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Thermoelectric Power Factor for various temperature gradients in Nanocrystalline Composites

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Abstract.
Nanocrystalline are polycrystalline material that are very tiny particles with the dimension less than 100 nanometers. Nanocrystalline material can be estimated using x-ray diffraction.

In this paper; thermoelectric power factor for nanocrystalline graphs are plotted and compared with various temperature gradients (10K, 100K and 200K) such as seeback coefficient, electrical conductivity, power factor, subband plot, transmission plot, potential energy – centerline, electron density – centerline, current density – centerline, density of states – centerline and areal current density; values for graphs are also noted for further study.

Keywords: Nanocrystalline; Nanotechnology; nanocrystalline composites; thermoelectric effect.

1. INTRODUCTION

Nanocrystalline materials have a unique characteristic feature; it has grain size phenomena down to a microstructural size, where materials loose crystallinity because of inclination of grain boundaries. [1] They have been described to be significantly stronger than their coarse grained counterparts, however their ductility is normally disappointingly low except for a few rare extraordinary reports. [2] Despite the fact, some nanocrystalline formed can remain even after long term heat treatment above 1473 K. The potential of nanocrystalline has not fully analyzed. [3] An extraordinary observation was made on superplasticity in electrodeposited nickel at $0.36T_m$.This is extraordinary lower than the minimum homologous temperature of >0.5 of superplastic temperature from 1050 to 650 degree Centigrade. [4] Recent research concentrates on bulk nanocrystalline materials that includes their synthesis, processing, thermal stability, their structural characterization and their behavior. [5] Nanocrystalline are subsequently analyzed using standard plasma spraying technologies. It was found that nanostructured crystalline had higher hardness, lower thermal diffusivity and better thermal shock resistance compared to conventional methods, although the grain sized influence to increase during annealing at high temperatures which could result in substantial degree of sintered density. [6]
To meet future energy requirements, devices are used for conversation of heat energy into electricity are semiconductor thermoelectric cells. It works on the principle of Seeback effect. [11] Thermoelectric materials play a very important role for efficient use of energy resources and waste heat recovery for future. [12] There has been recent progress in the area of thermoelectric applications of conducting polymers and its related composites. [13] Various attempts has been made for maximizing the power factor that include development of new materials, optimization of existing materials by doping and investigation of nanoscale materials. [14] Most important use of thermoelectric materials is that it can be used for solid power generation and heating/cooling applications. [15]

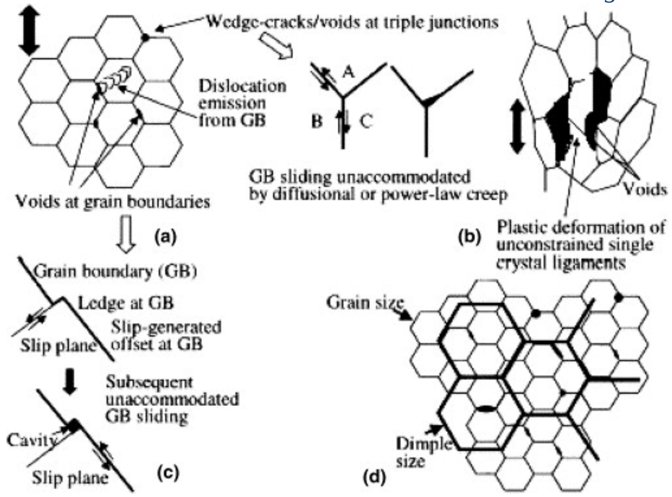

Figure. 1. illustratesmechanical properties of Nanocrystalline [Image Credit Reference No 7]

2. Experimental Simulation on Thermoelectric Power Factor for Temperature of 10K for Nanocrystalline composites

2.1 Simulation

A simulation was performed fornanocrystalline composites for temperature 10 K. [Ref 8]

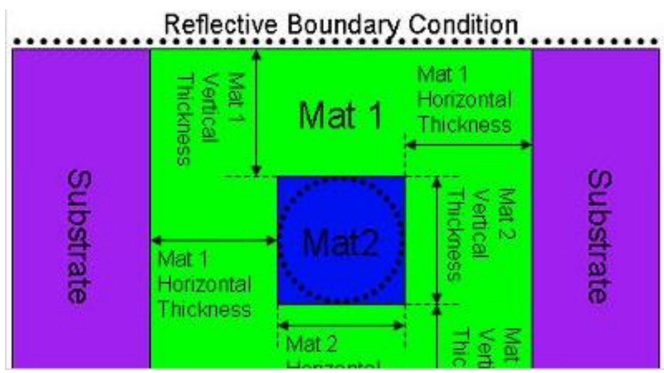

Figure. 2. Illustrates Reflective boundary condition for nanocrystalline composite[Image Credit Reference No 8]

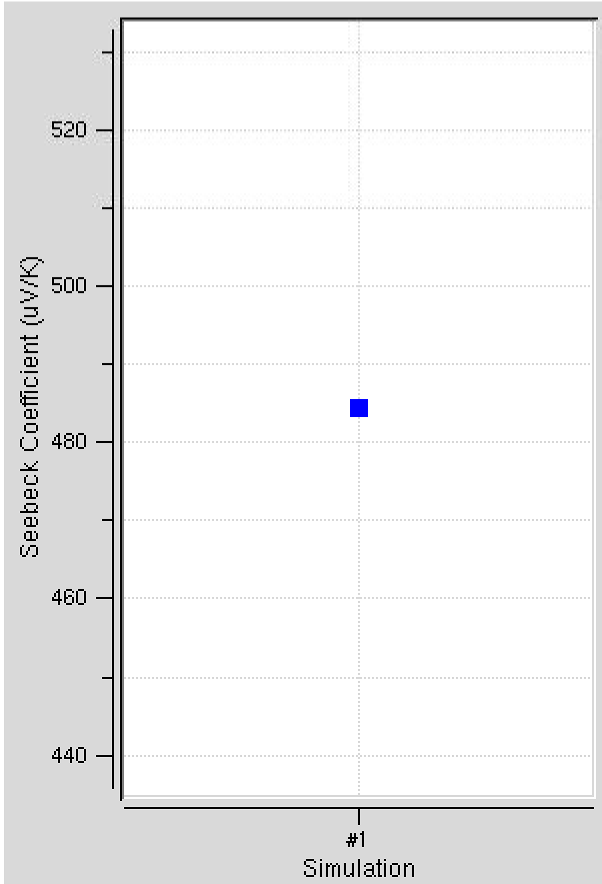

Figure. 3. Illustrates Seeback Coefficient (µV/K) is around 484.4 µV/K at temperature 10K

