Predicting Thermal Conductivity of Nanostructures by Implementation of Deep Neural Networks and Genetic Programming Based Symbolic Regression

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ABSTRACT

Predicting models for thermal conductivity (TC) of novel nanostructures have diverse applications. Within this process, new materials along with a better understanding of thermal management can be achieved. Although, the nature of TC makes it usually a troublous goal to predict. While experiments on this problem are quite expensive and inefficient to use, the classic models that have been used to predict TC are not effective neither when compared to those of density functional theory (DFT) nor molecular dynamics (MD) simulations. Providing researchers with a powerful tool to predict TC, DFT and MD acquire hours of CPUs and relatively high computing cost. This trouble seems to be more serious when the TC in larger scales is required. Herein, we use deep learning neural networks as well as proposing a genetic programming based Symbolic Regression (SR) approach to train the algorithms and obtain a better predicting model of nanostructure thermal conductivities. Our results show a five-fold reduction in simulation time versus current methods such as molecular dynamics or density functional theory.

OBJECTIVES

In this study we explore machine learning models with the concentration of extrapolations to investigate thermal conductivity of any lattice nanostructure provided enough input parameters such as bulk, shear, and young's modulus and environmental parameters are available.

MATERIALS & METHODS

In total, there are 347 nanostructure samples as our dataset all carried out based on DFT. We use a hybrid cross-validation approach including both K-Fold CV and holdout validations to compare these models. To evaluate our models, we use two well-known statistical criteria which are RMSE and R^2 as our metrics.

Our first model uses genetic programming for **Symbolic Regression (SR)** which can generate a physical formula connecting material input properties to thermal conductivity. For symbolic regression we conduct two different models refer to as GP1 and GP2, the latter is using richer functions as opposed to the former which is only allowed to use some simple functions. The second model is a **deep neural network model of a Multi-Layer Perceptron (MLP)** which benefits from Adam optimizer.

RESULTS

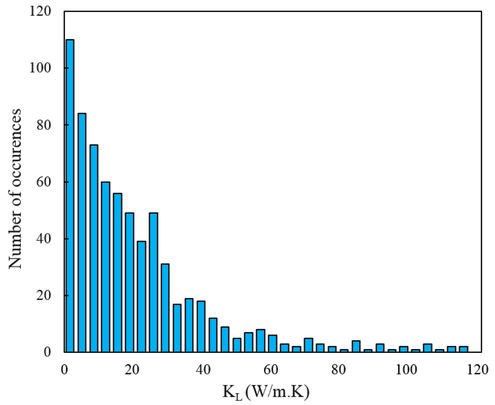
This was observed that neural networks are impressively strong in the process of training algorithm, and they outperform other models in all of our experiments during training. All models presented a weaker performance during extrapolation experiments comparing to cross-validation performance results. We believe this phenomenon occurs because of low distribution quality in our dataset since changing the set of data for training and using all the data in the domain has increased the efficiency.

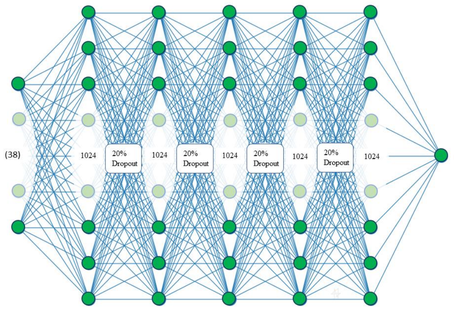
In some cases the GP1 model outperforms the GP2 models despite the fact that it generates a much simpler formula in terms of parameters and available functions. This is mostly because the GP2 model has to search an intensively larger space in comparison to the GP1 and while the models is limited in terms of operational space to generate a time efficient formula, it is clear to the authors that this model will perform better provided enough calculation time is available.

In our closest test to the actual extrapolation test, as we prevent the similarity of dataset may help the models to predict the thermal conductivity for evaluation block, The Neural Network model outperformed in this test.

