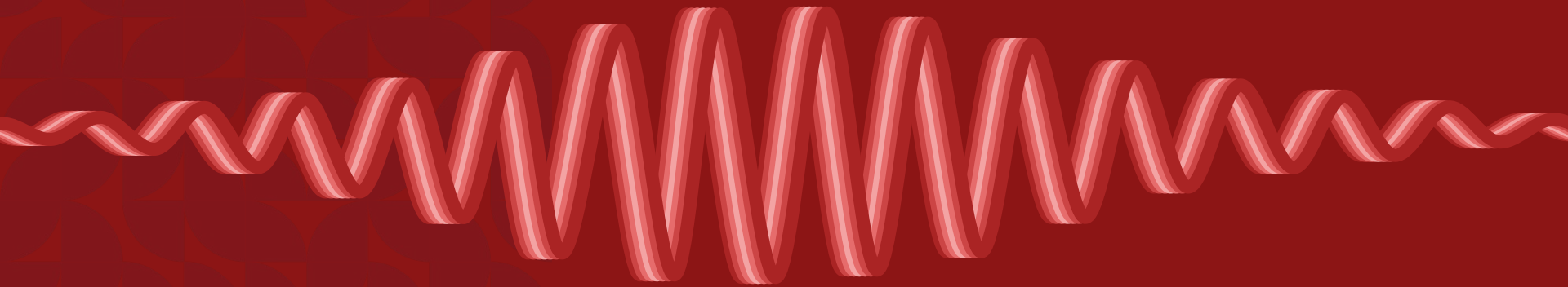
Bulk Thermal Conductivity Model for Un-doped Single-Crystal Semiconductor & Dielectric Materials



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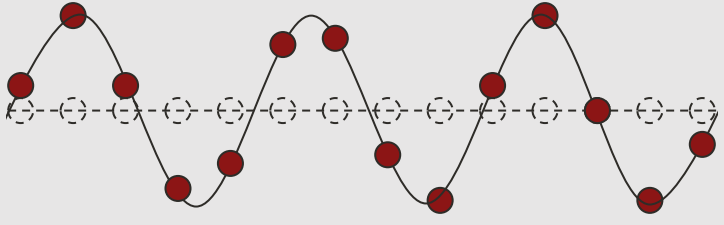
ME 233 - Automated Model Discovery
March 13th, 2025

Stanford University

Background & Physics

Semiconductor & Dielectric Materials:

- **Phonons are the dominant energy carrier** in dielectric/semiconductor materials.
- Phonons are quantized **atomic displacement waves** that carry energy through crystalline lattices.
  - Although massless, these quanta display particle/wave behavior similar to other energy carriers (e.g. photons, electrons).
  - **Acoustic phonons** (longitudinal & transverse) **are the main contributors to thermal conductivity**, relative to optical phonons, due to a much greater group velocity



Phonon Thermal Conductivity Integral:

$$k(T) = \frac{1}{3} v^2 \int_0^{\theta_D/T} C_s(x_\omega, T)\tau(x_\omega, T) dx_\omega, \quad \text{where } x_\omega = \frac{\hbar\omega}{k_B T}$$

Heat capacity per unit volume, C□

$$C_s = 9 n_a k_B \left(\frac{T}{\theta_D}\right)^3 \frac{x_\omega^4 \exp(x_\omega)}{[\exp(x_\omega) - 1]^2} = \begin{cases} \frac{12\pi^4}{5} n_a k_B \left(\frac{T}{\theta_D}\right)^3, & T << \theta_D \\ 3 n_a k_B, & T >> \theta_D \end{cases}$$

