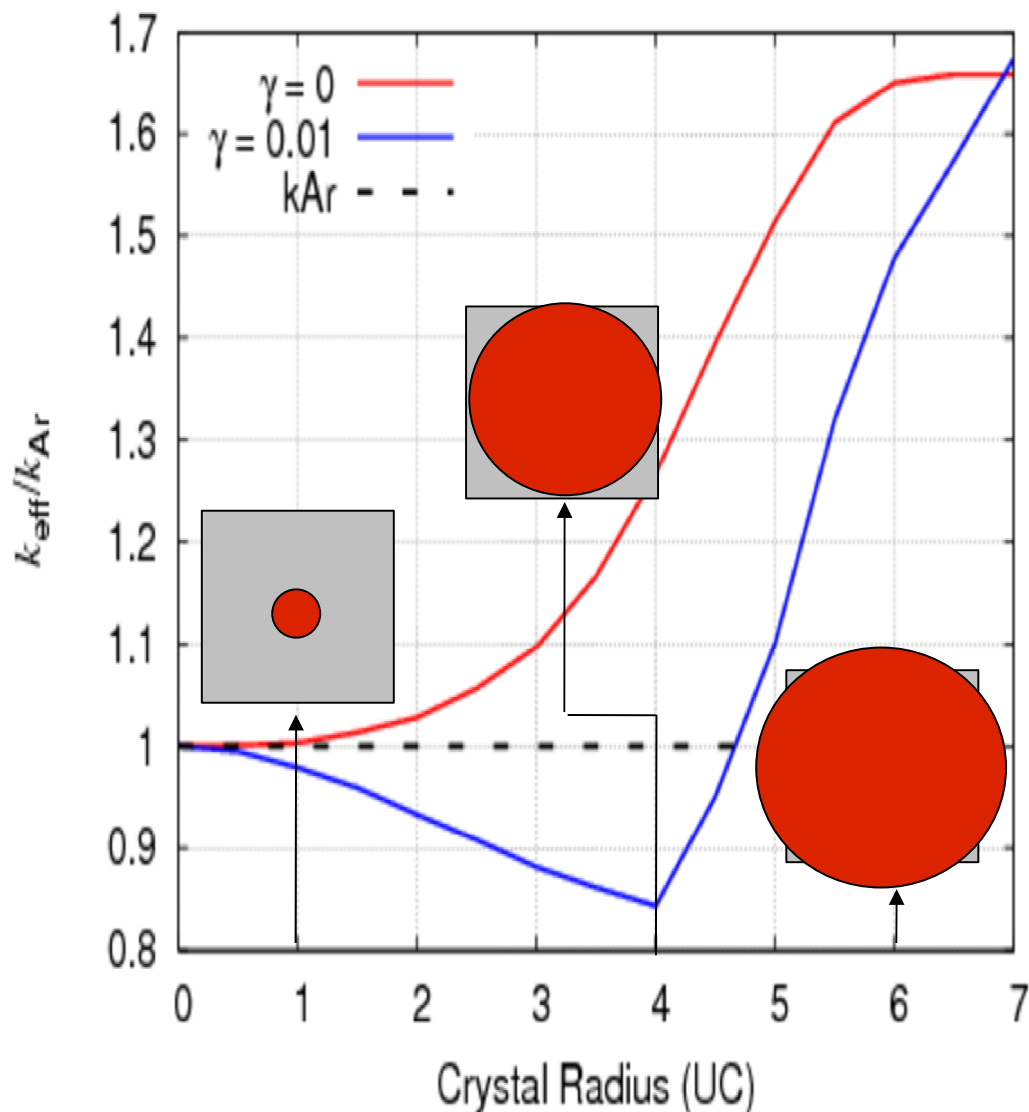


- $8 \times 8 \times 8$ ,  $16 \times 8 \times 8$ ,  $32 \times 8 \times 8$  and  $16 \times 16 \times 16$  FCC UC domains

- Varied the simulation parameter (crystal size, block size or number fraction)