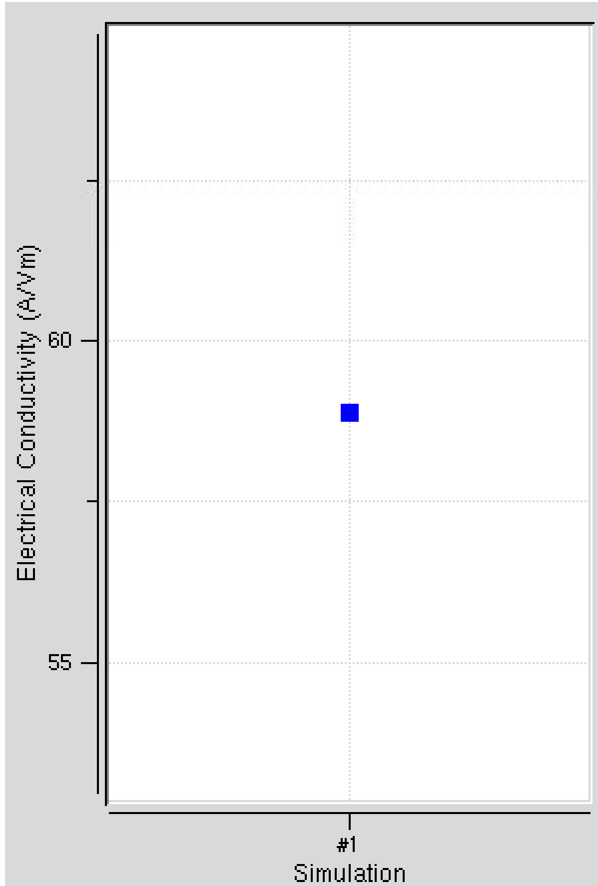

Figure. 4. Illustrates Electrical Conductivity (A/Vm) is around 58.8823 A/Vm at temperature 10K

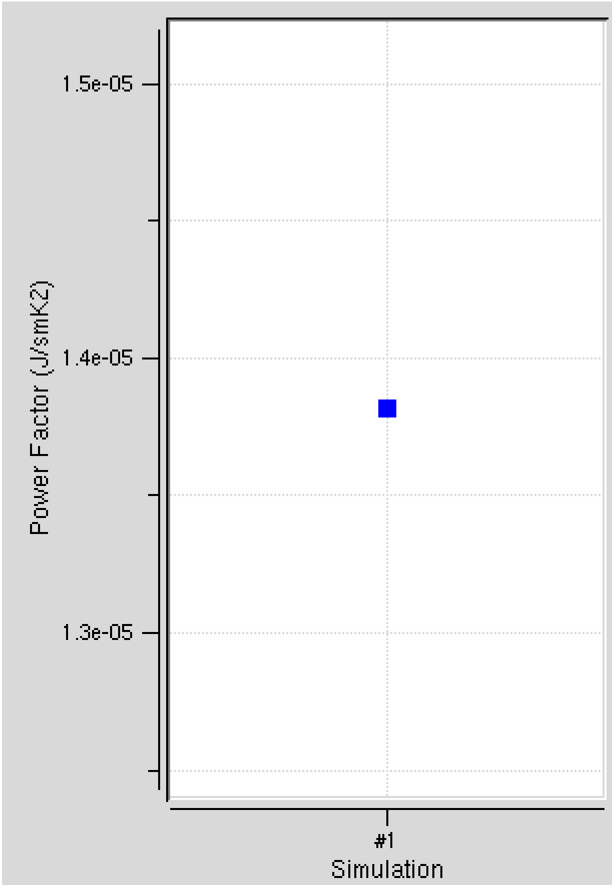

Figure. 5. Illustrates Power Factor (J/smK2) is around 1.38163e-05 J/smK2 at temperature 10K

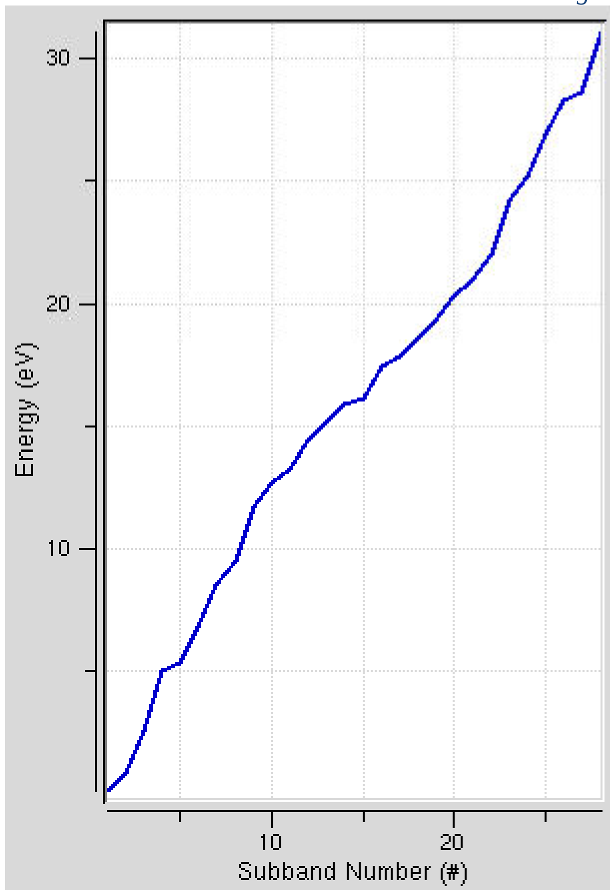

Figure. 6. Illustrates Subband Number (X-axis) and Energy (Y-axis) at temperature 10K

