International Journal of Electronic and Electrical Engineering.
ISSN 0974-2174 Volume 8, Number 1 (2015), pp. 77-90

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Thermoelectric Cooler based on AGNR/Bi_2Te_3 and Control using Lab-VIEW

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Abstract

Beyond maximum operating temperature, failure of electronics components can be caused by package or junction over temperature. Malfunction of electronics package due to self heating or environmental heating is a common problem. Heat-sinks and fans are realized which doesn't provide the desired cooling. Additional cooling techniques need to be developed and realized for reliable performance of devices.
The thermoelectric effect is conducive to the conversion of heat energy into electric power and vice versa. Peltier Effect is utilized in development of cooling system through thermocouples.
In this work combination of nanomaterial 'Armchair Graphene Nanoribbon', encompassing giant figure of merit and n type Bismuth Telluride have been investigated as thermocouple materials. With this arrangement maximum cooling achieved is 103K below the room temperature. NI Lab-VIEW based measurement and control software has been developed which, on sensing surrounding temperature rise, provides command to Thermoelectric cooling system to cool down the electronic system.
FEA model of peltier effect has been presented to implement heat equation, heat balance equation, Gauss theorem and Neumann boundary condition. Multiphysics simulation using PDE application mode has been performed to demonstrate cooling of thermocouple junction by peltier phenomenon.

Index Terms — Thermoelectric, Peltier Effect, Nanomaterials, Emf, Temperature, Measurement, Thermal control, FEA Model, Simulation.

I. INTRODUCTION

The thermoelectric (TE) effect refers to phenomena by which either a temperature difference creates an electric potential or an electric potential creates a temperature difference. Two dissimilar metals forming junctions at ends are called thermocouples which produces electric current. Nanomaterial 'Graphene' is 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 device. Graphene conducts electricity better than copper. It is 200 times stronger than steel but six times lighter. It is almost perfectly transparent since it only absorbs 2% of light. It impermeable to gases, even those as light as hydrogen or helium. Graphene burns at very low temperature 623K.

Graphene, however, is not a useful thermoelectric material. In order to improve the Seebeck coefficient grapheme needs to acquire a bandgap. This can be achieved by appropriate patterning of the graphene sheet into nanoribbons. Armchair GNRs (AGNRs) can be semiconductors with a bandgap inversely proportional to their width [1]. The resulting confinement gap, depends on the chirality of the edges (armchair or zigzag) and the width of the ribbon. AGNRs can be either metallic or semiconducting, depending on their width of Graphene.

Bismuth telluride (Bi_2Te_3) is a gray powder that is a compound of Bismuth and Tellurium. It is a Semiconductor which, when alloyed with antimony or selenium is an efficient thermoelectric material. The nanowire of n type Bi_2Te_3 is available as considerable thermoelectric material. Donor impurities of CuBr, I, and Te have been used for converting to n type Bi_2Te_3 to achieve good thermal stability of the *ZT*.[2]

The peltier effect is defined as "when an external voltage is applied, the resulting current flow is associated with a heat flow. Thermoelectric coolers using peltier effect are used commercially for small range of cooling. The efficiency of thermoelectric cooling is defined by figure of merit, ZT= $S^2\sigma T/\kappa$, where S is the thermoelectric power (also called Seebeck coefficient), σ the electrical conductivity, and κ the thermal conductivity of the material [3, 4].

The requirement of the Thermoelectric cooling system is narrow band-gap semiconductor, high mobility, and low thermal conductivity, highly anisotropic or symmetric and complex composition. Different metals and super lattice materials have been investigated as thermoelectric materials by various authors. The performance of such a device, using $(Bi,Sb)_2Te_3$-based thermoelectric elements, was examined from 270 to 55 °C.[5] Graphene/h-BN supper lattice consisting zigzag graphene nanoribbons (ZGNRs) and zigzag BN nanoribbons (ZBNNRs) has been investigated by Y. Yokomizo and J.Nakamura [4].

The maximum operating temperature of a component is limited not only to the performance of the active device, but also by the packaging material and joining technologies used to house the device. It is important to maintain the temperature of package and junction of these components.

