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## Study of thermoelectric phenomena, devices and behaviors

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### Abstract

In this work, 2-phenyl-4(3H)-3,1-benzoxazinone (1) was synthesized from benzoylation with simultaneous cyclization of anthranilic acid and benzoyl chloride. Compound 1 was treated with hydrazine hydrate to yield 3-amino-2-phenyl-4(3H)-quinazolinone (2). Reaction of compound 2 with aromatic aldehydes/ketones resulted Schiff bases 3-6. Furthermore, treated of compound 1 with thiosemicarbazide yield compound 7, which on reaction with chloroacetic acid in the presence of sodium acetate gave 3-[(4-oxo-1,3-thiazolidin-2-ylidene) amino]-2-phenylquinazolin-4(3H)-one (8). On the other hand, 2-substitutedquinazolin-4(3H)-one (9-12) were also synthesized from the reaction of anthranilic acid with different substituted amides in acetic acid. All newly synthesized compounds were characterized using different methods of spectroscopy such as IR, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR.

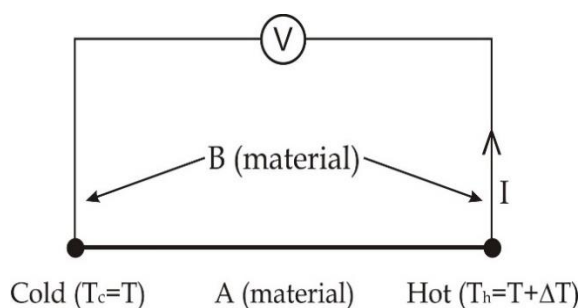
**Keywords:** Seebeck effect, Peltier effect, Thomson effect, thermoelectric device, phonon, figure of merit (ZT), thermoelectric materials also

### Introduction

The field of thermoelectric has long been recognized as a potentiality transformative power is now growing steadily to this ability to convert heat directly into electricity and to develop cost effective, pollution free form of energy conservation by using various thermoelectric device. Of course, thermal energy/ heat energy is available everywhere and other source of energy may not be available at all times or in places e.g. Solar energy is available only during the sunny days, hydro energy can only be generated at water sources, and fossil/fuel generators cannot operate without the availability of fuel such as oil, coal or natural gas. The thermoelectric devices can use body heat to indefinitely power some medical applications such as drug delivery, continuous diagnostics or vital signs monitoring.

The goal of this paper is to provide the reader with an overview about the thermoelectric devices and how they can be built and their behavior. The paper starts with explaining the principle of thermoelectric effects.

When two dissimilar metal wires are joined at two ends to form a loop, a voltage is developed in the circuit if two junctions are kept at different temperature. This voltage is proportional to the temperature difference (say  $\Delta T$ ) and this phenomenon is called Seebeck effect because this effect observed by Seebeck in 1821 and hence the name of the effect is Seebeck effect. The ratio of the voltage generated to the temperature gradient is an intrinsic property of the material and it is called thermoelectric power or Seebeck coefficient (S). i.e.



**Fig 1:** Seebeck effect

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$$S = -\frac{\Delta V}{\Delta T} \tag{1}$$

The temperature difference results in moving the mobile charge carriers towards the cold junction from the hot junction and leaving behind the oppositely charged at the hot junction. The movement of charge results in the rise of a thermoelectric voltage as shown in fig.1. The effect is due to conversion of thermal energy to electrical energy. The potential different in the circuit whose junctions are maintained at temperature.  $T_h$  and  $T_c$  is given by

$$\Delta V = SAB (T_h - T_c) \text{ It may be written as in the form}$$

$$\text{Thermoelectric Voltage (V)} = (S_A - S_B) \Delta T \tag{2}$$

Where,  $S_{AB} = S_A - S_B$  and  $\Delta T = T_h - T_c$

The second thermoelectric effect was discovered by Jean Peltier in 1834 and really, this effect is the converse of Seebeck effect. When a current flows through a circuit containing junction of two dissimilar metals, it leads to an absorption or liberation of heat at the junctions. Heat is given out or absorbed depending on the pairs of metal and the direction of current as shown in fig. 2.