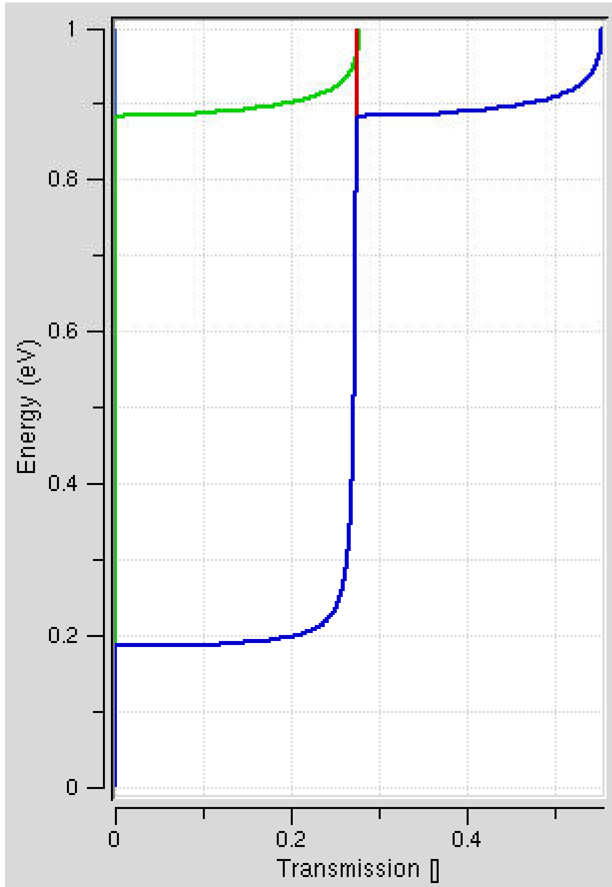

Figure. 7. Illustrates Transmission (X-axis) and Energy (Y-axis) at temperature 10K

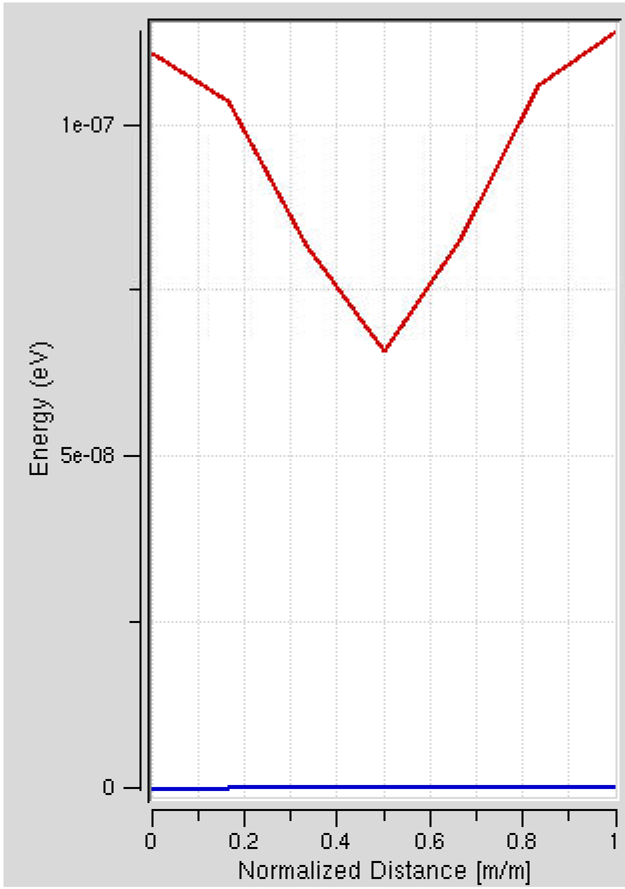

Figure. 8. Illustrates Potential Energy and Normalized Distance (X-axis) and Energy (Y-axis) at temperature 10K

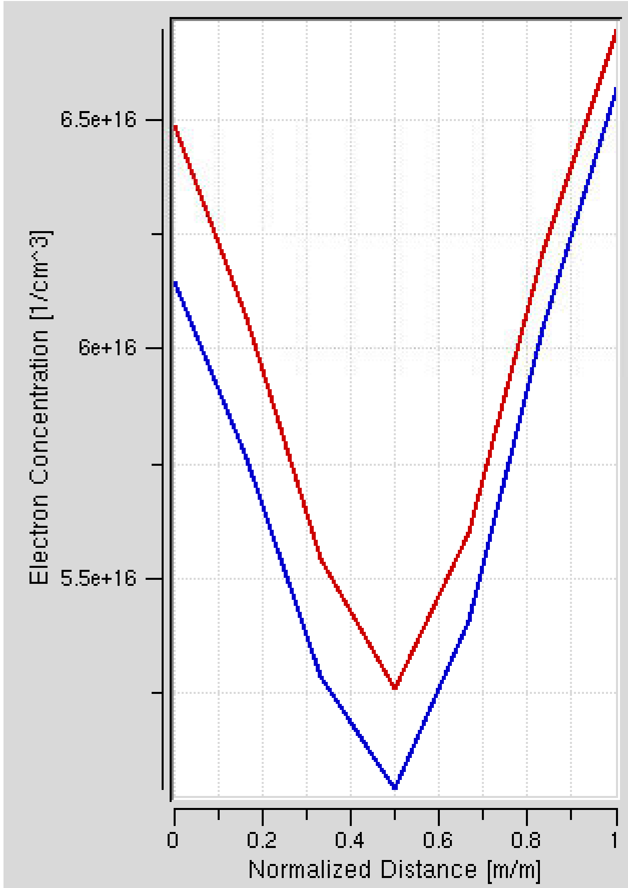

Figure. 9. Illustrates Electron Density and Normalized Distance (X-axis) and Electron Concentration (Y-axis) at temperature 10K

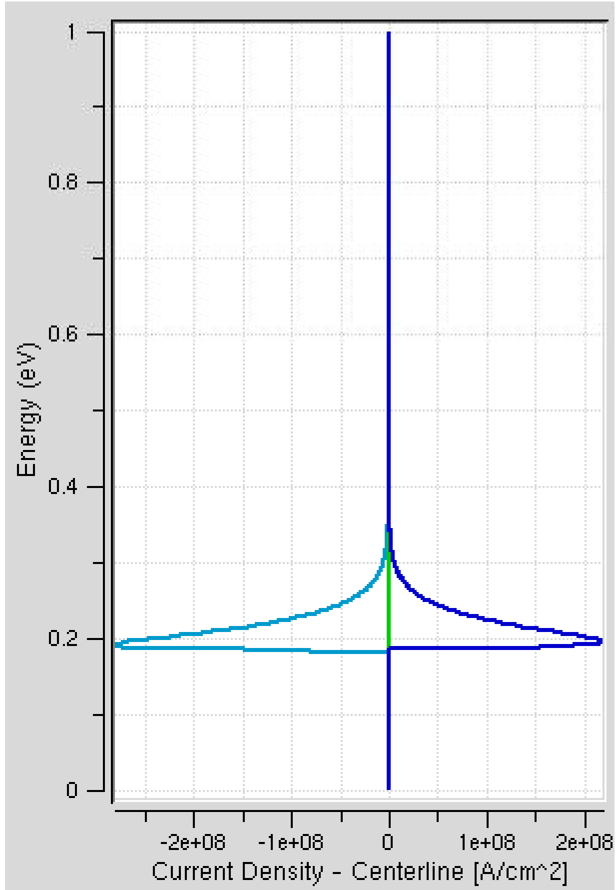

Figure. 10. Illustrates Current Density and Current Density (X-axis) and Energy (Y-axis) at temperature 10K