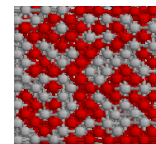
- Argon
- Krypton

# Analytic Model

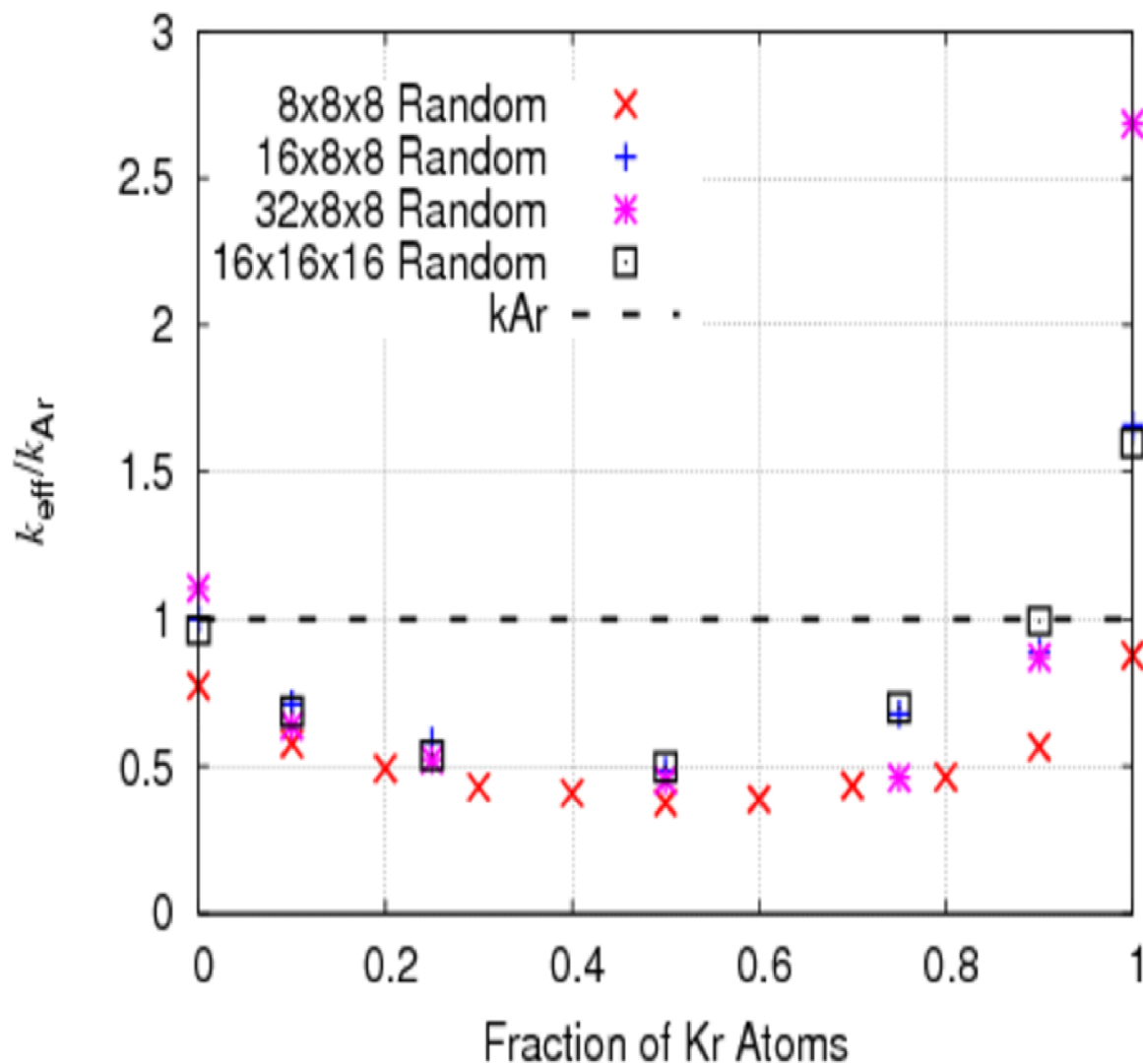


$$k_{eff} = \left[ \frac{(1 - n_{Kr})}{k_{Ar}} + \frac{n_{Kr}}{k_{Kr}} + \gamma A_S \right]^{-1}$$

- Smooth transition from primary to secondary
- Thermal conductivity minimized when interface is maximized