In this work 6-AGNR and n-type Bi_2Te_3 has been investigated as thermoelectric combination for cooling. Both are wonder materials in the field of thermoelectric cooling and generation. K-type thermocouple has been employed for measure the temperature of the surrounding of the electronic packages. K-type thermocouple is combination of Alumel and chromel. The NI Lab-VIEW based measurement and control system has been developed to sense and display surrounding temperature. Based on set working temperature the Lab-VIEW based controller provide control voltage output to the Thermoelectric cooling system. As the temperature increases the control output increases and vice versa.

FEA model of peltier phenomenon has been presented to implement heat equation, heart balance equation, Gauss' theorem and Neumann boundary condition. Multiphysics simulation using PDE application mode has been performed to demonstrate peltier phenomenon.

This work validates the nanomaterials proposed as thermoelectric combination yields great cooling efficiency and can be utilized in the electronic packages where reliability is the issues and fan or heat sink are partially efficient.

II. THERMOELECTRIC COOLER DESIGN

Thermoelectric combination of 6-AGNR and n-type Bi_2Te_3 is utilized as basic cooling element. Two legged thermocouple with one leg of 6-AGNR and second of Bi_2Te_3, is shown in "Fig. 1". The dimension of each leg is 1000µm X 200 µm X 200 µm.

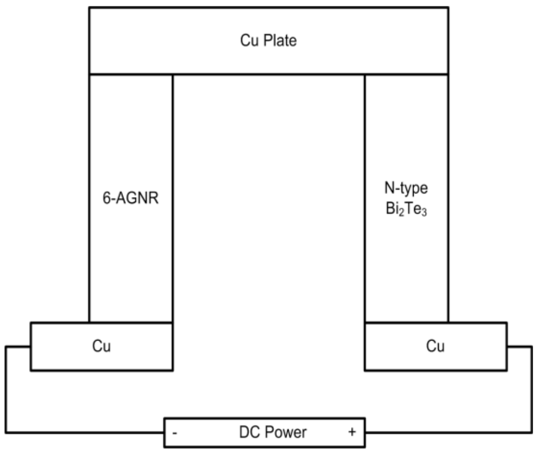

Figure 1: Single Unit of Two legged thermoelectric cooler consisting 6-AGNR and n-type Bi_2Te_3

One unit shall not be enough to provide sufficient cooling of the object. Hence Thousands of such unit is combined and kept thermally in parallel and electrically in series. Two free end are given DC voltage which is variable based on required cooling. Five such elements are shown in "Fig. 2".

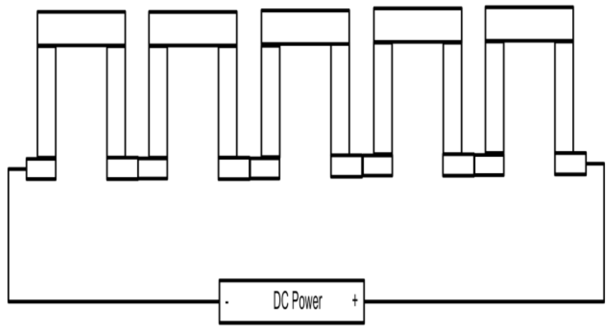

Figure 2: Five such units of Thermoelectric cooler has been connected in parallel thermally and in series electrically

The combination of multiple elements has two ends hot junction and cold junction. Hot junctions are open to atmosphere through heat-sink or cooling fans. The hot junction temperature is not allowed to rise beyond a predefined temperature range using heat sink or other traditional cooling devices A heat sink is a device that is attached to the hot side of thermoelectric module. It is used to facilitate the transfer of heat from the hot side of the module to the ambient. A cold sink is attached to the cold side of the module. It is used to facilitate heat transfer from whatever is being cooled (liquid, gas, solid object) to the cold side of the module [6]. Copper has been used as intermediate junction, being isothermal the copper junction do not produce thermoelectric voltage. K Type thermocouple is located over the object whose temperature rise is to be restricted or integrated with the electronic packages.

6-AGNR is wonder material having giant thermoelectric Properties and n-type Bi_2Te_3 has been proven as good thermoelectric material. Dynamics study has shown that high ZT of 6 can be obtained with 6-AGNR which is attributed to a high Seebeck coefficient as 4 mV/K [4]. Properties of the utilized thermoelectric materials have been detailed in "Table I".