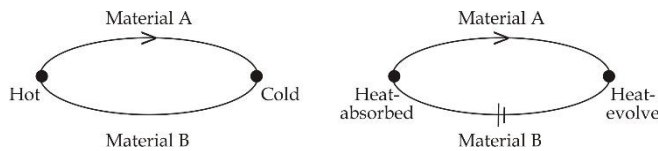


Fig 2: Peltier effect

The effect is due to the difference in the Fermi energy of the two materials.

The amount of heat  $Q$  liberated to (or absorbed from) the surroundings in order that the junction may be kept at the same temperature is proportional to the current ( $I$ ) passing through the junction. i.e.

$$Q = \pi_{AB} I$$

Or,

$$Q = (\pi_A - \pi_B) I \tag{3}$$

where,  $\pi_A$  and  $\pi_B$  are called the Peltier coefficient of materials A and B respectively and  $I$  is the current passed through the materials.

The third thermoelectric effect is the combination of Seebeck effect and Peltier effect called Thomson effect (later well known as Lord Kelvin) and was discovered by William Thomson in 1854. The Thomson effect may be considered by a simple picture as shown in fig. 3. A conductor has free charge

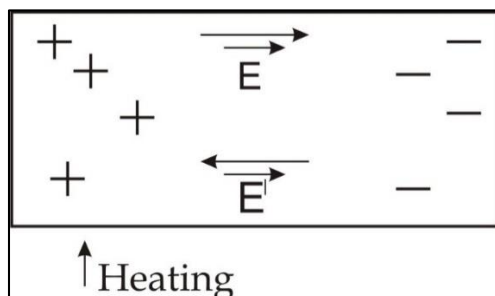


Fig 3: Thomson effect

Carriers, which are electrons in metals, electrons and holes in semiconductors and ions in case of ionic conductors. Consider a electron of such a conductor whose one end is hotter than the other end. The charge separation sets up an electric field  $\vec{E}$ . Diffusion of carriers would stop when the attractive force on the carriers due to field  $\vec{E}$  strong enough to retard the motion of the carriers due to the thermal effect. Now, we can represent the effect of the thermal gradient responsible for the diffusive motion of the carriers by an effective field  $\vec{E}'$ . This effective field is proportional to the thermal gradient and can be written as

$$E' = \sigma \frac{dT}{dX} \tag{4}$$

Where  $\sigma$  is known as Thomson coefficient for the material of the conductor. The Thomson electromotive force  $E_{Th}$  is given by

$$E_{Th} = \int_{T_1}^{T_2} \vec{E}' dx = \int_{T_1}^{T_2} \sigma dT \tag{5}$$

Where  $T_1$  and  $T_2$  are the temperature at the two ends of the rod.

When a current  $I$  is passed through a homogenous conductor with a temperature gradient, the rate of heat production per unit volume is given by

$$Q = \rho I^2 - \sigma I \frac{dT}{dX} \tag{6}$$

Where  $\rho$  is the resistivity of the material,  $\sigma$  is the Thomson coefficient and  $\frac{dT}{dX}$  is temp. gradient along the conductor.

The conversion efficiency of thermoelectric materials is related to a quantity, called the figure of merit ( $ZT$ ) is defined as follows:

$$ZT = \frac{S^2 \sigma_e T}{K} \tag{7}$$

Where  $S$  is the Seebeck coefficient,  $\sigma_e$  and  $K$  are the electrical and thermal conductivity respectively,  $T$  is the absolute temperature. It should be noted that thermal conductivity ( $K$ ) of thermoelectric materials consists of two parts: lattice thermal conductivity ( $K_l$ ) and electronic thermal conductivity ( $K_e$ ).

The thermoelectric efficiency in power generation mode and the coefficient of performance  $\eta$  in refrigeration mode (heat is pumped from  $T_c$  to  $T_h$ ) of a thermoelectric couple are given by

$$\epsilon = \frac{T_H - T_C}{T_H} \left[ \frac{(1 + ZT_m)^{\frac{1}{2}} - 1}{(1 + ZT_m)^{\frac{1}{2}} + (T_C / T_H)} \right] \tag{8}$$

And,

$$\eta = \frac{[T_c (1 + ZT)^{\frac{1}{2}} - T_H / T_c]}{(T_c / T_H) [(1 + ZT)^{\frac{1}{2}} + 1]} \tag{9}$$

