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Design and Simulation of a Graphene Based Thermoelectric Device

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Abstract

The thermoelectric effect refers to phenomena by which either a temperature difference creates an electric potential or an electric potential creates a temperature difference and any device which utilizes this effect is known as thermoelectric device. So thermoelectric devices are used as generators and coolers to convert thermal energy into electrical energy or vice versa. A highly efficient thermoelectric material is desired in either case. Graphene, a 2D allotrope of carbon, has a very high electrical conductivity but its application in thermoelectric devices is limited by the high thermal conductivity and low Seebeck coefficient. However, various modification methods has been suggested to enhance the Seebeck coefficient and to reduce the thermal conductivity which will make it an amazing thermoelectric material. In this paper, we propose to design a thermoelectric device utilizing graphene and create a simulation to explore the prospects of graphene in thermoelectric devices.

Keywords: Graphene, simulation, Ansys, thermoelectric.

1. Introduction

Thermoelectric generator (TEG) and thermoelectric cooler (TEC) are thermoelectric devices which depend on the principle of thermoelectric effect. TEG is a device which can produce electrical energy by converting temperature differences. This effect is called Seebeck effect which is a form of thermoelectric effect. In case of TEC, when voltage is applied in one direction, one side of the device creates heat while the other side absorbs heat, becoming cold. This is known as the Peltier effect. A large amount of waste heat is generated in various operations which can be properly used by applying thermoelectric effect that can recharge our batteries. TEC is very suitable device in the applications that require heat removal. The efficient performance of TEG and TEC depend on the thermoelectric property of material used in respective devices which can be measured by a dimensionless term ZT, also known as thermoelectric figure of merit.

$$ZT = \frac{S^2 \sigma T}{k} \tag{1}$$

where S is the Seebeck coefficient, σ the electric conductivity, k the thermal conductivity of material [1]. It clearly shows the importance of material for greater thermoelectric effect. Greater Seebeck coefficient of a material gives greater figure of merit which shows the ability of a material to produce thermoelectric power efficiently. Seebeck coefficient is defined as the amount of generated potential when a temperature gradient is applied to the sides of a material and it is described as $S = V/\Delta T$. The temperature gradient (ΔT) can be attained between the ambient temperature (air) and any heat-waste source such as a hot exhaust engine [3]. Bismuth Telluride (Bi_2TE_3) is widely used thermoelectric material for application at room temperature which has Seebeck coefficient approximately -150 $\mu v/^0c$ (maximum value -287 $\mu v/^0c$ observed at 54^0c) at room temperature [2]. Recent years have witnessed considerable interest devoted to the electronic properties of graphene. Graphene, a one-atom-thick sheet of carbon atoms arranged in a honeycomb crystal, exhibits unique properties like high thermal conductivity, high electron mobility and optical transparency, and has the potential for use in nano-electronic and optoelectronic devices [1]. The figure of merit needs to be as large as possible to get the best performance of thermoelectric generator. So, graphene has a great possibility in the field of thermoelectric generator. This paper shows the comparative study of graphene as thermoelectric material, the research opportunities and the possibilities of graphene in the field of thermoelectric devices**.**

2. Graphene as a thermoelectric material

For a material to have a high thermoelectric figure of merit, it is required to have high electrical conductivity and Seebeck coefficient and low thermal conductivity. So the figure of merit also depends on the power factor of the material which is given by equation (2). Also in solids, conduction is mediated by the combination of vibrations and collisions of molecules, of propagation and collisions of phonons, and of diffusion and collisions of free electrons. Thus the thermal conductivity in solids are written as,

$$P = \sigma S^2 \tag{2}$$

$$k_{tot} = k_e + k_{ph} \tag{3}$$

where k_{tot} is the total thermal conductivity, k_e is the electronic contribution to thermal conductivity and k_{ph} is the thermal conductivity due to phonon conductance. Phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, like solids and some liquids, often designated a quasiparticle which represents an excited state in the quantum mechanical quantization of the modes of vibrations of elastic structures of interacting particles [4]. Graphene has very beneficial charge transport properties as a potential thermoelectric material, but is limited by very large thermal conductivity. In graphene, the high phonon thermal conductivity is the main factor limiting the thermoelectric conversion. So graphene has a high power factor but a low figure of merit. The common strategy to enhance ZT is therefore to introduce phonon scatterers to suppress the phonon conductance while retaining high electrical conductance and Seebeck coefficient.