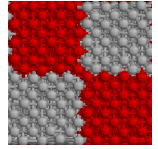
# Random Distribution of Atoms



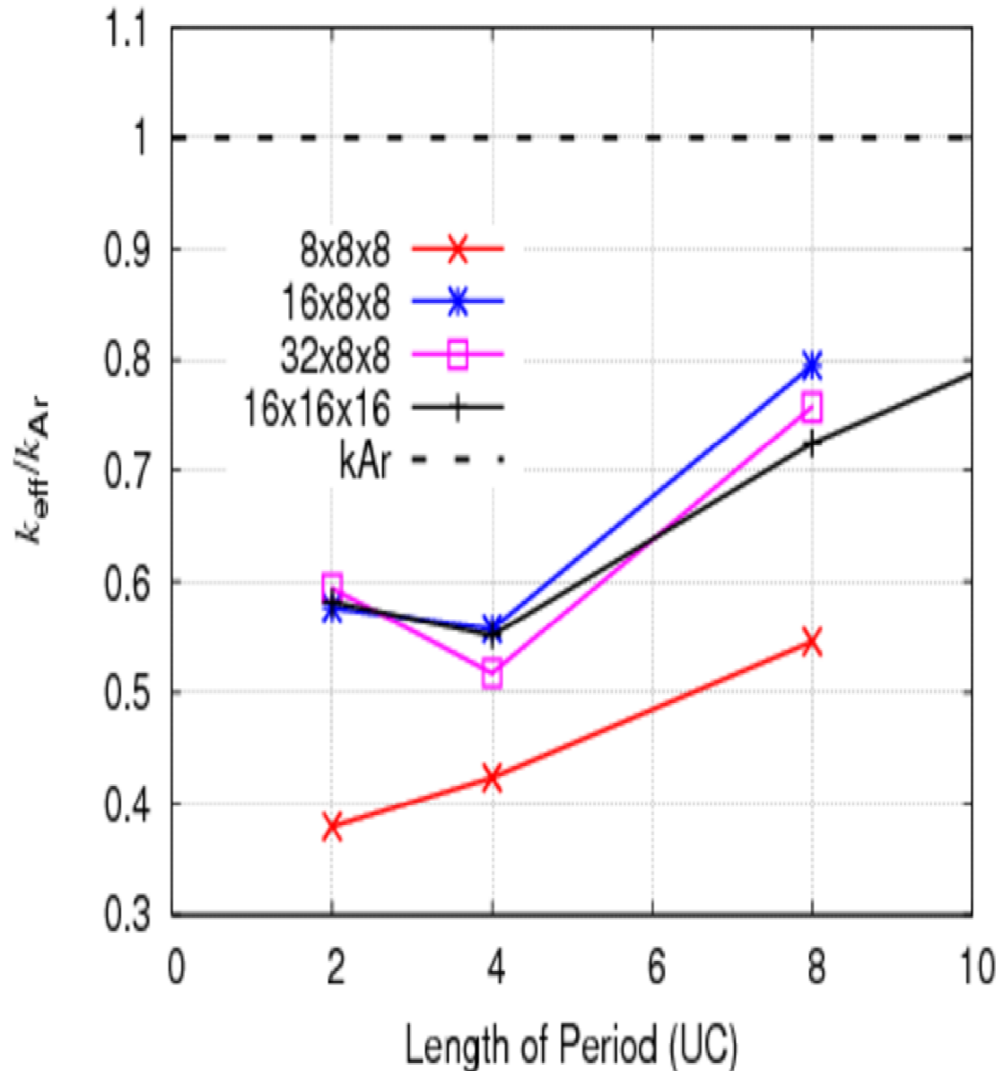
- 50% atomic number fraction has the lowest thermal conductivity of all configurations being 0.49 for 8x8x8

- Greater reduction of thermal conductivity found in larger simulations (Maximum of 59% achieved in 32x8x8 case)

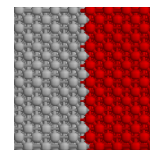
- This is assumed to be the alloy limit for Argon/Krypton



