

Evaluation of Efficiency Factors of Commercial Thermoelectric Materials Using COMSOL Multiphysics® Software

S. Seif¹, K. Cadien¹, T. Thundat¹

1. Department of Chemical & Materials Engineering, University of Alberta, Edmonton, AB, Canada

Introduction: Many challenges have been raised about the applicability and reliability of the dimensionless figure of merit (ZT) in estimating the efficiency factor (Φ) of different thermoelectric (TE) materials. To avoid these challenges, we have developed special program using Comsol Multiphysics to compute Φ of TE materials without using conventional ZT parameters. The obtained Φ in eight TE materials are within the range as those reported in the literature between $0.091 \mu\text{Wcm}^{-2}\text{K}^{-2} \leq \Phi \leq 0.001 \mu\text{Wcm}^{-2}\text{K}^{-2}$. This work has shown that Comsol Multiphysics is a powerful tool for analysis of TE materials and can be used to predict Φ without using conventional ZT.

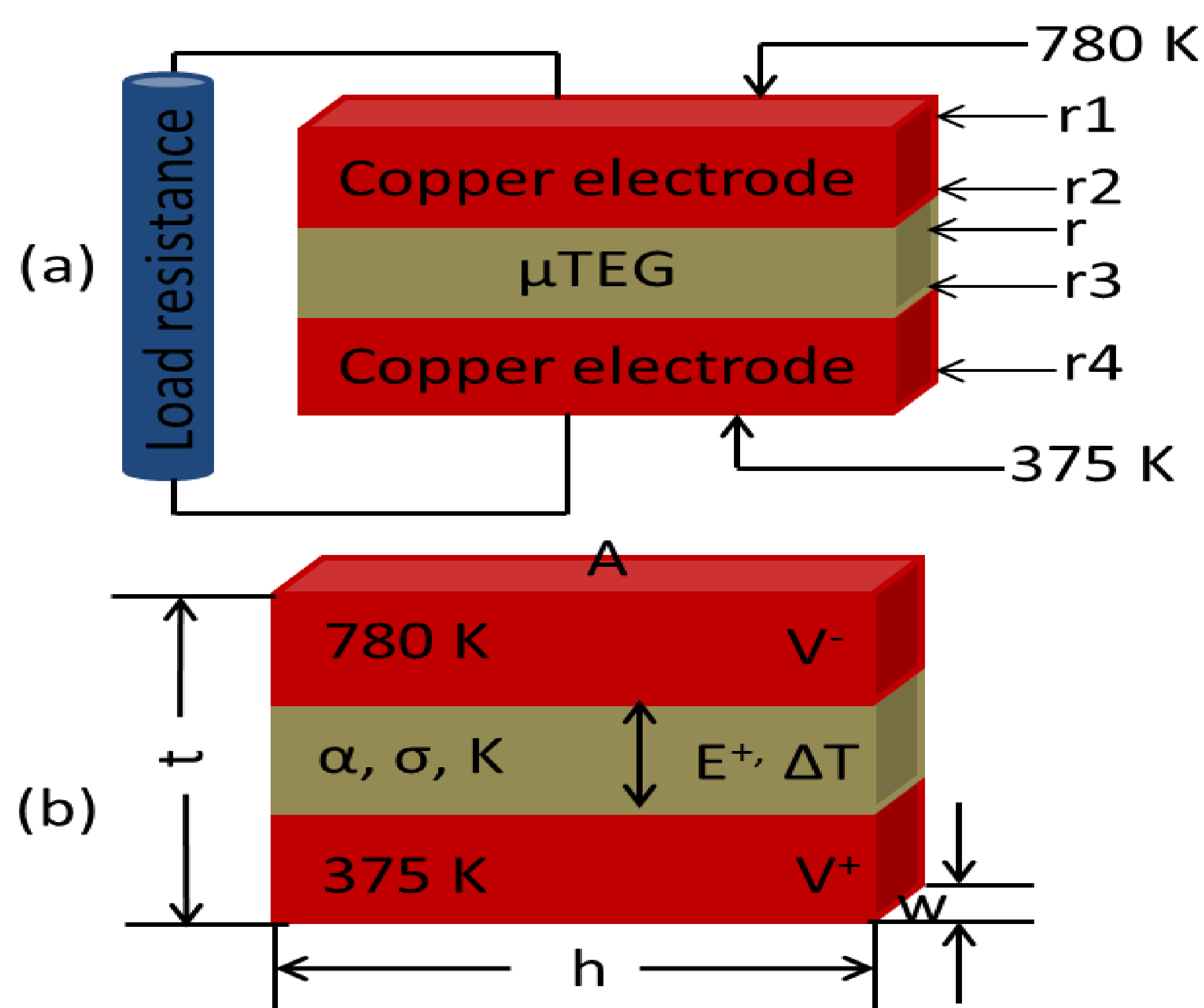


Figure 1. (a) Single leg model, (b) parameters used for simulation.

Computational Methods: The following equations were used to insert TE parameters in Partial Differential Equation (PDE).

$$\nabla \cdot (-c\nabla u) = f \dots \dots \dots (1)$$

$$c = \begin{pmatrix} \lambda + \sigma\alpha^2 & \sigma\alpha T \\ \sigma\alpha & \sigma \end{pmatrix} \dots \dots \dots (2)$$

$$f = \begin{pmatrix} \sigma((\nabla V)^2 + \alpha \nabla T \nabla V) \\ 0 \end{pmatrix} \dots \dots \dots (3)$$