CONCLUSION

There are admittedly both benefits and drawback to all machine learning models have been used in this study. The symbolic regression models are computationally expensive although the advantage is that it yields to an unprecedented formula with a physical insight. Having said that, it is impossible to apply this model to many problems as it is quite restrictive in terms of what it can do and not every property can be expressed with an explicit expression. Predicting such an expression may not be appropriate in complicated cases. On the contrary, the Neural Network models are believed to be able to make a relation between enough input data of almost any problem to the desired results provided the architecture is well-established and minding the overfitting not happen as well.





	GP1	GP2	MLP	Analytical	Best
Formula	$\frac{0.63Mn}{n_p}$	$\sqrt{Bn.cos^2\left(\frac{14.21}{n}\right)}$	-	$A.\frac{(\theta_c)^3 M^3\sqrt{Vn_p}}{n^{4/3}Ty_a^2}$	
Training RMSE	7.607	5.610	4.598	22.249	MLP
Testing RMSE	43.524	44.856	43.934	36.043	MLP
$Training\ R^2$	0.199	0.650	0.750	0.079	MLP
$Testing\ R^2$	-1.43	-2.009	-1.813	-1.109	MLP

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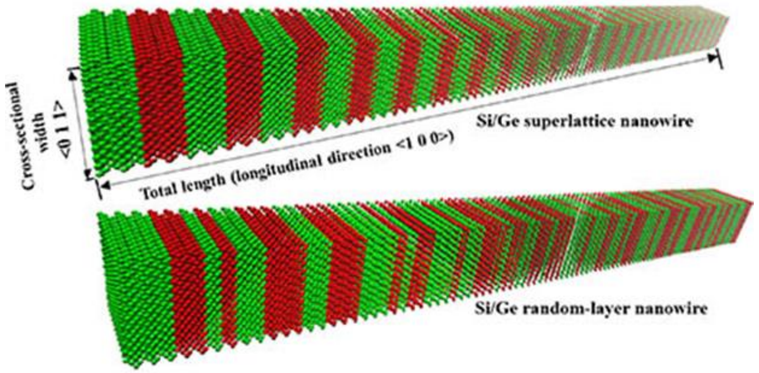
Superlattice and the need to investigate heat transfer in them

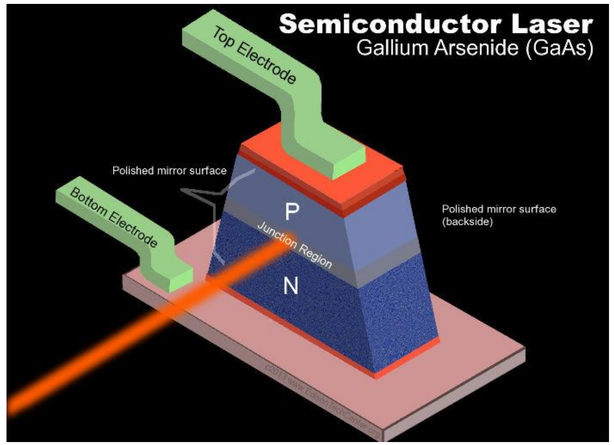
Superlattice

A superlattice is a periodic structure of layers of two (or more) materials. Typically, the thickness of one layer is **several nanometers**.