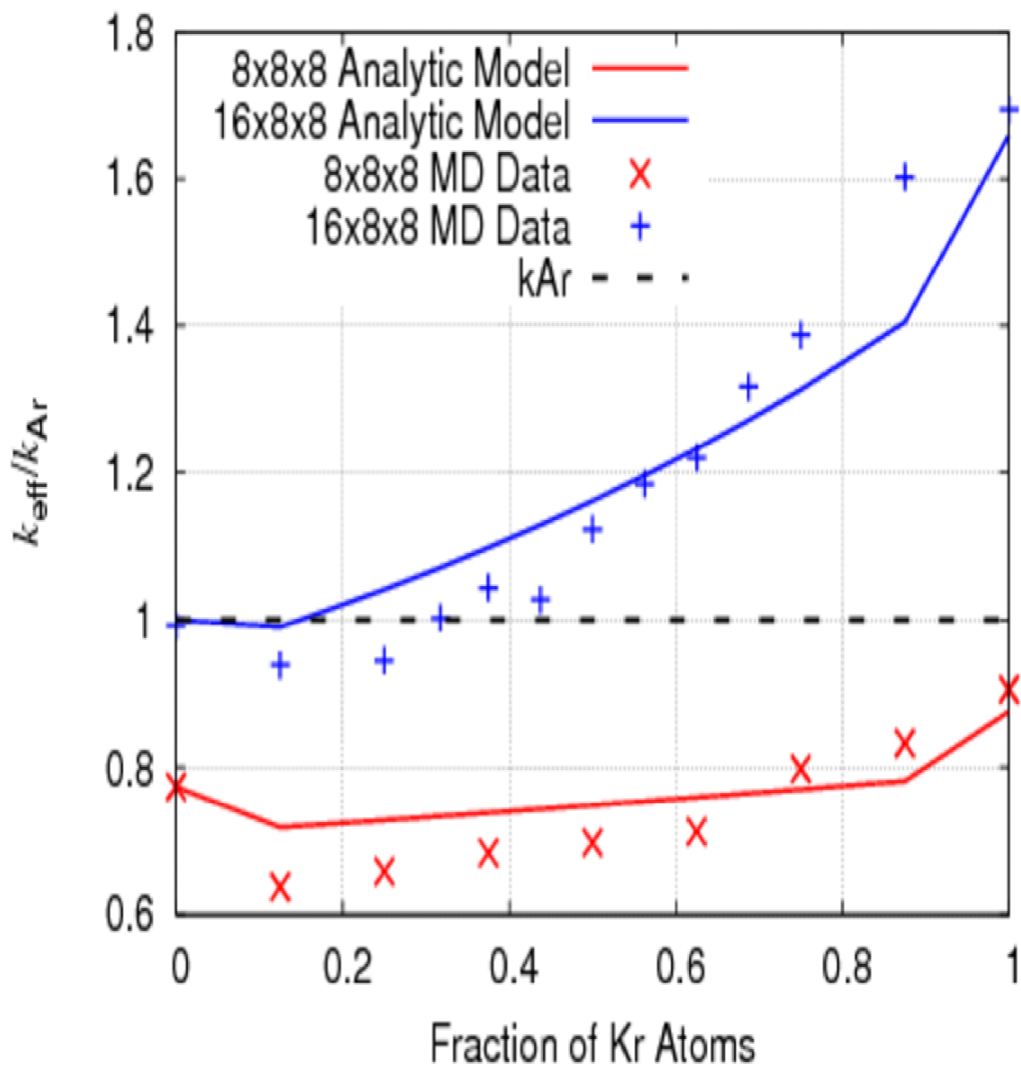
# Constant Number Fraction Results



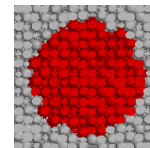
- Thermal conductivity is reduced by decreasing the period of “blocks”
- Greater than 50% reduction
- Optimal period length in larger domains
- 16 UC lengths include longer wavelength phonons