3. Ansys workbench

Ansys is a software implementation of finite element simulations. Its functionalities include structural, mechanical, fluid, electromagnetic, heat transfer, etc. [5]. Ansys features a number of products which are used for different types of analysis. For example, Ansys Fluent, CFD, CFX are used as Computational Fluid Dynamics software whereas Ansys Maxwell and Ansys HFSS are used in electromagnetic and electromechanical fields. The Ansys Workbench provide multiple Ansys tools in a single package. It is an intuitive up-front finite element analysis suite that is used in conjunction with CAD systems and/or Design Modeler. ANSYS Workbench is a software environment for performing structural, thermal, and electromagnetic analyses with the capabilities of coupling different fields in a single simulation.

4. Design and simulation

A number of parameters has to be considered before designing the simulation. The compatibility factor of the materials, the geometry for each component in both size and shape, mesh sizing, material properties, contact region behaviors etc.

4.1. Compatibility factor

The materials used in TEG/TEC are guided by the compatibility factor. A material's compatibility factor s is defined as,

$$s = \frac{\sqrt{1-\mathrm{ZT}}-1}{ST} \tag{4}$$

When the compatibility factor from one segment to the next differs by more than a factor of about two, the device will not operate efficiently [6]. In both cases of the compatibility factor was found within the acceptable range which also indicates a potential practical use of the TEG/TEC utilizing graphene and Bi_2Te_3.

4.2. Ansys workbench parameters

The simulation was created using the Thermal-Electric template from the Toolbox in Ansys workbench. It is a coupled field of solid state thermal and electrical analysis using the Mechanical APDL solver. The mesh sizing was kept at a medium range and kept constant in both simulation. Copper alloy was selected for both simulations as the default conductor plates.

Table 1. Properties of copper alloy (Default Ansys values)

Name of the properties	Values
Density	8300 kg m^-3
Coefficient of Thermal Expansion	1.8e-005 K^-1
Specific Heat	385 J kg^-1 K^-1
Thermal Conductivity	401 W m^-1 K^-1

To create a simulation of thermoelectric generator (TEG) and thermoelectric cooler (TEC) in Ansys, a basic geometry identifying a single cell was drawn on Solidworks. This basic geometry was created in accordance with widely popular model of TEC of Bismuth Telluride (Bi2Te3) but in an enlarged scale of a single cell. Two simulations are prepared. One with the popular Bi2Te3 configuration and another using graphene in conjuncture with Bi2Te3. This geometry will stay constant in both simulations. The geometry was imported to Spaceclaim, the integrated design modeler of Ansys workbench. The boundary conditions of hot junction and cold junction temperatures were also kept same for both simulations.

Table 2. Contact region parameters

Name of the properties	Values
Type	Bonded
Scope Mode	Automatic
Behavior	Program Controlled
Trim Contact	Program Controlled
Trim Tolerance	5.7502e-004 m

Table 3. Mesh parameters

Name of the properties	Values
Size Function	Adaptive
Relevance Center	Coarse
Element Size	Default
Initial Size Seed	Active Assembly
Transition	Fast
Error Limits	Standard Mechanical
Target Quality	Default (0.050000)
Smoothing	Medium
Nodes	8574
Elements	1466

4.3. Simulation of TEG/TEC using only Bi_2Te_3

For the first simulation using P type and N type Bi_2Te_3, the parameters are given in table 1.

Table 4. Thermoelectric properties of Bi_2Te_3

Name of the component	*S* *(µv/k)*	*ρ* *(Ωm)*	*k* $(Wm^{-1}K^{-1})$	*ZT*	Ref.
P type Bi_2Te_3	140	0.6× 10-5	1.3	0.8	7
N type Bi_2Te_3	-150	4× 10-5	0.21	0.8	8