TABLE I THERMOELECTRIC MATERIALS PROPERTIES

	6-AGNR	**n-type Bi_2Te_3**	**Copper (Cu)**
Thermal Conductivity (W/m.K)	218	1.6	350
Electrical Conductivity (S/m)	2.725E3	1.1E5	5.9E8
Density(kg/m^3)	300	7740	8920
Specific Heat at constant Pressure(J/kg.K)	2100	154.4	385
Seebeck Coefficient (µV/K)	+ 4000	-228	+6.5

III. FEA Model Of Thermoelectric Cooler

The thermoelectric device is combination of two materials having good electrical conductivity and low thermal conductivity. The model deals with heat equations and transport of electron phenomenon. “Fig. 3” shows the basic model of the TE device.

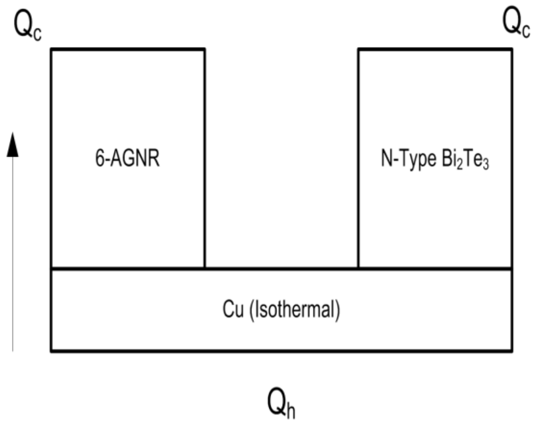

Figure 3: Thermoelectric cooler model and heat flow

The nomenclature used in the model as follows.

Q	Heat generation (W/m^3)
q	Heat Flux(W/m^2)
A	TE element area(m^2)
L	TE element length(m)
c	Specific heat(J/Kg.K)
h	Heat Transfer Coefficient(W/m^2.K)
N	Number of TEC elements
Q	Heat Flux(W/m^2)
T	Time(s)
T_c	Cold Side temperature(K)
T_h	Hot Side Temperature(K)
S	Seebeck Coefficient(V/K)
P	Peltier Coefficient(V)
k	Thermal Conductivity(W/m.K)
ρ	Specific electrical resistivity(Ω.m)
R	Electrical Resistance(Ω)
J	Current Density(A/m^2)
i	Current(A)

The purpose of the model is to get maximum cooling below room temperature and maximize the time averaged heat flux capacity Qc of the thermoelectric during the cool down period represented by

$$Q_c = \frac{1}{t_c}\int_0^{t_c} q(t)dt \tag{1}$$

Where q(t) is instantaneous heat pump to cold side. t_c is the time to achieve final cold side temperature.

The amount of heat flux generation is given by [7, 8]

$$q_c = SI_cT_c - \frac{A_c}{L_c}(T_H - T_C) - \frac{1}{2}I_c^2\rho\left(\frac{L_c}{A_c}\right) \quad (2)$$

Applying energy balance at the cold side of a single TE couple (two elements)

$$q_c = SI_cT_c - k(T_H - T_C) - \frac{1}{2}I_c^2R \quad (3)$$

Where $k=A_c/L_c$ and $R=\rho(L_c/A_c)$

The first term describes the thermoelectric heat pumping due to peltier effect, second term defines the Joule heating and third term describes the conducted heat.

For the Single Element or one Legged TE element the Heat being rejected from hot side is found by using first law of thermodynamics

$$q_h = q_c + i.V \quad (4)$$

Applied Voltage 'V' is given by

$$V = i.R + S.\Delta T \quad (5)$$

Where ΔT is difference is Hot and Cold Temperature.

Current required to pump the maximum amount of heat flux is derived by

$$\frac{dq_c}{dt} = 0 \quad (6)$$

Resulting in, maximum current given by

$$\mathrm{I}_{\max} = \frac{ST_c}{R} \quad (7)$$

The rate of heat flux pump shall be

$$q_c = \frac{1}{2}\frac{S^2T_c^2}{R} - k\Delta T \quad (8)$$

The maximum temperature drop would occur if there is no external heat input to the cold side at this current pumped.

$$\Delta T = \frac{1}{2}\frac{S^2T_c^2}{Rk} \quad (9)$$

In the model length of each leg is 1000 μm and width is 200 μm. Using properties of 6-AGNR and n-type Bi_2Te_3 and using "Equation (7)" , the maximum current to be supplied is 6.496A for 6-AGNR and 14.95A for n-type Bi_2Te_3. Considering 6.494 A as the current to be fed maximum voltage for pumping is 30.75V.