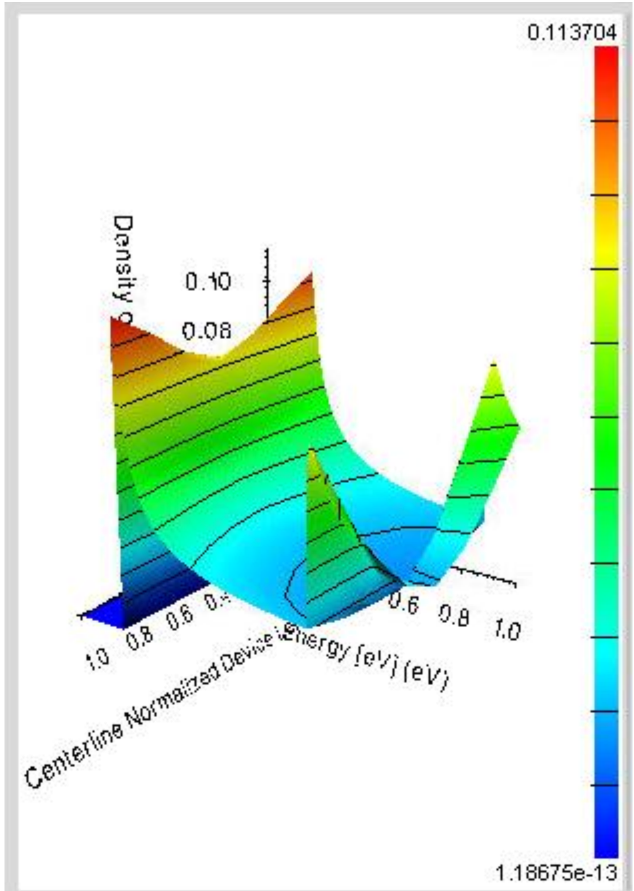

Figure. 11. Illustrates Density of States and its graphical representation at temperature 10K

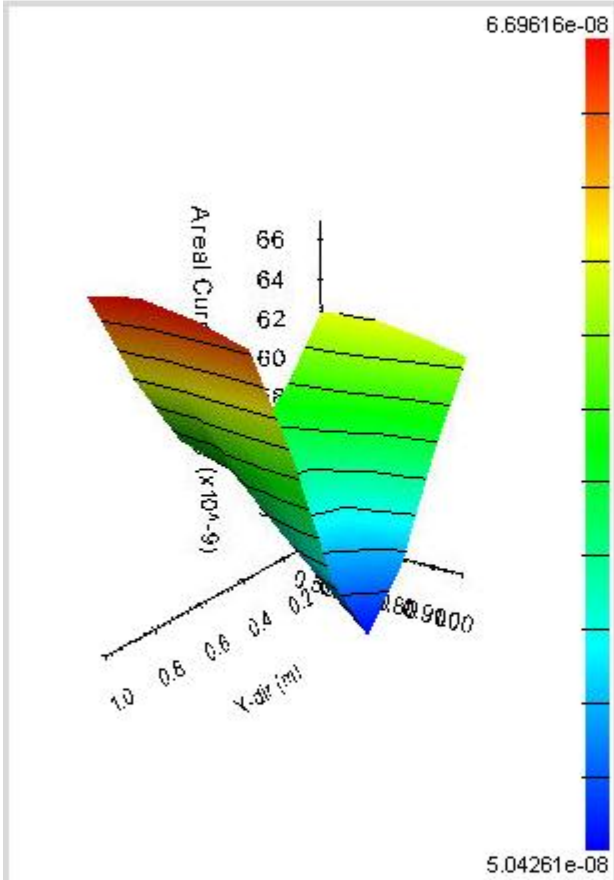

Figure. 12. Illustrates Areal Current and its graphical representation at temperature 10K

TABLE 1
SIMULATION NOTES FOR TEMPERATURE GRADIENT OF 10K

Sl No:	Source Parameters	Values
1	Temperature	300K
2	Temperature Gradient	10K
3	Silicone Doping	1e+18/cm3
4	Germanium Doping	1e+18/cm3
5	Substrate concentration Si(x) Ge (1-x)	1
6	Material 1	Silicon
7	Material 2	Germanium
8	Material 1 Horizontal Thickness	0.2nm
9	Material 1 Vertical Thickness	0.2nm
10	Material 2 Horizontal Thickness	0.2nm
11	Material 2 Vertical Thickness	0.2nm

TABLE 2
SIMULATION NOTES FOR TEMPERATURE GRADIENT OF 10K
ADVANCED PARAMETERS

Sl No:	Advanced Parameters	Values
1	Base Number of Energy Integration Steps	600
2	Poisson Self-Consistent Method	Anderson Mixing
3	Simple Mixing Parameter	0.2
4	Anderson Mixing Parameter (w):	10
5	Number of Previous Terms	5
6	Energy AMR	on
7	Energy AMR Maximum Divisions	5
8	Material 1 Horizontal Thickness	0.2nm
9	Material 1 Vertical Thickness	0.2nm
10	Material 2 Horizontal Thickness	0.2nm
11	Material 2 Vertical Thickness	0.2nm

2.2 Observations

Below are the observations that are noted for 10K for nanocrystalline composites

1. Seeback Coefficient is around 484.4 µV/K
2. Electrical Conductivity is around 58.8823 A/Vm
3. Power Factor is around 1.38163e-05 J/smK2
4. Subband Plot is noted
5. Transmission Plot is noted
6. Potential Energy is plotted and its low peak value is around 6.5611e-08eV @ 0.5
7. Electron Density is plotted and filled electrons are 5.25883e+16 @ 0.5 (red color) and free electrons are 5.04261e+16 @ 0.5 (blue color)
8. Current Density is plotted and Drain Current Subband is 0.190317eV @ -2.81537e+08 (light blue color) and Source Current Total is 0.193656eV @ 2.15539e+08 (dark blue color)
9. Density of States is plotted
10. Areal Current density is plotted