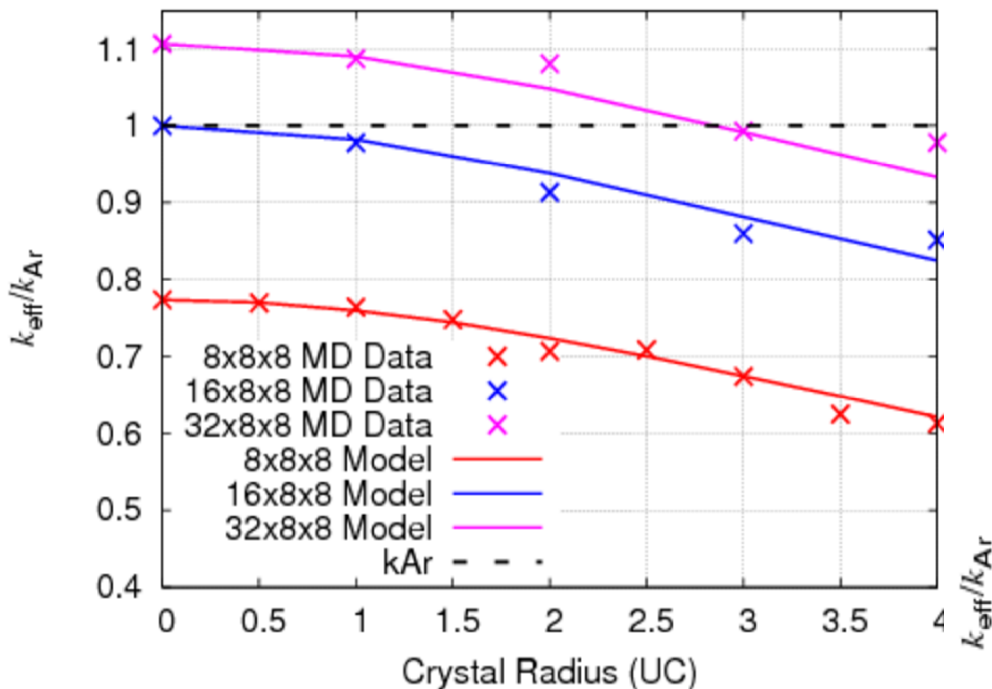
# Constant Interface Area Results



- Constant interfacial area of  $64 \text{ UC}^2$
- No interfacial area at number fractions of 0 and 1 (interface not within domain)
- Reasonable agreement with model, same fit parameter as in single crystal