Ignoring Joule heating, thermoelectric equations for heat flux and Current Density in PDE general form are given as

$$q = -k\nabla T + PJ \quad (10)$$

$$J = -\sigma\nabla T - \sigma S\nabla T \quad (11)$$

Energy and Current Balance or continuity equations for the junction are given as

$$Q = \rho C \frac{dT}{dt} + \nabla.q \tag{12}$$

$$\nabla.J = 0 \tag{13}$$

Multiplying Energy balance Continuity Equation by Test function T_{test} and integrating over computation domain Ω.

$$\int_{\Omega} QT_{test} d\Omega = \int_{\Omega} \rho C \frac{dT}{dt} T_{test} d\Omega + \int_{\Omega} (\nabla.q) T_{test} \tag{14}$$

Using Vector identity theorem

$$\nabla.(T_{test} q) = q.\nabla T_{test} + T_{test} \nabla.q \tag{15}$$

"Equation (14)" is modified as

$$\int_{\Omega} QT_{test} d\Omega = \int_{\Omega} \rho C \frac{dT}{dt} T_{test} d\Omega + \int_{\Omega} \nabla.(T_{test} q) d\Omega - \int_{\Omega} q.\nabla T_{test} d\Omega \tag{16}$$

Applying Gauss theorem

$$\int_{\Omega} \nabla.(T_{test} q) d\Omega = \int_{d\Omega} T_{test} q.n d\Omega \tag{17}$$

"Equation (16)" is modified as

$$\int_{\Omega} \left[-\rho C \frac{dT}{dt} T_{test} + q.\nabla T_{test} + QT_{test} \right] d\Omega - \int_{d\Omega} (q.n) T_{test} d\Omega = 0 \tag{18}$$

Using expression for Heat flux

$$\int_{\Omega} \left[-\rho C \frac{dT}{dt} T_{test} + (-k\nabla T).\nabla T_{test} + (PJ).\nabla T_{test} + QT_{test} \right] d\Omega - \int_{d\Omega} (q.n) T_{test} d\Omega = 0 \tag{19}$$

"Equation (19)" is the expression for total heat flux generation, where last term is Neumann Boundary condition for heat. Q is a source of heat and first two terms are heat flux generation due to thermal phenomenon. The weak contribution due to peltier effect is.

$$Weak_{peltier} = (PJ).\nabla T_{test} \tag{20}$$

For three dimensional object

$$Weak_{peltier} = (PJ_x).\frac{dT_{test}}{dx} + (PJ_y).\frac{dT_{test}}{dy} + (PJ_z).\frac{dT_{test}}{dz} \tag{21}$$

Hence heat generation at the junction due to peltier effect greatly depends on peltier Coefficient of materials and Current or Voltage Applied.

IV. AUTOMATIC TEMPERATURE CONTROL USING LAB-VIEW

Measurement of surrounding temperature and control based on the feedback is required for the Thermoelectric cooling system. This necessarily demands for automation being continuous and high frequency operation. For the purpose Lab-VIEW software has been utilized for measurement and automatic control of temperature. The Lab-VIEW graphical language is an intuitive way for engineers to develop their measurement and control applications. It is easy to learn and use, the language also delivers the performance needed for advanced applications[9] . The system takes feedback and gives voltage output as shown in “Fig 4”.

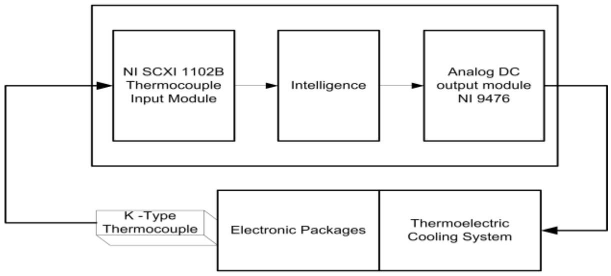

Figure 4: Thermoelectric Cooling control loop: feedback from k-type thermocouple is received by NI SCXI 1102 module and intelligence or software generated command through NI for cooling depending on set temperature.

NI SCXI 1102B module has been used to measure the surrounding temperature with help, of K-type thermocouple. The module has internal Cold junction compensation. The set temperature for the electronic package is provided using GUI. The difference in actual and set temperature generates control output. The control output is thrown to thermoelectric coolers using analog voltage output module NI PXI 9476. The module is capable to pump 6V to 36V to thermoelectric cooler. The graphical user interface (GUI) of the temperature measurement and automatic cooling though cooling voltage generation has been shown in “Fig. 5”.