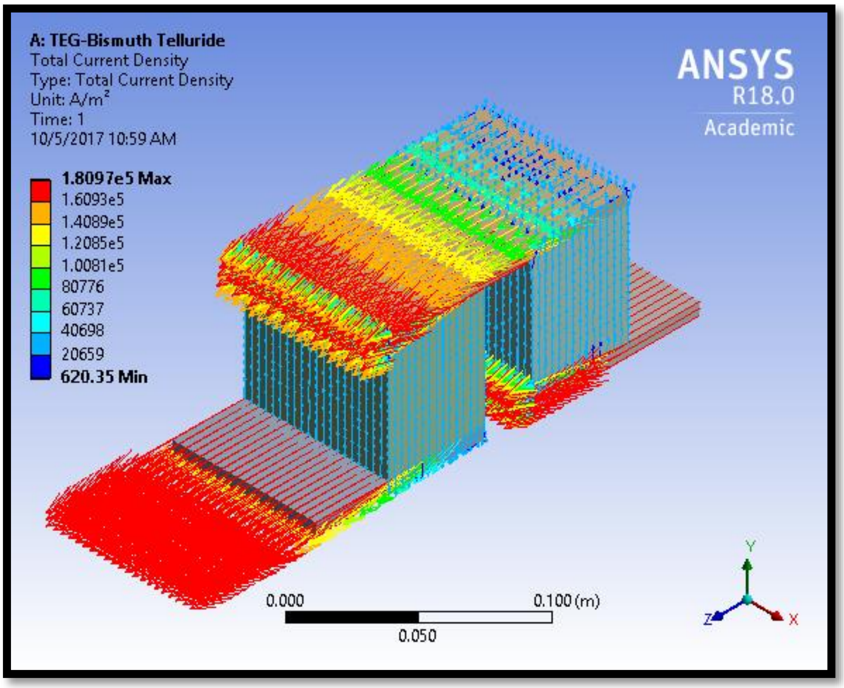

Fig 1. Simulation of TEG/TEC using only Bi_2Te_3 (Current density)

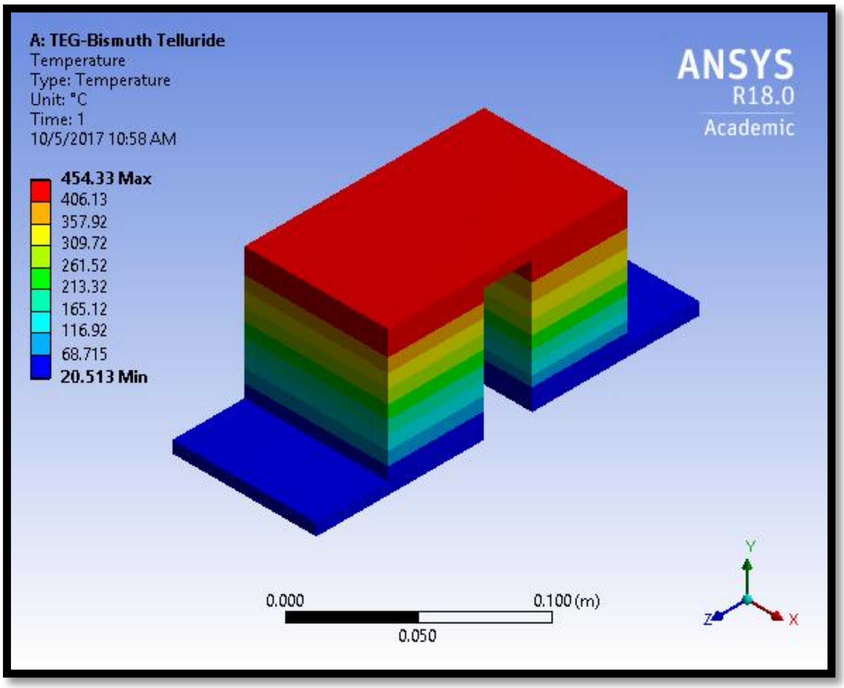

Fig 2. Simulation of TEG/TEC using only Bi_2Te_3 (Heat Distribution)

4.4. Simulation of TEG/TEC using Graphene and Bi_2Te_3

For the second simulation using P type graphene and N type Bi_2Te_3, the parameters are given in table 2.

Table 5. Thermoelectric properties of Bi_2Te_3 and graphene

Name of the component	*S* *(μv/k)*	*ρ* *(Ωm)*	*k* *($Wm^{-1}K^{-1}$)*	*ZT*	Ref.
P type graphene	150	1.67× 10-7	50.4	0.8	9
N type Bi_2Te_3	-150	4× 10-5	0.21	0.8	8