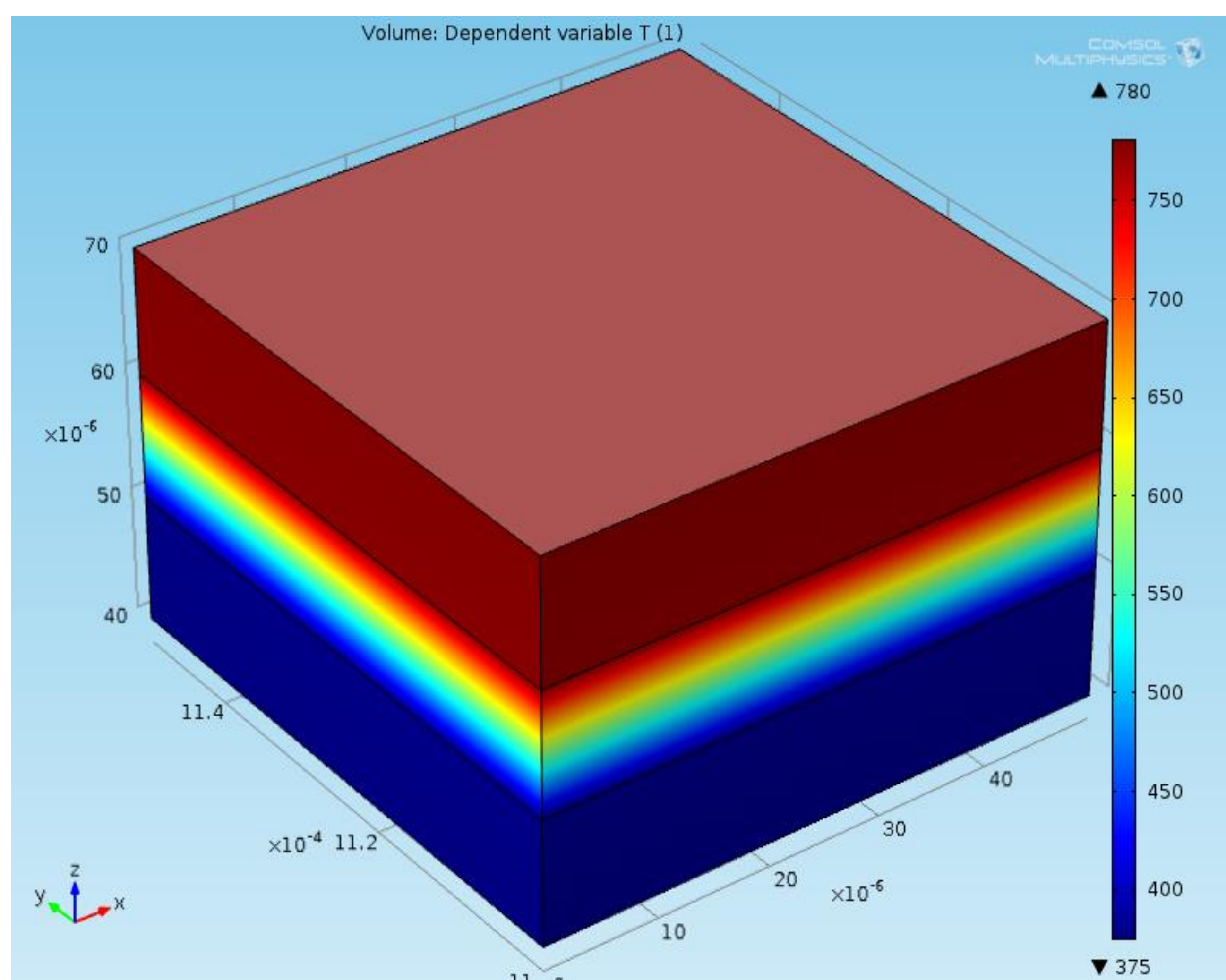


Figure 2. Temperature distribution in a single leg model.

$$P = [\sigma A(\alpha \nabla T - E)] * V \dots \dots \dots (4)$$

$$\Phi = \Delta P (\Delta T)^{-2} * A^{-1} \dots \dots \dots (5)$$

Results: The product of electric currents per meter and voltages per meter were calculated using PDE and the results were reported as power per unit area or (W.m^{-2}). The Φ were calculated using parametric programming in PDE by using special probe to capture change in power (ΔP), ΔT , and area (A), thus ($\Phi = \Delta P * A^{-1} * \Delta T^{-2}$).