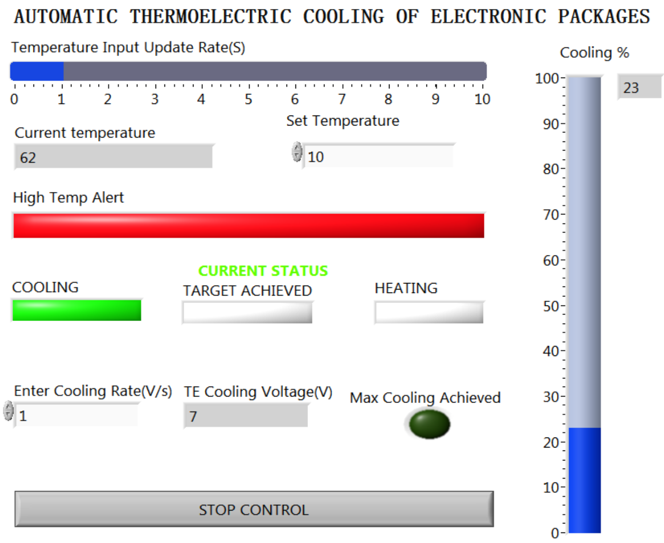

Fig. 5 Lab-VIEW based Temperature Measurement and Automatic Cooling: Front Panel

The control panel and software logic has been shown in “Fig. 6”.

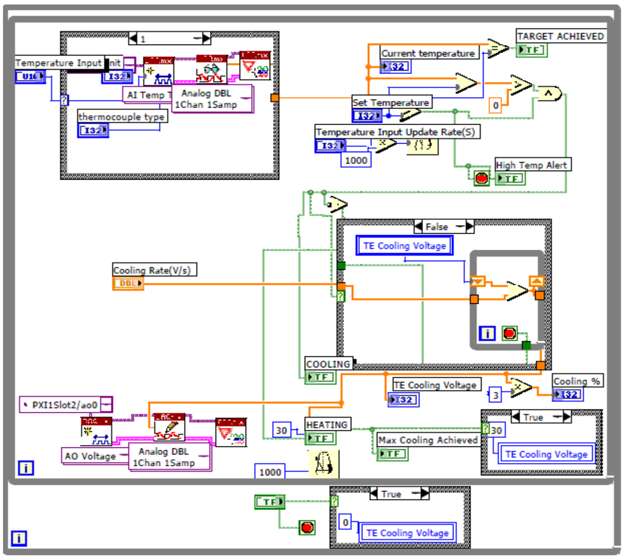

Figure 6: Lab-VIEW based Temperature Measurement and Automatic Cooling: Control Panel

V. Simulation Results

Simulation has been performed using Heat transfer and electric current module of COMSOL Multi-physics. Five unit of two legged thermoelectric cooler has been connected thermally parallel and electrically in series. 6-AGNR and n-type Bi_2Te_3 make junction cold and hot junction. Copper plate is laid over cold junctions. The hot junction is kept at room temperature 298K as heat boundary condition. Two extreme free end of the system is given electric energy. 6-ANGR being positive side has been grounded as part of electrical boundary condition and Bi_2Te_3 has been provided variable voltage source.

Heat distribution at the thermoelectric elements has been observed. The cooling effect at the cold junction has been analyzed. The cooling efficiency for raised surrounding temperature has been studied. Finally control loop using Lab-VIEW GUI has been verified.

Cooling profile of the cold junction with increasing thermoelectric voltage has been studied. Cooling at 1V, 9V, 19V and 31 V have been shown in “Fig. 7”, “Fig. 8” , “Fig. 9” and “Fig. 10” respectively.

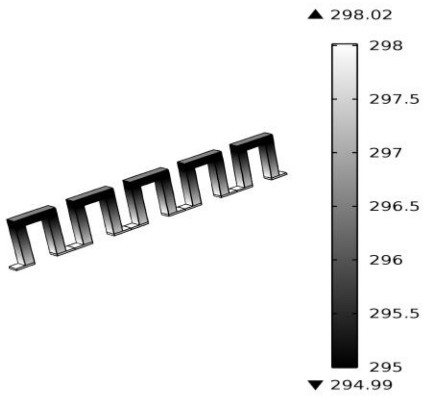

Figure 7: On applied thermoelectric voltage 1V, cold junction is cooled 3K below room temperature.