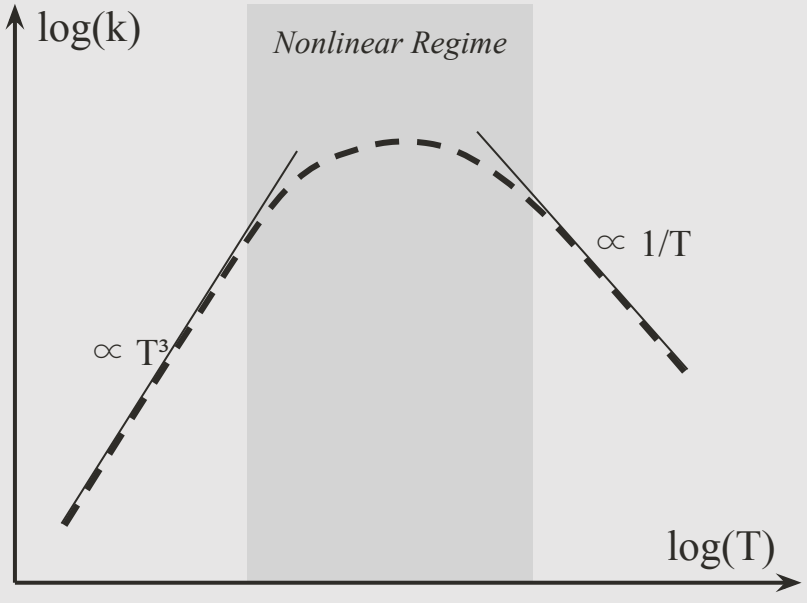
Relaxation time, τ

$$\tau^{-1}(x_\omega, T) = \tau^{-1}_{phonon-phonon} + \cancel{\tau^{-1}_{phonon-impurity}} + \cancel{\tau^{-1}_{phonon-boundary}}$$
$$= A T^\gamma \omega^n \exp(-B x_\omega)$$

Assumptions:

- Neglecting other energy carrier contributions (e.g. electrons)
- Materials are **undoped/pure** (no impurity scattering)
- Properties are **not limited by size effects** (no boundary scattering)
- Isotropic material properties

Project Objectives



Goals:

- **Rediscover known scaling behavior**:
  - $k \propto T^3$, for small T
  - $k \propto 1/T$, for large T
- Discover change in regime using smooth Heaviside function
- Discover model for **predicting/interpolating nonlinear regime**

Principle Objective:

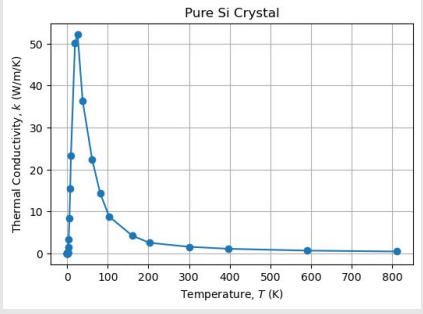
- Discover (ideally sparse) **universal model** for thermal conductivity curves

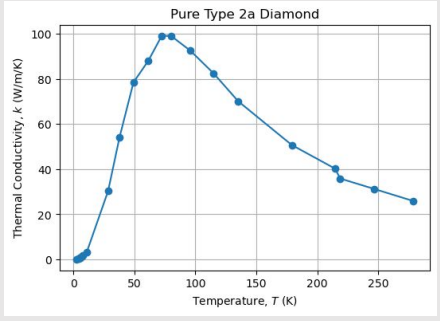
Data

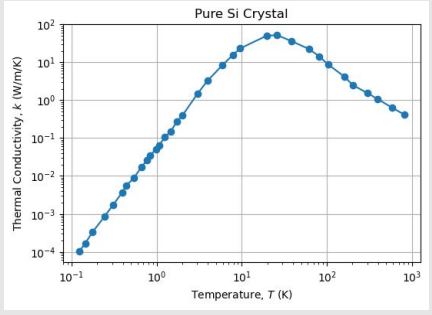
Undoped material data found in literature:

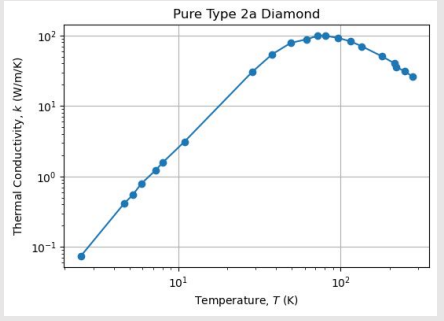
- Semiconductor materials: Si, Ge
- Dielectric materials: Diamond, NaCl

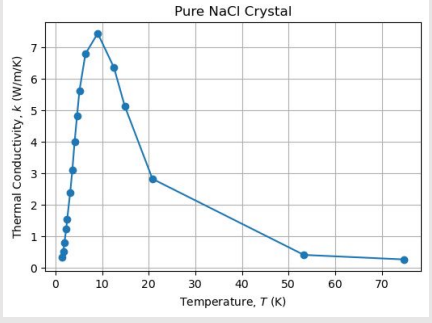
(log-log scaling to improve model learning performance)