3. Experimental Simulation on Thermoelectric Power Factor for temperature of 100K for Nanocrystalline Composites

3.1 Simulation for nanocrystalline composites for temperature 100 K

A simulation was performed for nanocrystalline composites for temperate of 100 K

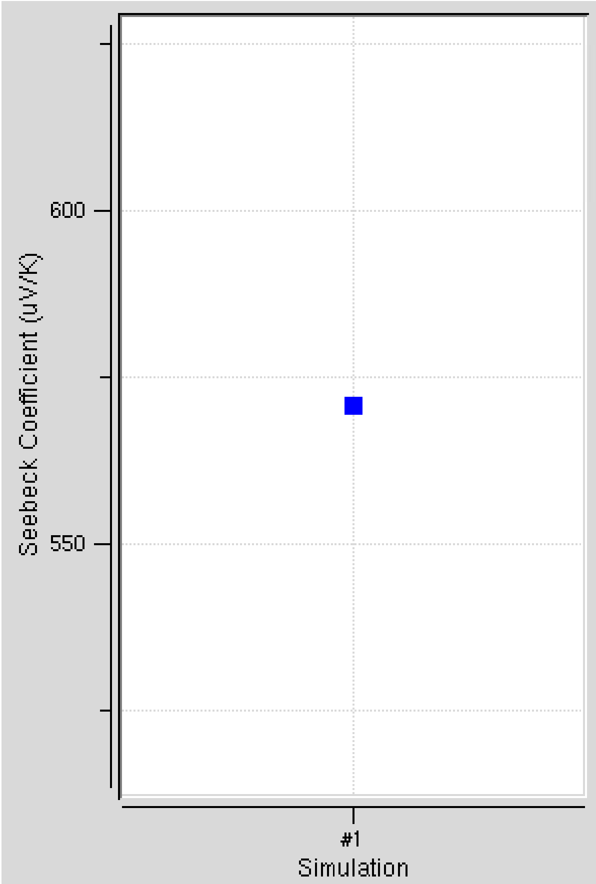

Figure. 13. Illustrates Seeback Coefficient (µV/K) is around 570.843 µV/K (approximately) at temperature 100K

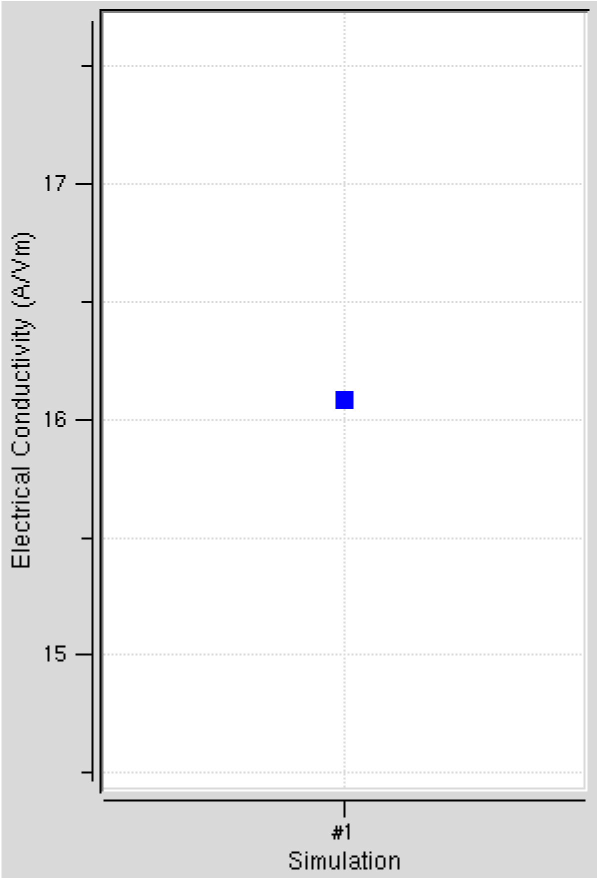

Figure. 14. Illustrates Electrical Conductivity (A/Vm) is around 16.0819 A/Vm (approximately) at temperature 100K

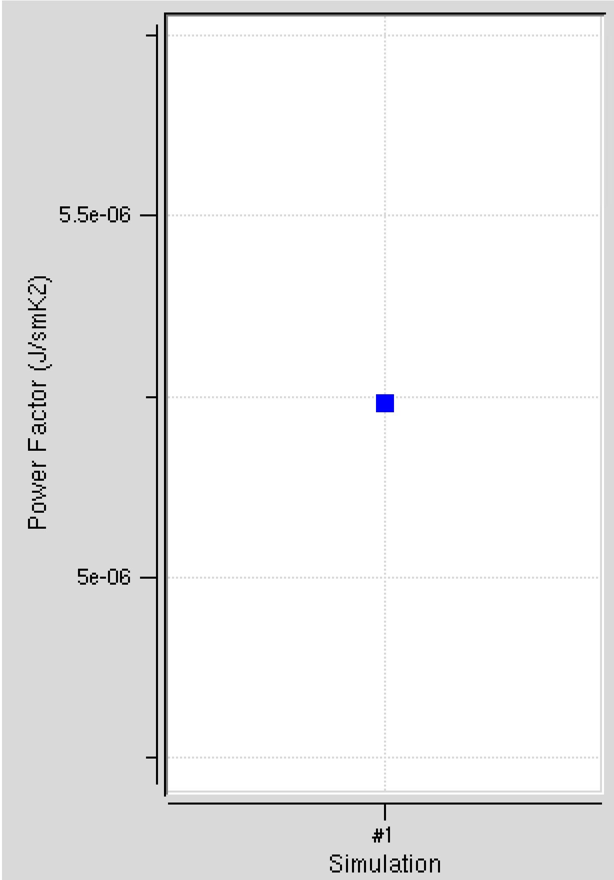

Figure. 15. Illustrates Power Factor (J/smK2) is around 5.24066e-06 J/smK2 (approximately) at temperature 100K