Where  $T_H$ ,  $T_C$  and  $T_m$  are hot side, cold side and average temperature respectively and  $\mathcal{E}_c$  is the carrier efficiency and can be expressed as

$$\mathcal{E}_c = \frac{T_H - T_C}{T_H} \quad (10)$$

The thermoelectric power or Seebeck coefficient of the material as the ratio of the induced thermoelectric voltage to the temperature difference across it. The thermopower of a good thermoelectrical material is usually in the range of  $100\mu\text{V/K}$  and is given by

$$S = \frac{8\pi^2 K_0^2}{3eh^2} m^* T \left( \frac{\pi}{3n} \right)^{2/3} \quad (11)$$

Where,  $K_0$  is the Boltzmann's constant,

$e$  is the electronic charge,

$h$  is the Planck's constant,

$T$  is the temperature.

$m^*$  is the effective mass of the carrier and  $n$  is the concentration of charge (or carrier)

From the equation 11, it is clear that

$$S \propto \frac{m^*}{n^{2/3}} \quad (12)$$

Thus, for large thermopower, the material should have high effective mass and low charge concentration. This is because, semiconductors have large Seebeck coefficients compared with metals.

The measurement of ability of material to conduct electric current is called electrical conductivity and it may be defined as

$$\sigma_e = \frac{1}{\rho_e} = ne\mu \quad (13)$$

Where  $\mu$  is the mobility of the charge carriers, which obtained from the equation given below

$$\mu = \frac{e\tau}{m^*} \quad (14)$$

Where  $\tau$  is the mean scattering time between the collisions for the carriers. The ability of the material to transfer heat under the effect of temperature gradient across it points is called thermal conductivity and it is related to the transfer of heat either through the electron or through the vibration of the lattice, known as phonon. Hence the thermal conductivity can be written as

$$K = K_e + K_l \quad (15)$$

Where  $K_e$  and  $K_l$  are the thermal conductivities due to electrons and phonons, respectively. Also,  $K_e$  and  $K_l$  are defined as the following equation below

$$K_e = \frac{\pi^2 n k_0^2 T \tau}{m}$$

$$\therefore K_e = \frac{\pi^2 n^2 k_0^2 T \mu}{e} \quad (16)$$

And

$$K_l = \frac{Cv l}{3} \quad (17)$$

Where  $C$  is the phonon heat capacity per unit volume.  $v$  is the average velocity of phonon and  $l$  is the phonon mean free path.

Peltier effect is used for refrigerating, cooking of electrical components, portable boters, cameras, climate controlled jackets, space crafts, satellite and others. The efficiency of the device is directly related to the figure of merit as explained theoretically in equation (7) and (8) and the coefficient of performance for the thermoelectric cooler is explained by equation (9) discussed above.

In 1995 Slack described the characteristics required for a material to be good thermoelectric material as material with high carrier mobility and low thermal conductivity, he also indicated that the best thermoelectric material should have the electrical properties of crystalline material and the thermal properties of glass material i.e. phonon glass electron crystal and theoretically there is no restriction on the values of figure of merit.

Finally, bulk thermoelectric materials can be used for a wide range of power generation and cooling applications, it is difficult to accommodate them for micro-scale applications. In such cases, a thin film approach is needed, where the films can be directly deposited on the substrate. Since the films are not formed under equilibrium condition, the properties of the materials may differ from their bulk counterpart. Using thin films instead of bulk material will result is a significant increases in the figure of merit. Harman reported that the figure of merit of this film materials is enhanced compared with bulk materials.

## Conclusions

It is of interest to note that the good thermoelectrical material should have high electrical conductivity but low thermal conductivity. Electrical conductivity increases with the increases of the carrier concentration and/or the carrier mobility. Hence, improvement can be achieved by developing material structure or fabrication process that increases the mobility or the carrier concentration, or both.

Thermoelectric devices will be used extensively for personal electronic tools like watches or cloths, to biomedical applications such as drug delivery and vital signs monitoring as well as to many industrial applications. Modern technology can provide devices for micro-thermoelectric applications but to reach the full potential of these applications, a cost of effective mass production techniques needs to be developed and conversion efficiency of the devices should be optimized. In conclusion, thermoelectric devices have a great potential in both personal and industrial electronics components. However, a more efficient material need to be developed and mass production techniques need to be developed to reach this potential.

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