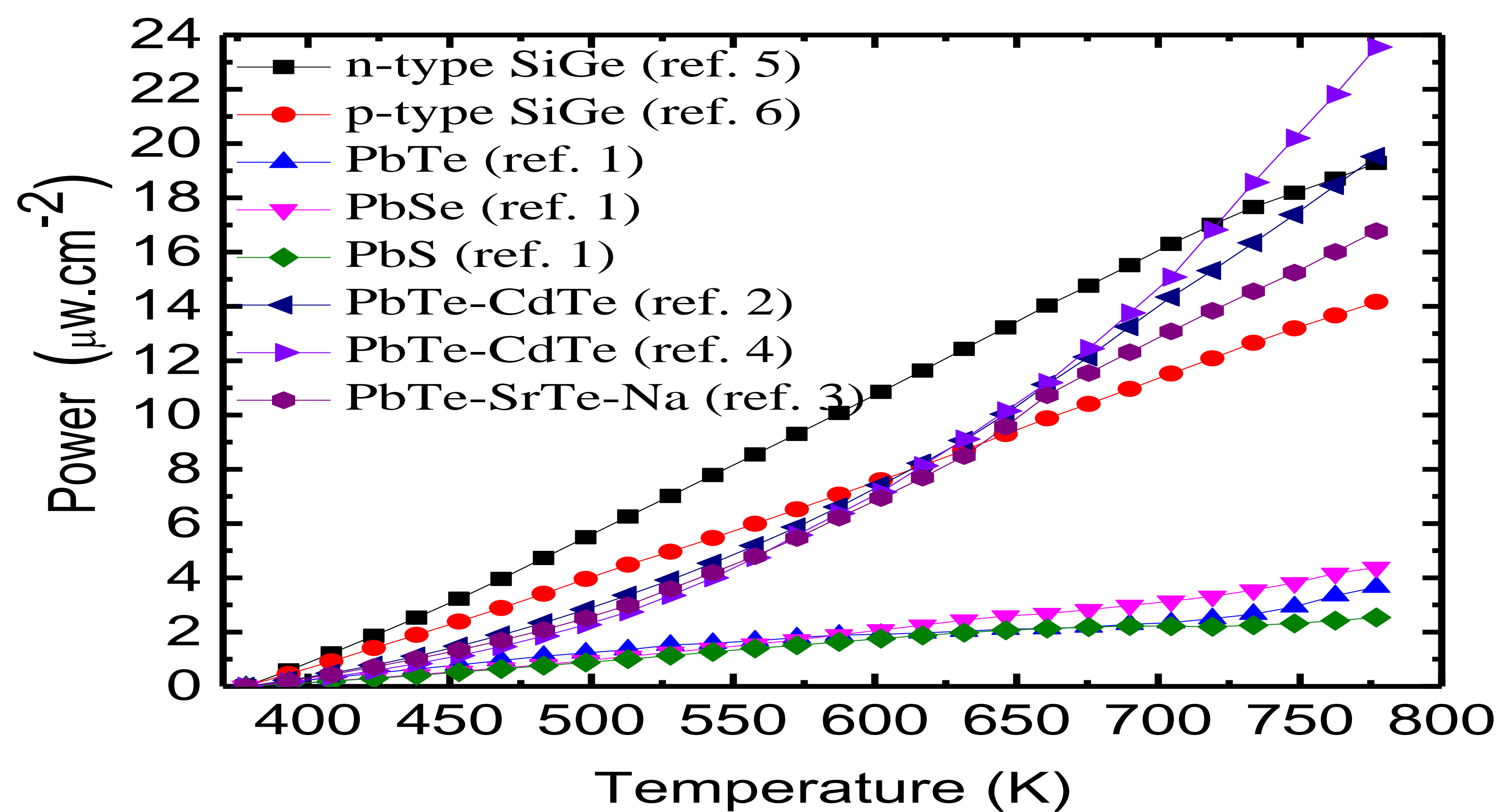


Figure 3. Power versus temperatures.