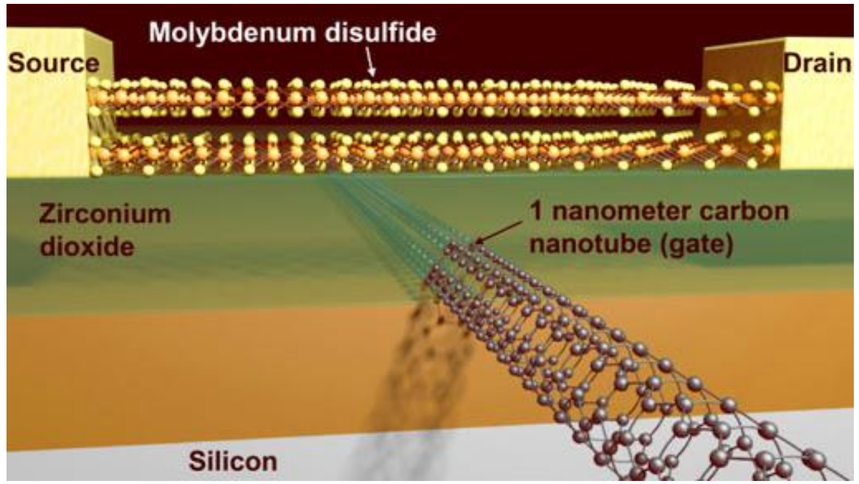
Zan Wang, Xingyu Cai, Tiezhu Mao. (2019) Thermal Transport in Silicon-Germanium Superlattices at Low Temperatures. *Journal of Nanomaterials* **2019**, 1-9.

