F-2-07 Extended Abstracts of the 2020 International Conference on Solid State Devices and Materials, VIRTUAL conference, 2020, pp369-370

Accurate thermoelectric generator performance evaluation by deep learning using artificial neural network

Dai Peng[1], Daniel W. Newbrook[1], C.H. (Kees) de Groot[1] and Ruomeng Huang[1*]

[1] School of Electronics and Computer Science, University of Southampton
University Road, Southampton, SO17 1BJ
*Email:r.huang@soton.ac.uk Phone: +442380599305

Abstract

Thermoelectric (TE) generators convert waste heat into electricity and have attracted increasing interests in the search of cleaner, more sustainable energy sources. Along with the substantial improvement achieved on the performance of thermoelectric materials, the design of TE generators is also crucial as it bridges the TE materials and applicable TE products. However, designing thermoelectric devices is a difficult task due to the complexity in the multiple parameter optimization and is always relied on extensive, time and computational resource consuming simulations. Here we report, for the first time, the use of artificial neural network (ANN) to achieve a rapid and accuracy performance evaluation of thermoelectric generator. An average prediction error of 0.013 is reported with a 12 million times reduction of computation time.

1. Introduction

Sustainable energy generation is a growing issue for the world. Conventional fossil fuel energy production is both inherently unsustainable as the fuel is finite, but it is also increasing greenhouse gases leading to climate change. Thermoelectric power generation is one possible energy source that can be both sustainable and low emission. It is based on the Seebeck effect in which a voltage is produced by a constant temperature difference [1]. Output efficiency of these devices is dependent on both the materials used, characterized by the figure of merit $(ZT = \alpha^2\sigma/\kappa)$, and the design of the thermoelectric generator (TEG). Design of TEGs is often a challenging task as there are multiple parameters that need to be optimized, and this optimization can also be application specific. Methods for optimization include mathematical modelling which can be inaccurate depending on the models used [2], or finite element method (FEM) simulation which can be computationally expensive [3].

Here we apply deep learning technology to predict the performance of TEG. An artificial neural networks (ANN) is firstly trained through a dataset produced by FEM simulations using COMSOL Multiphysics®. The architecture of the ANN will be introduced, and the prediction performance of the ANN will be evaluated by the training loss as well as the prediction error.

2. Results and Discussion

A conventional TEG structure is adopted in this work as shown in Fig. 1. The geometric parameters including the dimensions of the n and p legs, electrical interconnects are labelled accordingly.

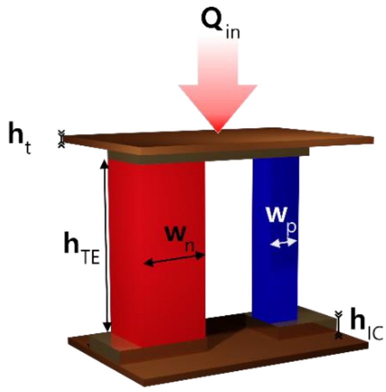

Fig. 1 Schematic of TEG simulated in this work showing parameters.

A dataset of 4112 TEG structures and their power performance were generated for the ANN training. This includes the first generation of 4112 random parameter sets. Table 1 lists the ranges and resolutions of each parameter. Fill factor (FF) is defined as the ratio of the thermoelectric area to the whole device area, where Q_{in} is the input heat flow which is fixed at 5,000 W/m^2. The cold side temperature was fixed at 300 K, and the height of the ceramic was fixed at 0.5 mm. The materials used for the metal interconnects and the ceramic are copper and quartz from the built-in COMSOL material library. PbTe and BiSbTe were used as the n and p type materials and their TE properties were taken from literature [4,5]. This parameter set was then simulated in COMSOL to obtain the power performance of each set. It should be noted that although the dataset needs to be generated by simulation, it is a one-time investment. Once the ANN has been properly trained, it can replace any simulation needed for future design, significantly reducing computational time.

Table I The range and resolution of each TEG parameter.

Parameter	Range	Resolution
w_n	1-10 mm	1 µm
w_p	1-10 mm	1 µm
h_{TE}	1-100 mm	1 µm
h_{IC}	0.5-5 mm	1 µm
FF	0.05-0.95	0.001

The dataset was then divided into three sub-groups for training (3330), validation (370) and testing (412) of the ANN. The architecture of the fully connected ANN used in this work is presented in Fig. 2. TEG parameters (i.e. p_1 to p_n) and the heat flow Q_{in} were fed into the input layer of the network which were connected to the output layer of power performance through a number of hidden layers. The hyper-parameter of the hidden layer was set to be 3 layers and 100 neurons per layer in this work.