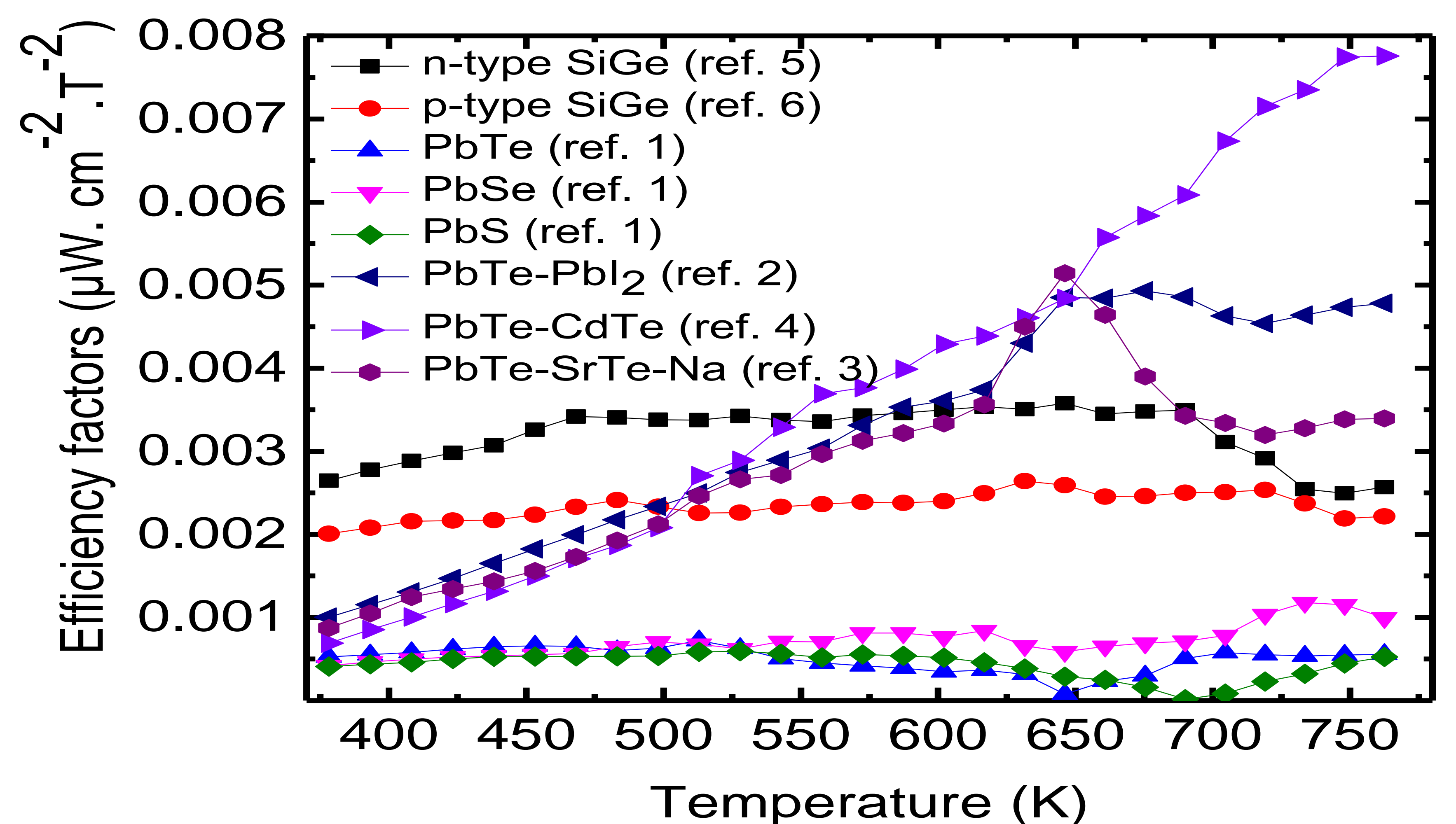


Figure 4. Efficiency factors versus temperatures.

Conclusions: We noted that our results are within the range as those reported in the literature, showing that Φ can be from $0.091 \mu\text{W.cm}^{-2}\text{K}^{-2} \leq \Phi \leq 0.001 \mu\text{W.cm}^{-2}\text{K}^{-2}$. We have also shown that Comsol Multiphysics is a powerful tool for computing Φ of different TE materials without using conventional ZT parameters.

References

- [1]. Y. Ling Pei, Y. Liu, Electrical and thermal transport properties of Pb-based chalcogenides, PbT PbSe, and PbS, J. of Alloys and Compounds. 514 (2012) 40-44.
- [2]. C. Long, X. Hou, Y. Gelbstein, J. Zhang, B. Ren, and Z. Wang, Preparation and thermoelectric Properties of N-type PbTe doped with In and PbI₂, In Proc. of IEEE 25th Inter. Conf. on Thermoelectrics. (2006) 382-385.
- [3]. K. Biswas, J. He, I. D. Blum, C. I. Wu, T. P. Hogan, D. N. Seidman, V. P. Dravid, and M. G. Kanatzidis, High-performance bulk thermoelectric with all-scale hierarchical architectures, Nature Materials. 489, 7416 (2012) 414-418.
- [4]. Y. Pei, A. D. LaLonde, N. A. Heinz, and G. J. Snyder, High Thermoelectric figure of merit in PbTe alloys demonstrated in PbTe-CdTe, J. Adv. Energy Material. 2, 6 (2012) 670-675.
- [5]. X. W. Wang, H. Lee, Y. C. Lan, G. H. Zhu, G. Josh, Enhanced thermoelectric figure of merit in nanostructured n-type silicon germanium bulk alloy, J. App. Phys. Letters. 93, 193121 (2008).
- [6]. G. Josh, H. Lee, Y. Lan, X. Wang, G. Zhu, D. Wang, R. W. Gould, D. C. Cuff, M. W. Tang, M. S. Dresselhaus, G. Chen, and Z. Ren, Enhanced thermoelectric figure-of-merit in nanostructured p-type silicon germanium bulk alloys, Nano letters. 8, 12 (2008) 4670-4674.