Applications



Semiconductor Lasers

Available @ http://edisontechcenter.org/Lasers.html



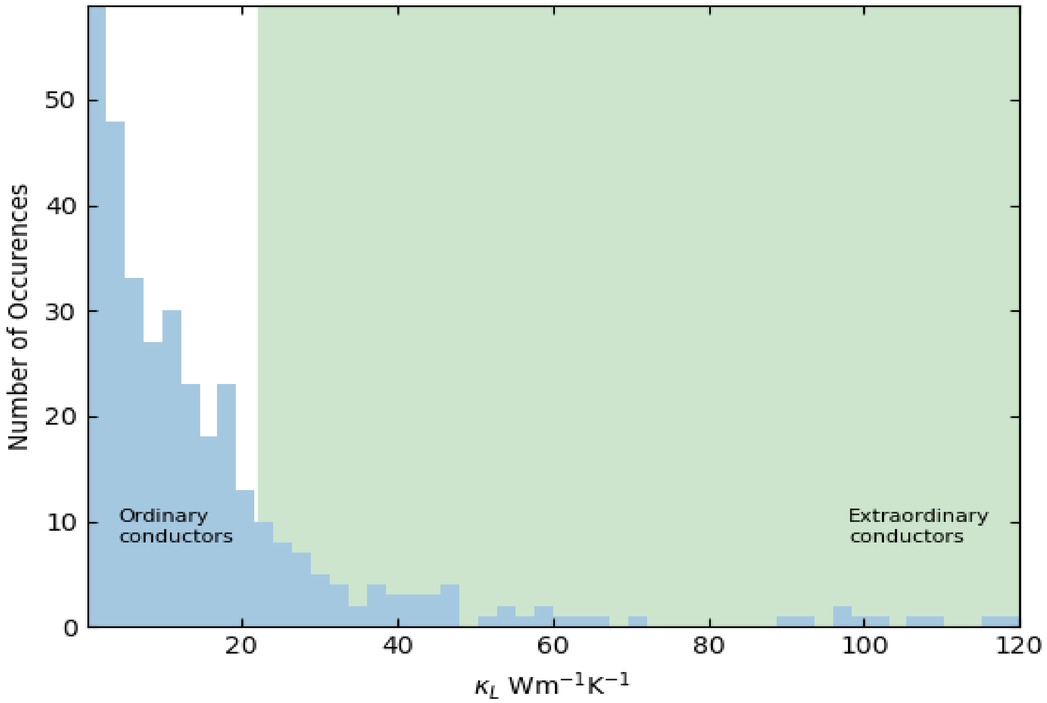
Nano Transistors

Available @ https://www.nanowerk.com/nanotechnology-news/newsid=44741.php

Materials, Data, and List of Descriptors

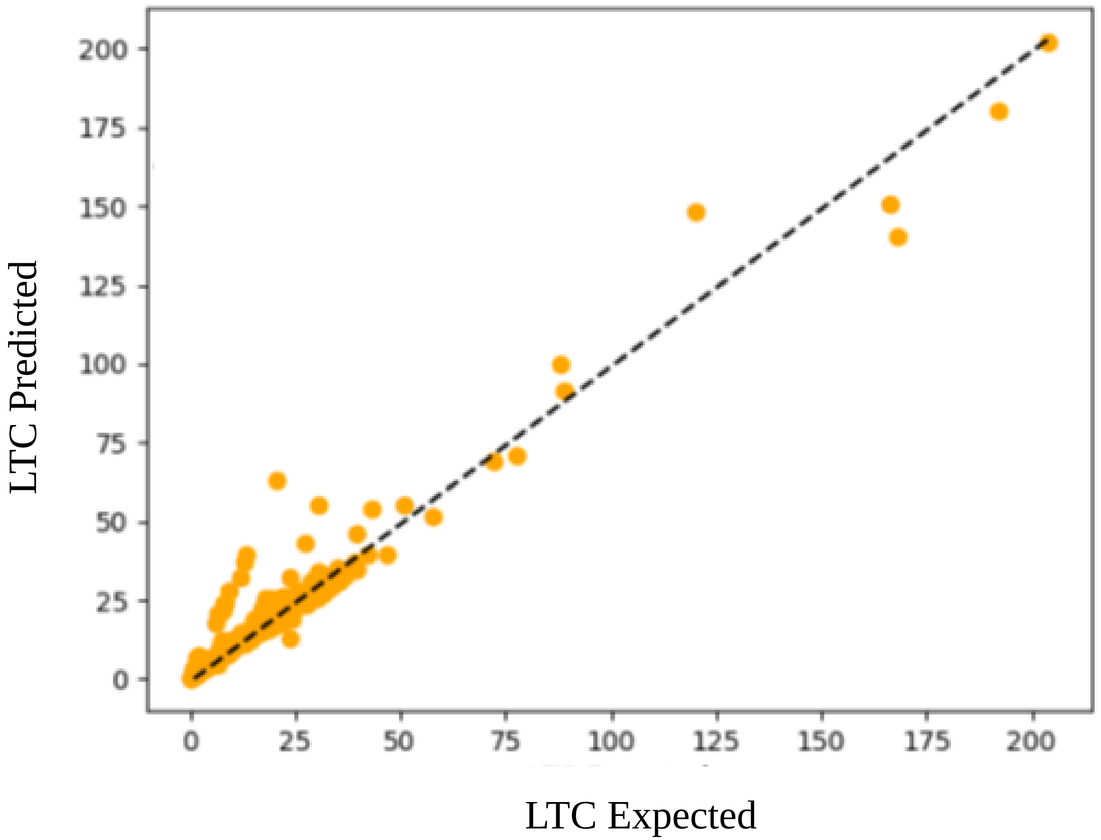
Dataset

- To prepare the dataset, all the first-principles calculations are carried out based on density functional theory (DFT) as implemented in the Vienna ab-initio Simulation Package (VASP)
- In total, there are 347 samples.



Variable Symbol	Definition
V	Volume per atom
T	Temperature (constant: 300 K)
M	Average atomic mass
n	Total number of atoms in unit cell
n_p	Total number of atoms in primitive cell
B	Bulk modulus calculated from C_{ij} [a]
G	Shear modulus calculated from C_{ij}
E	Young's modulus
ν	Poisson's ratio
H	Estimated hardness
B'	(δ B/δ.V)
G'	(δ G/δ.V)
ρ	Mass density
v_L	Sound velocities of the longitude
v_S	Sound velocities of the shear
v_a	Corresponding average velocity
Θ_D	Debye temperature
γ_L	Longitude acoustic Grüneisen parameters
γ_S	Shear acoustic Grüneisen parameters
γ_a	Average acoustic Grüneisen parameters
A	Empirical parameter

Verifying Effectiveness of Symbolic Regression



GP Model:

$$K_L = \frac{\theta e^2 \sqrt[3]{nM^2 \gamma e \sqrt[9]{\theta e^2}}}{n \sqrt[3]{T^7}}$$