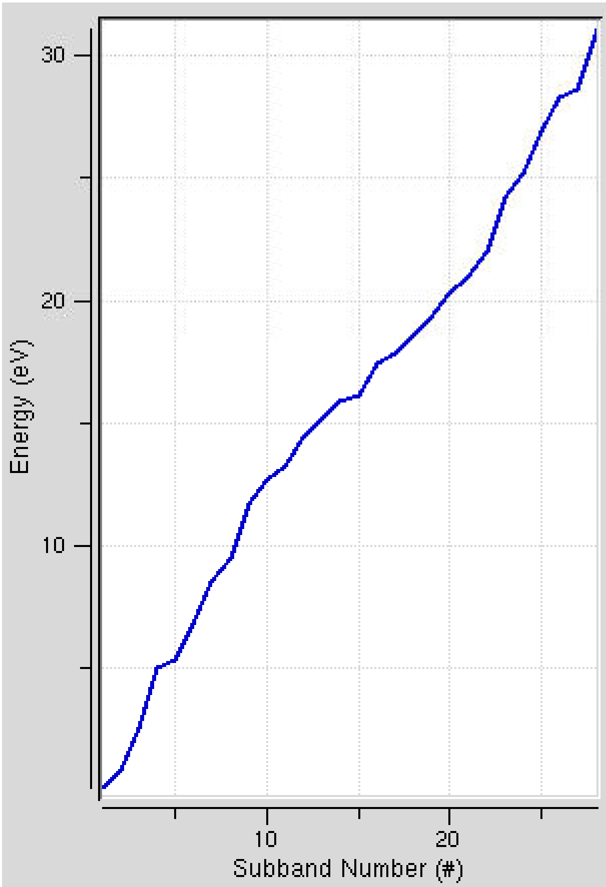

Figure. 16. Illustrates Subband Number (X-axis) and Energy (Y-axis) at temperature 100K

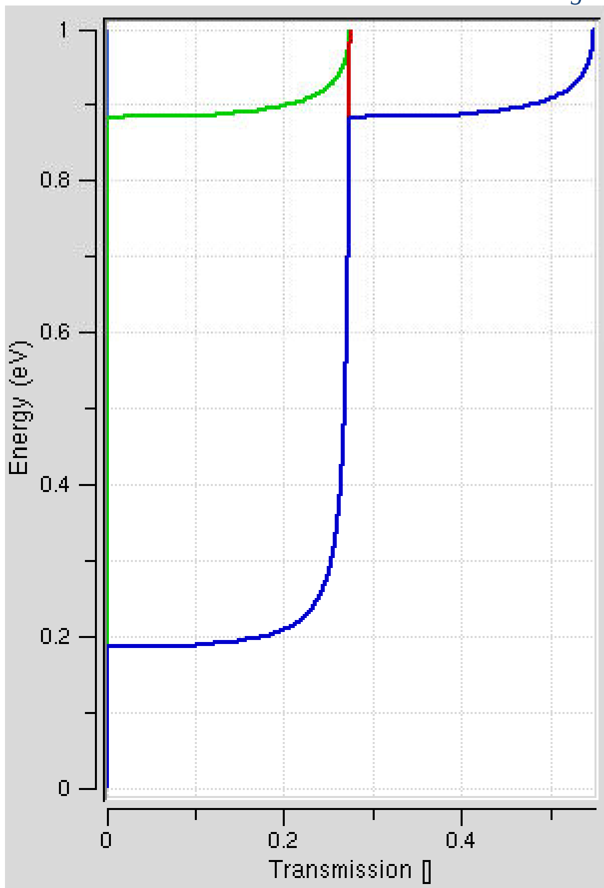

Figure. 17. Illustrates Transmission (X-axis) and Energy (Y-axis) at temperature 100K

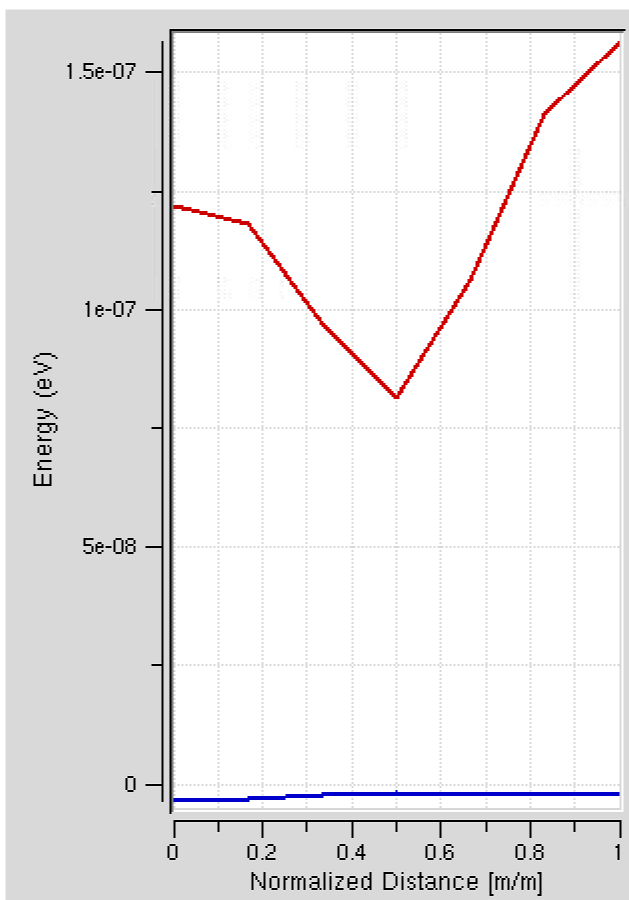

Figure. 18. Illustrates Potential Energy and Normalized Distance (X-axis) and Energy (Y-axis) at temperature 100K

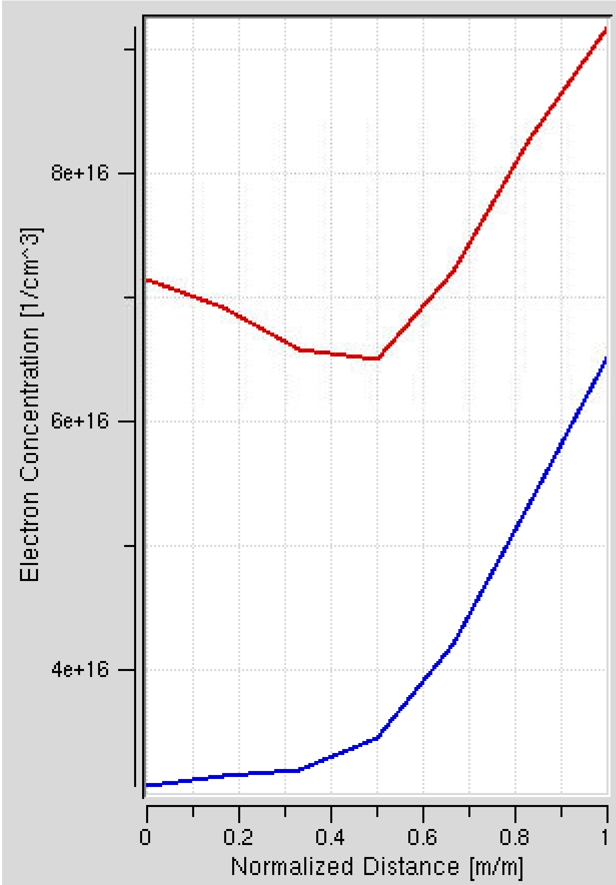

Figure. 19. Illustrates Electron Density and Normalized Distance (X-axis) and Electron Concentration (Y-axis) at temperature 100K