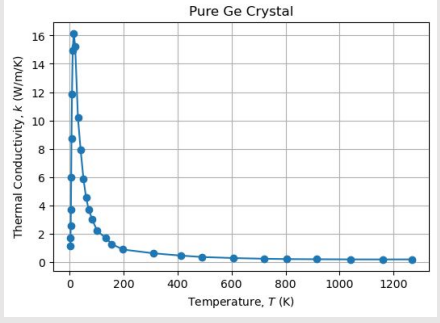


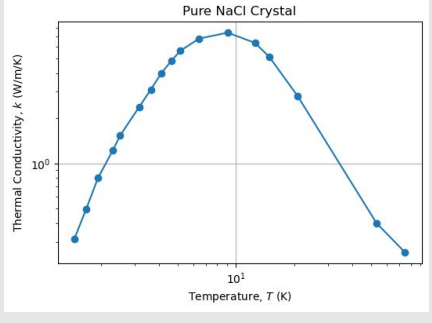


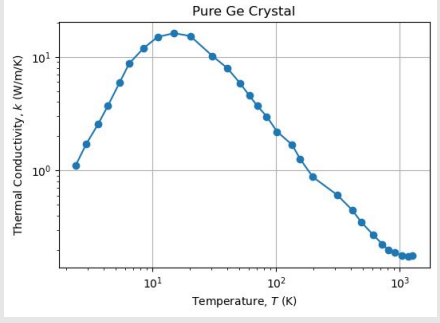






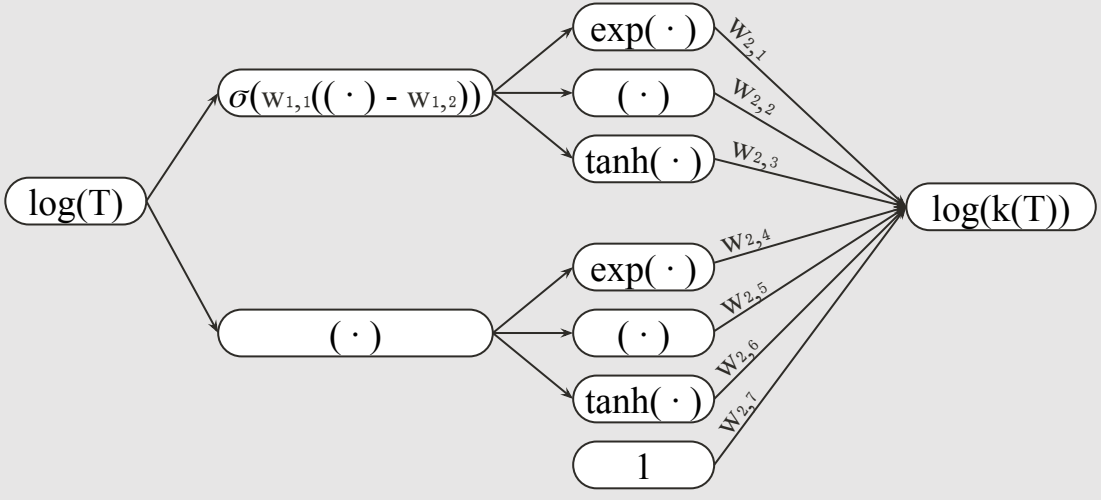






Neural Network & Model Parameters

Neural Network Architecture:



Loss Function:

$$\Rightarrow \quad L(\theta; log(T)) = ||\widehat{log(k)} - log(k)(\theta; T)||_2^2 + \alpha||\theta||_1$$

Evaluation Metric:

$$\Rightarrow \quad R^2 = 1 - \frac{||\log(k) - \widehat{\log(k)}||_2^2}{||\log(k) - \overline{\log(k)}||_2^2}$$