Analytical Model:

$$K_L = A. \frac{(\theta_e)^3 M \sqrt[3]{V n_p}}{n^{4/3} T {\gamma_a}^2}$$

Interpolation Test:10-Fold cross-validation

Model	GP1	GP2	MLP	Analytical	Best
	Round 1	Round 2	Round 3	Round 10	
Formula	$\frac{G}{H.n_p}$	$\frac{\sqrt[6]{V}.n\sqrt{n}}{\sqrt[12]{\cos(\cos(E))}}$	-	$A.\frac{(\theta_e)^3 M^3\sqrt{V n_p}}{n^{4/3} T {\gamma_a}^2}$ ...	
RMSE	15.914	16.184	11.816	16.349	**MLP**
R^2	0.368	0.346	0.651	-1.206	**MLP**

Extrapolation Test: 5-fold Cross Validation

Extrapolation Tests

	GP1	GP2	MLP	Analytical	Best
Formula	$\frac{Mn}{n_p}$	$\ln\left(\left\lvert\sqrt[3]{B\cos(\ln(\lvert p\rvert))}\right\rvert\right)^3.\left\lvert\ln\left(\left\lvert ln^3\left(\lvert\sqrt{G}\rvert\right)\right\rvert\right)\right\rvert$	-	$A.\frac{(\theta_e)^3 M\sqrt[3]{Vn_p}}{n^{4/3}T{\gamma_a}^2}$	
Training RMSE	21.458	19.759	18.792	20.697	MLP
Testing RMSE	5.089	5.558	4.166	4.727	MLP
$Training\ R^2$	-0.059	0.102	0.188	0.053	MLP
$Testing\ R^2$	-38.381	-45.97	-45.97	-32.971	GP1

	GP1	GP2	MLP	Analytical	Best
Formula	$\frac{0.31B}{n_p}$	$B^{\frac{1}{2}}n_p^{\frac{1}{9}}\cos(\cos(\sin(\cos V)))\cos(\frac{1}{\tan(e^n)^3})^2$	-	$A.\frac{(\theta_e)^3 M\sqrt[3]{Vn_p}}{n^{4/3}T{\gamma_a}^2}$	
Training RMSE	20.293	18.398	17.332	19.392	MLP
Testing RMSE	4.788	5.825	4.992	14.029	GP1
$Training\ R^2$	0.159	0.309	0.387	0.036	MLP
$Testing\ R^2$	-6.718	-10.424	-7.391	-65.266	GP1

	GP1	GP2	MLP	Analytical	Best
Formula	$\frac{0.68Mn}{n_p}$	$4ln^2(n).\sqrt[3]{Bn.cos^2\left(\frac{15.49}{n}\right)}.\sqrt[9]{\frac{B}{sin^2(M)}}$	-	$A.\frac{(\theta_e)^3 M\sqrt[3]{Vn_p}}{n^{4/3}T{\gamma_a}^2}$	
Training RMSE	5.534	4.729	3.113	19.451	MLP
Testing RMSE	45.257	44.038	43.979	37.999	MLP
$Training\ R^2$	0.196	0.413	0.745	0.083	MLP
$Testing\ R^2$	-1.98	-1.821	-1.814	-1.101	MLP

	GP1	GP2	MLP	Analytical	Best
Formula	$\frac{G}{8.36B}$	$\sqrt{Ecos(ln^2(\lvert\cos(\ln(\lvert\cos(n_p)\rvert))\rvert))}$	-	$A.\frac{(\theta_e)^3 M\sqrt[3]{Vn_p}}{n^{4/3}T{\gamma_a}^2}$	
Training RMSE	8.396	7.206	5.423	18.808	MLP
Testing RMSE	42.99	40.869	40.922	36.101	GP2
$Training\ R^2$	-0.01	0.256	0.579	0.124	MLP
$Testing\ R^2$	-0.353	-0.223	-0.226	0.046	GP2