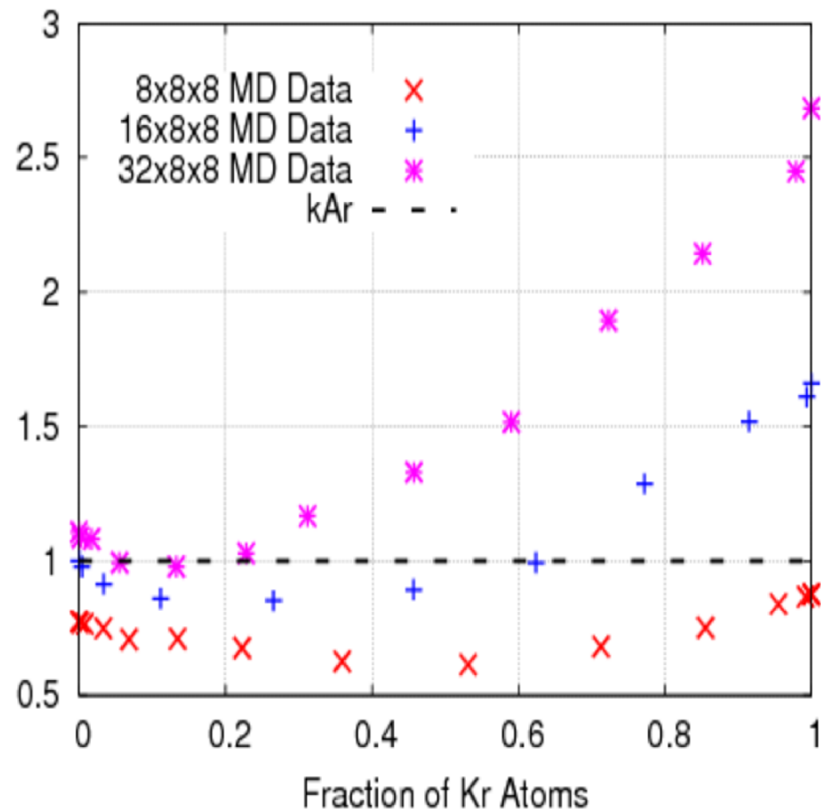


# Single Crystal Results

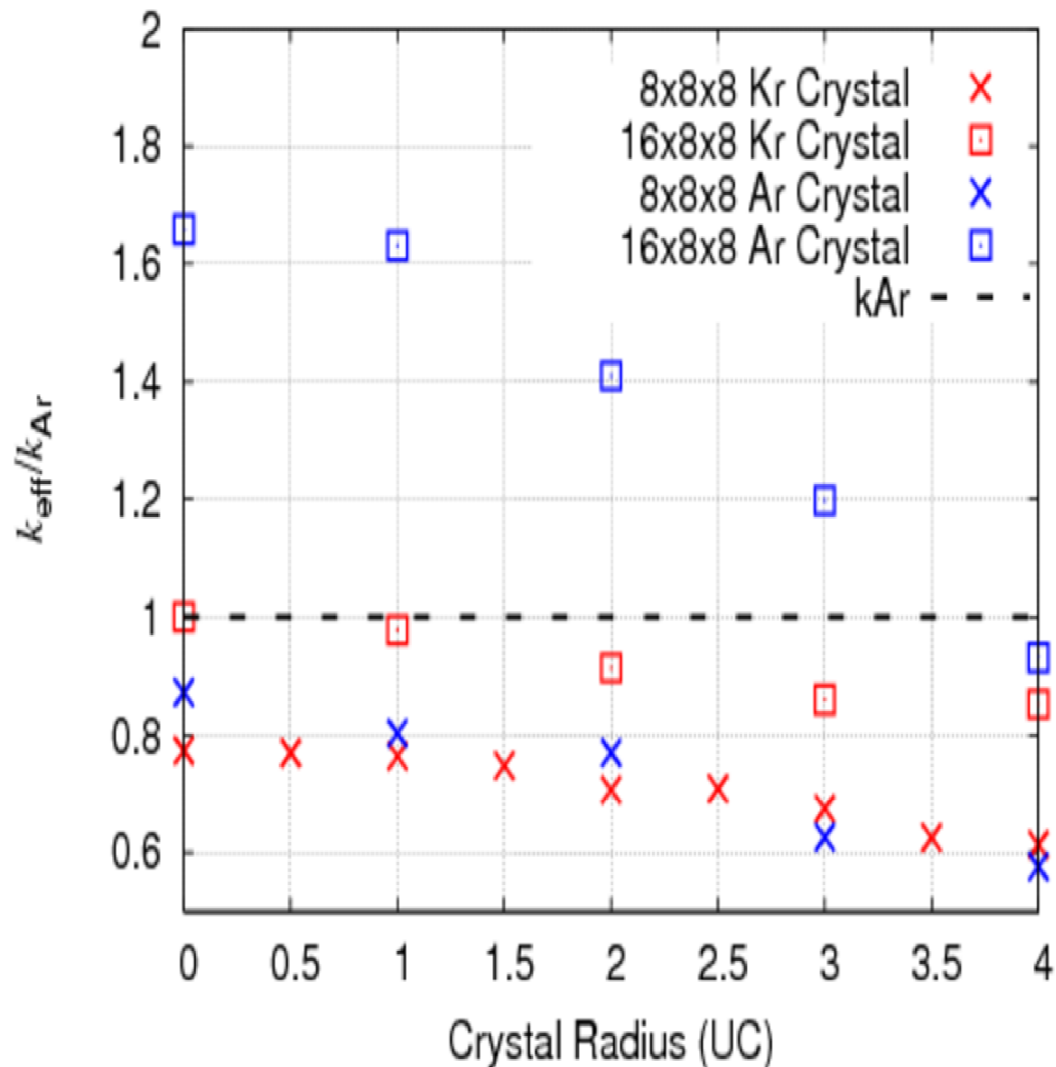
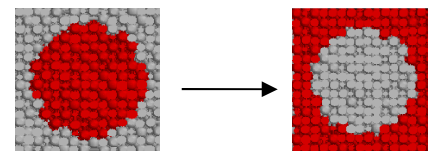


- Interface dominates thermal conductivity
- Decreases until the crystal becomes an inscribed sphere