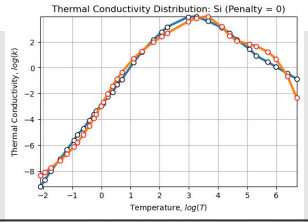
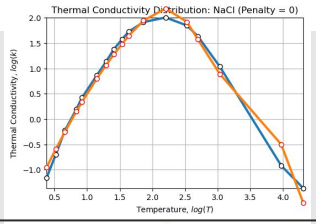
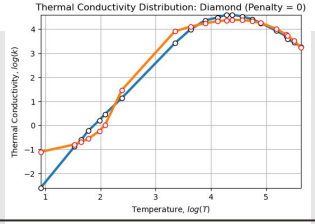
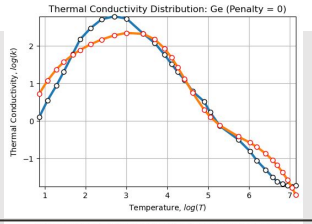
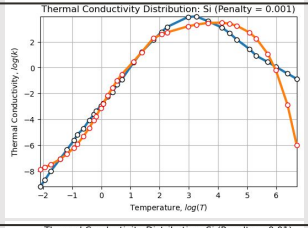
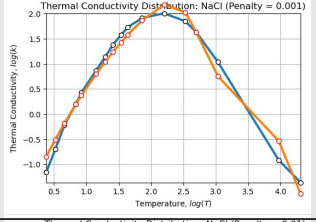
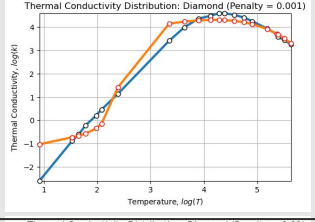
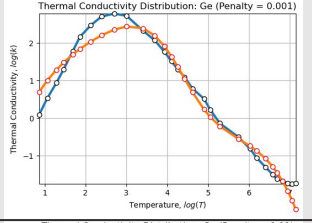
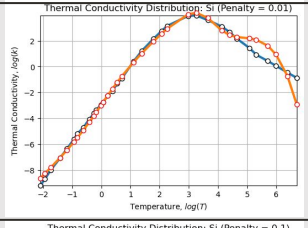
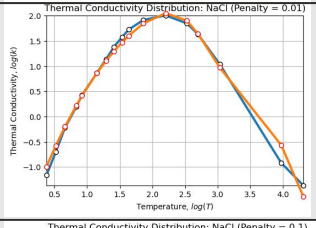
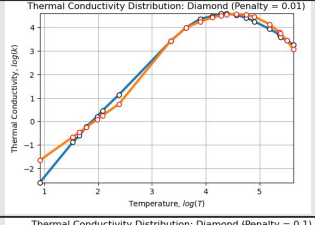
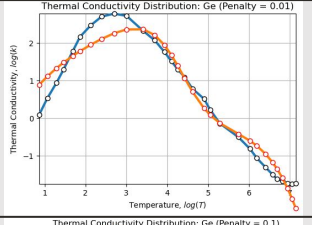
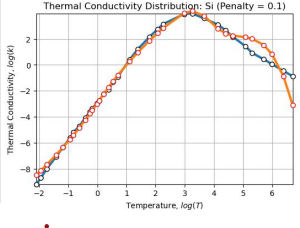
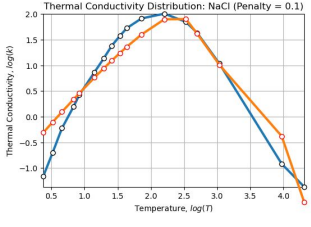
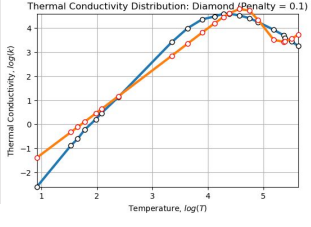
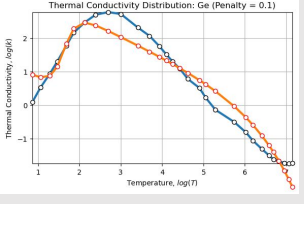
Optimization:

- Adam optimizer with exponential decaying learning rate:
  - initial_learning_rate = 5e-4
  - decay_steps = 5000
  - decay_rate = 0.95

Model Parameters:

- num_epoches = 10000
- batch_size = 10
- $\alpha \in [0, 0.001, 0.01, 0.1]$

Results - L1 Regularization

	Si	NaCl	Diamond	Ge
$\alpha = 0$				
$\alpha = 0.001$				
$\alpha = 0.01$				
$\alpha = 0.1$				