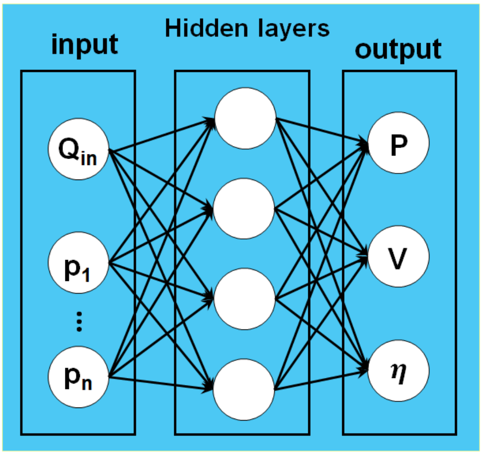

Fig. 2. The architecture of the fully connected artificial neural network used in this work.

The training and validation losses of the ANN are shown in Fig. 3. A low loss of 10^{-4} was achieved after 10,000 epochs, indicating a good training process. This is further verified by the low validation loss of *ca.* 3×10^{-4}.

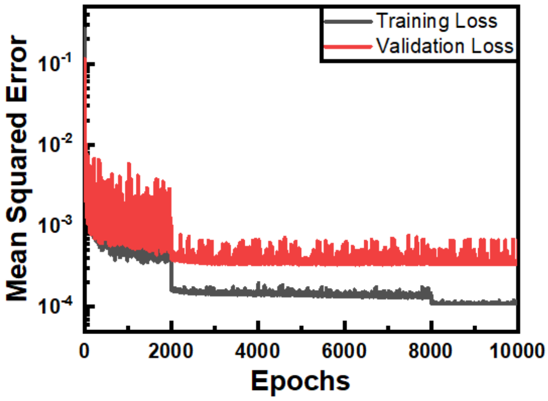

Fig. 3. The training (black) and validation (red) losses of the artificial neural network.

The prediction performance of the ANN is evaluated by the relative error of the predicted and true power output. This is calculated by the following equation,

$$Relative\ error = (P_{predicted} - P_{true})/P_{true}$$

and the distribution of the relative error is shown in Fig. 4. It is clear that a majority of the relative error is below 0.03. The average error is calculated to be 0.013, indicating an extremely high prediction accuracy of the network. The prediction time for 1000 TEGs is only 5 ms while the same simulation will cost *ca.* 17 hours using the same computer configuration. This translates to a significant saving of time and computational resource of 12 million times.

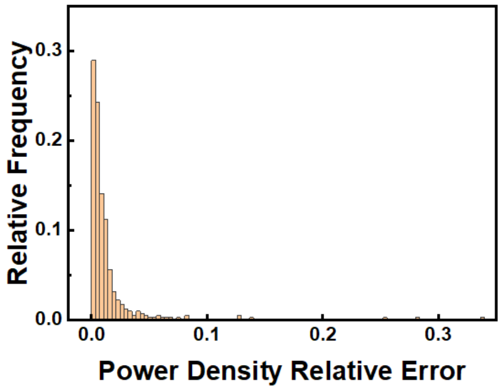

Fig. 4. The distribution of the relative error of the power density for the artificial neural network trained in this work.

3. Conclusions

This work reports the use of artificial neural network to obtain rapid and accurate prediction of the power performance for TEGs. A fully connected ANN containing 3 hidden layers and 100 neurons per layer was trained by a dataset with the size of 3330. An extremely high prediction accuracy manifested by the low average relative error of 0.013 was achieved. This network also enables a 12 million times saving of the time and computational resources. The successful demonstration of applying ANN in TEG design offers exciting prospects for further development of this technology in thermoelectric applications.

Acknowledgements

We would like to express sincere thanks to all the contributors to the Conference for their cooperation in the Conference program. The authors acknowledge the use of the IRIDIS High Performance Computing Facility, and associated support services at the University of Southampton, in the completion of this work.

References

[1] G.J. Snyder, E.S. Toberer, Complex thermoelectric materials, Nat. Mater. 7 (2008) 105–114.

[2] D.W. Newbrook, R. Huang, S.P. Richards, S. Sharma, G. Reid, A.L. Hector, C.H. (Kees) de Groot, Mathematical model and optimization of a thin-film thermoelectric generator, J. Phys. Energy. 2 (2019) 014001.

[3] Min Chen, L.A. Rosendahl, T.J. Condra, J.K. Pedersen, Numerical Modeling of Thermoelectric Generators With Varing Material Properties in a Circuit Simulator, IEEE Trans. Energy Convers. 24 (2009) 112–124.

[4] J. Zhang, D. Wu, D. He, D. Feng, M. Yin, X. Qin, J. He, Extraordinary Thermoelectric Performance Realized in n-Type PbTe through Multiphase Nanostructure Engineering, Adv. Mater. 29 (2017) 1–7.

[5] B. Poudel, Q. Hao, Y. Ma, Y. Lan, A. Minnich, B. Yu, X. Yan, D. Wang, A. Muto, D. Vashaee, X. Chen, J. Liu, M.S. Dresselhaus, G. Chen, Z. Ren, High-Thermoelectric Performance of Nanostructured Bismuth Antimony Telluride Bulk Alloys, Science (80-.). 320 (2008) 634–638.