• Conductivity increases with increasing fraction of Krypton atoms beyond inscribed sphere

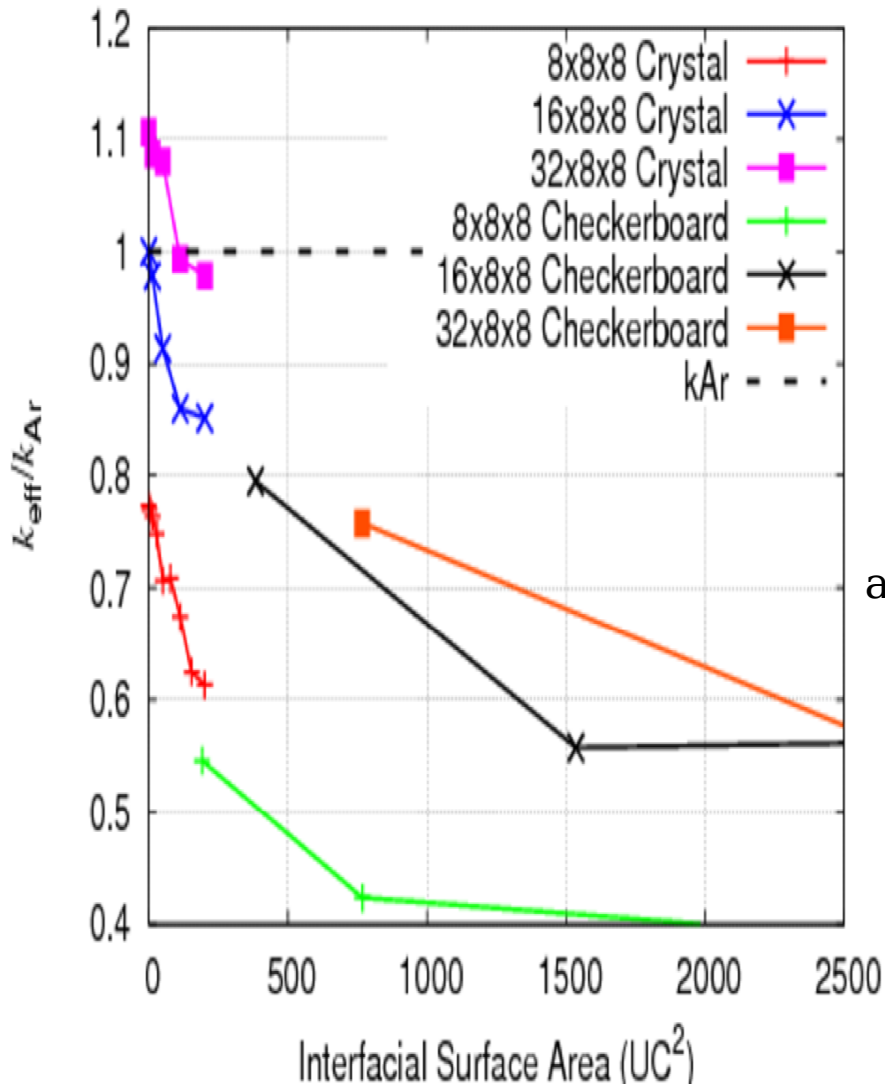


# Argon Krypton Switch



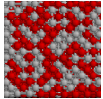
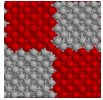
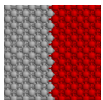
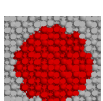
- Lower thermal conductivities found when the crystal was composed of the heavier material (Krypton) than when composed of the lighter material (Argon)
- Greater reduction found when the crystal was composed of the lighter material

# Summary of Results



- Much greater reduction in thermal conductivity in the checkerboard cases over single crystal
- Conductivity is related to interfacial area

alloy →

Device	Min $k_{eff}/k_{Ar}$	Parameter
	0.49	$n_{Kr} = 0.5$
	0.52	$l_p = 4$ UC
	1.00	$x = 8$ UC
	0.85	$r = 4$ UC

# Conclusions

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- Single crystal results were comparable to observations from the literature
- Single crystal should be as large as possible within the domain to maximize interfacial area
- Embedded material of lower conductivity adds to effect of interface

# Acknowledgements

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