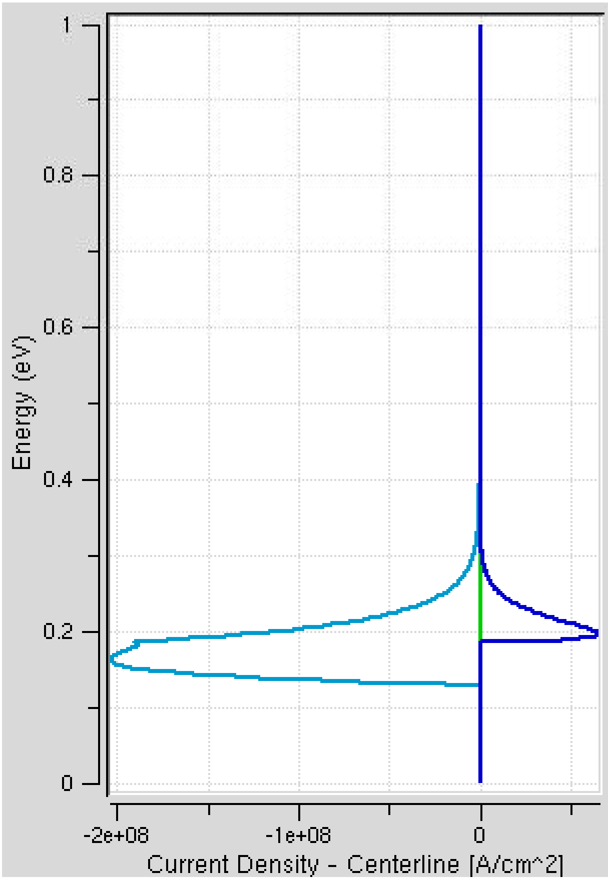

Figure. 20. Illustrates Current Density and Current Density (X-axis) and Energy (Y-axis) at temperature 100K

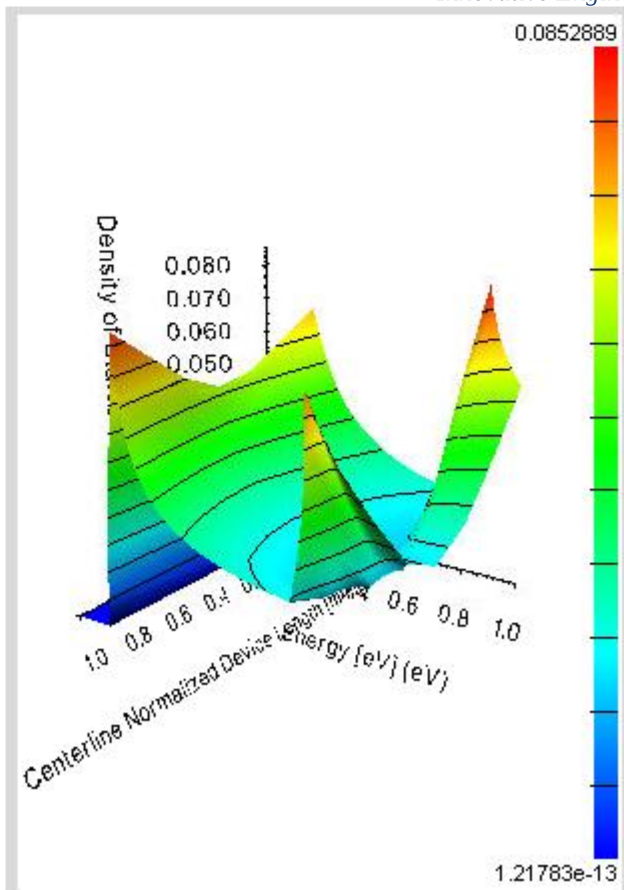

Figure. 21. Illustrates Density of States and its graphical representation at temperature 100K

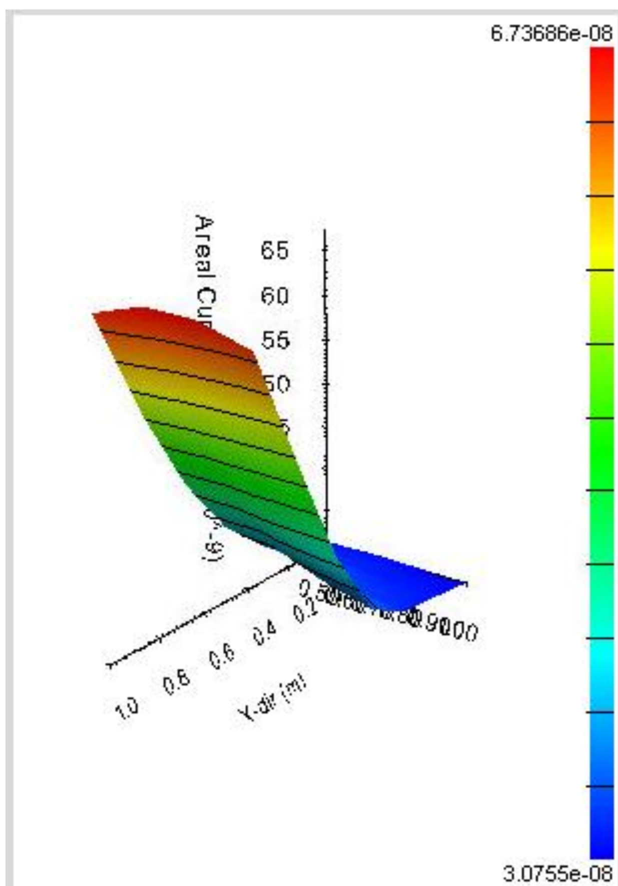

Figure. 22. Illustrates Areal Current and its graphical representation at temperature 100K