Effectively 3K below room temperature is achieved at 1V. 38K cooling is observed on thermoelectric voltage 9V.

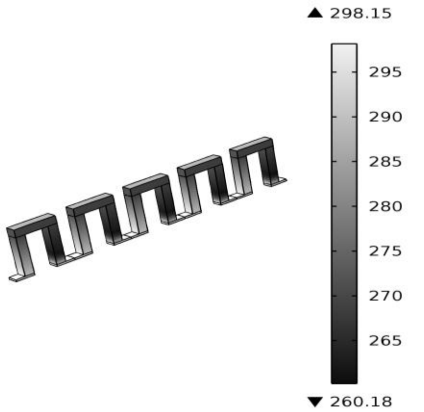

Figure 8: On applied thermoelectric voltage 9V, cold junction is cooled 38K below room temperature.

On further increment of thermoelectric voltage the cooling effect dominate and cold junction temperature further gets down. For 19V and 29 V the cooling below room temperature is 71 K and 103 K respectively.

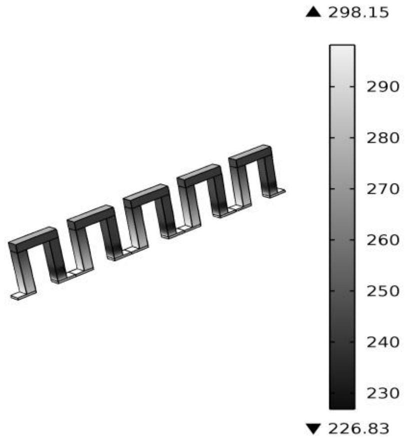

Figure 9: On applied thermoelectric voltage 19V, cold junction is cooled 71K below room temperature.

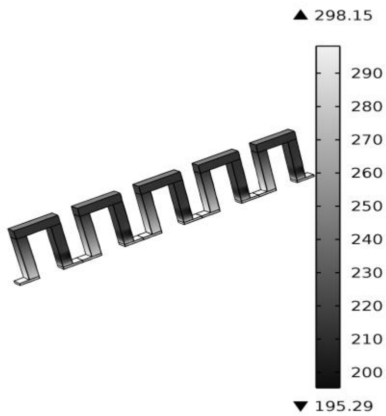

Figure 10: On applied thermoelectric voltage 31V, cold junction is cooled 103 K below room temperature.

The cold junction cooling with increasing thermoelectric voltage is almost linear as shown in "Fig. 11".

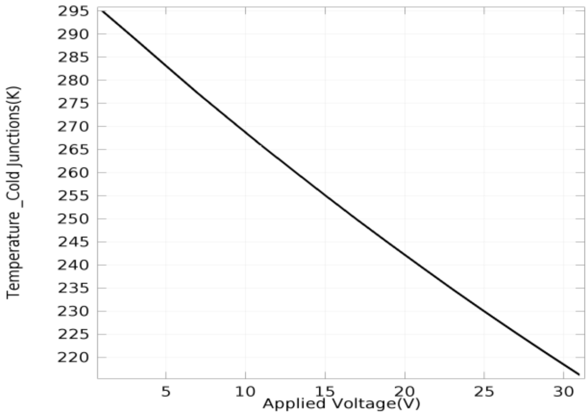

Fig. 11 Cooling effect is dominated with increasing thermoelectric voltage and relation is linear

VI. Conclusion and Future Scope

I designed a thermoelectric cooling system for electronic packages, which can provide maximum cooling of 100K. The cooling system has been realized by making thermoelectric junction of wonder nanomaterials 6-AGNR and n-type Bismuth Telluride. Multiple units are connected thermally parallel and electrically in series to design effective cooling system. Lab-View based automatic temperature measurement and control system has been developed.

Five cooling units have been demonstrated and simulated using multi-physics software. Increasing cooling with voltage has been demonstrated.

The cooling system can be used in the electronics packages where temperature rise is not tolerable for reliable application.

The designed system is intended to use in the rocket motors where pressure, vibration and acoustic levels are abnormally high. Modeling and Simulation to study effectiveness of the system in this environment can be the interest for analysis in future.

Acknowledgment

I would like to thank department of electrical, IIT Roorkee. Instrumentation and Signal Processing Group has given motivation towards this work while pursuing M Tech.

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