Results - Learned Model Weights and R^2

	Si	NaCl	Diamond	Ge	Si	NaCl	Diamond	Ge	Si	NaCl	Diamond	Ge	Si	NaCl	Diamond	Ge
	a = 0	a = 0	a = 0	a = 0	a = 0.001	a = 0.001	a = 0.001	a = 0.001	a = 0.01	a = 0.01	a = 0.01	a = 0.01	a = 0.1	a = 0.1	a = 0.1	a = 0.1
w_1,1	3.9384	4.4522	6.0648	2.3931	8.3909	5.6488	6.8676	2.0785	2.9153	4.0872	7.9840	2.3680	2.9267	7.4892	6.4518	6.4599
w_1,2	3.9880	2.6474	2.4755	4.2583	1.5422	2.7429	2.4713	4.2351	3.7523	2.7257	3.2696	4.3753	3.6933	2.6672	4.8974	1.5550
w_2,1	-0.0097	-0.0835	-0.0125	-0.0021	-0.0154	-0.0753	-0.0086	-0.0027	-0.0131	-0.0686	-0.0188	-0.0028	-0.0133	-0.0846	0.0004	-0.0017
w_2,2	1.3637	1.8962	1.0744	0.4097	0.7934	1.6742	0.5762	0.6919	2.1926	1.3862	1.8005	0.6242	2.1732	1.5746	1.7462	-0.5773
w_2.3	2.6462	0.9600	-1.8159	3.0462	3.2878	1.0606	-0.2216	1.9121	1.1258	1.9800	-0.3588	1.1452	1.0472	0.0001	-0.0566	0.0017
w_2,4	-2.0959	-0.6929	-0.5344	-1.5165	-0.2970	-0.8010	-0.3715	-1.9132	-1.7944	-0.9790	-1.1451	-0.7153	-2.9272	-0.7843	-1.8975	1.3959
w_2,5	-0.9297	-1.2446	1.2860	-0.9124	0.3526	0.1753	2.6601	-0.2082	-1.3702	-0.3130	2.7478	-0.7597	-0.0004	-0.0001	-0.0002	0.0019
w_2,6	1.4883	-0.2919	3.7637	-0.0395	1.3911	-1.6817	2.6933	-1.4594	-0.9271	-0.3783	0.9724	-2.5921	-0.0004	-0.0001	0.0003	0.0024
w_2,7	-0.8124	-1.2067	-0.2163	-0.2427	-2.7414	-0.9596	-1.0129	0.6889	-1.1565	-1.1543	-1.8633	0.2745	-0.0003	0.0001	-1.0590	0.0016
R^2	0.9836	0.9804	0.9672	0.9580	0.9097	0.9740	0.9578	0.9628	0.9803	0.9876	0.9864	0.9492	0.9789	0.9036	0.9604	0.9351

$\sigma(w_{1,1}((\cdot) - w_{1,2}))$

$w_{2,1}\exp(\sigma(w_{1,1}((\cdot) - w_{1,2})))$

$w_{2,2}\sigma(w_{1,1}((\cdot) - w_{1,2}))$

$w_{2,3}\tanh(\sigma(w_{1,1}((\cdot) - w_{1,2})))$

$w_{2,4}\exp(\cdot)$

$w_{2,5}(\cdot)$

$w_{2,6}\tanh(\cdot)$

$w_{2,7}$

$$\Rightarrow \begin{cases} \log(k) = w_{2,2}\sigma(w_{1,1}(\log(T) - w_{1,2})) + w_{2,4}\exp(\log(T)) \\ k \sim T + \exp(-T) \end{cases}$$

Remarks/Conclusions:

- α too small → no sparsity induced
- note, α too large → poor convergence/oscillating loss function
- Small, random variations in R^2 value for both different materials and different values of α
- $w_{2,2} \neq -4$, $w_{2,2} \neq 3$, as anticipated by defined phonon scattering theory
- The global fit is decent (> 0.9) but not explainable by known physics
- Smooth heaviside function is inconsistent
- Insufficient model architecture and function space
- Insufficient data distributions (need a larger temperature range)

Limitations on Objectives:

☒ Rediscover known scaling behavior
☒ Discover change in regime using smooth Heaviside function
☐ Discover model for predicting/interpolating nonlinear regime
☐ Discover (ideally sparse) universal model for thermal conductivity curves

Thank You