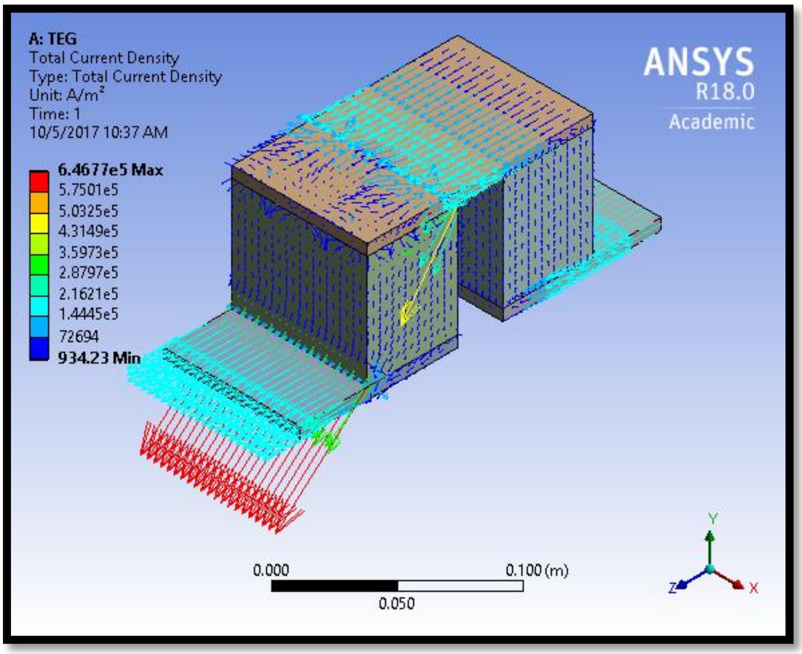

Fig 3. Simulation of TEG/TEC using graphene and Bi_2Te_3 (Curent density)

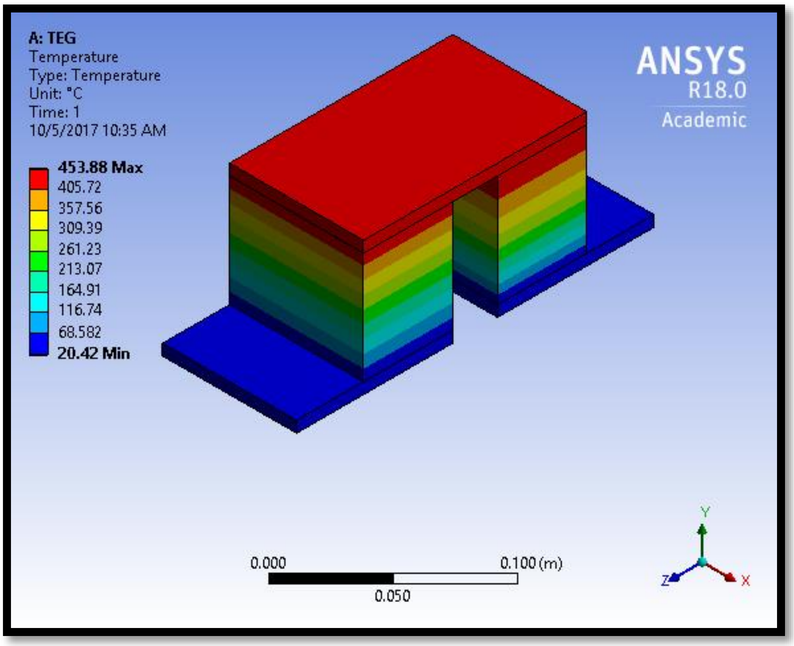

Fig 4. Simulation of TEG/TEC using only graphene and Bi_2Te_3 (Heat Distribution)

5. Results and discussion

The results are demonstrated in table 3. It is clear that the TEG/TEC with graphene incorporated gives a higher current output and a much larger absorbed heat.

Table 6. Results

Name of the simulation	Generated current *(A)*	Heat absorbed *(W)*
P type and N type Bi_2Te_3	84.452	54.579
P type graphene and N type Bi_2Te_3	94.46	1311.8

The geometry of the single cell was taken much larger to minimize simulation difficulties hence the large values found in the result. The vectors in both simulation are depicting the direction of current and in H In reality a number of cells are used in an interconnected system. Nonetheless, these simulations were able to demonstrate the usefulness of using graphene in TEG/TEC.

6. Conclusion

It is apparent that graphene has a lot of potential as a thermoelectric material despite the disadvantages it faces due to large thermal conductivity. The aim of this paper was to highlight this unique material in terms of thermoelectric application. Much research is needed to verify the theoretical and simulation results with actual practical scenario.

7. References

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