TABLE 3
SIMULATION NOTES FOR TEMPERATURE GRADIENT OF 100K

Sl No:	Source Parameters	Values
1	Temperature	300K
2	Temperature Gradient	100K
3	Silicone Doping	1e+18/cm3
4	Germanium Doping	1e+18/cm3
5	Substrate concentration Si(x) Ge (1-x)	1
6	Material 1	Silicon
7	Material 2	Germanium
8	Material 1 Horizontal Thickness	0.2nm
9	Material 1 Vertical Thickness	0.2nm
10	Material 2 Horizontal Thickness	0.2nm
11	Material 2 Vertical Thickness	0.2nm

TABLE 4
SIMULATION NOTES FOR TEMPERATURE GRADIENT OF 100K
ADVANCED PARAMETERS

Sl No:	Advanced Parameters	Values
1	Base Number of Energy Integration Steps	600
2	Poisson Self-Consistent Method	Anderson Mixing
3	Simple Mixing Parameter	0.2
4	Anderson Mixing Parameter (w):	10
5	Number of Previous Terms	5
6	Energy AMR	on
7	Energy AMR Maximum Divisions	5
8	Material 1 Horizontal Thickness	0.2nm
9	Material 1 Vertical Thickness	0.2nm
10	Material 2 Horizontal Thickness	0.2nm
11	Material 2 Vertical Thickness	0.2nm

3.2 Observations

Below are the observations that are noted for 100K for nanocrystalline composites
1. Seeback Coefficient is around 570.843 µV/K
2. Electrical Conductivity is around 16.0819 A/Vm
3. Power Factor is around 5.24066e-06 J/smK2
4. Subband Plot is noted
5. Transmission Plot is noted
6. Potential Energy is plotted and its low peak value is around 8.11646e-08eV @ 0.5
7. Electron Density is plotted and filled electrons are 6.50548e+16 @ 0.5 (red color) and free electrons are 3.45178e+16 @ 0.5 (blue color)
8. Current Density is plotted and Drain Current Subband is 0.165275eV @ -2.03707e+8 (light blue color) and Source Current Total is 0.195326eV @ 6.47464e+07 (dark blue color)
9. Density of States is plotted
10. Areal Current density is plotted

4. Experimental Simulation on Thermoelectric Power Factor for temperature of 200K for Nanocrystalline Composites

4.1 Simulation for nanocrystalline composites for temperature 200 K

A simulation was performed for nanocrystalline composites for temperate of 200 K

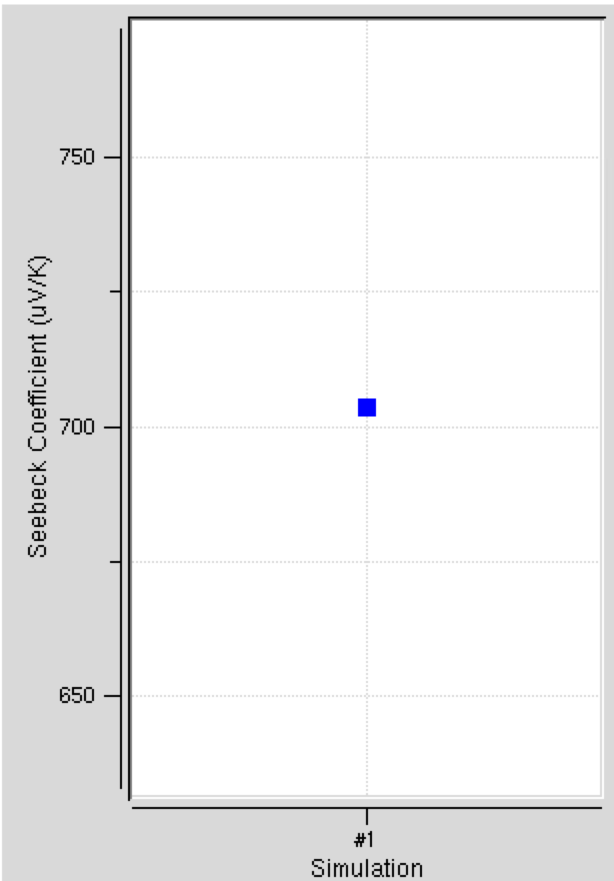

Figure. 23. Illustrates Seeback Coefficient (µV/K) is around 703.625 µV/K at temperature 200K

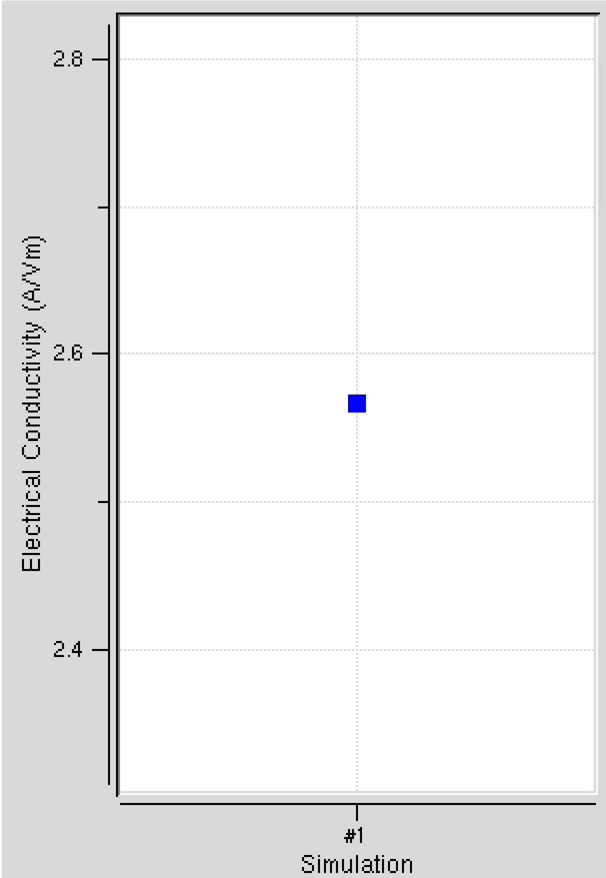

Figure. 24. Illustrates Electrical Conductivity (A/Vm) is around 2.56678 A/Vm at temperature 200K

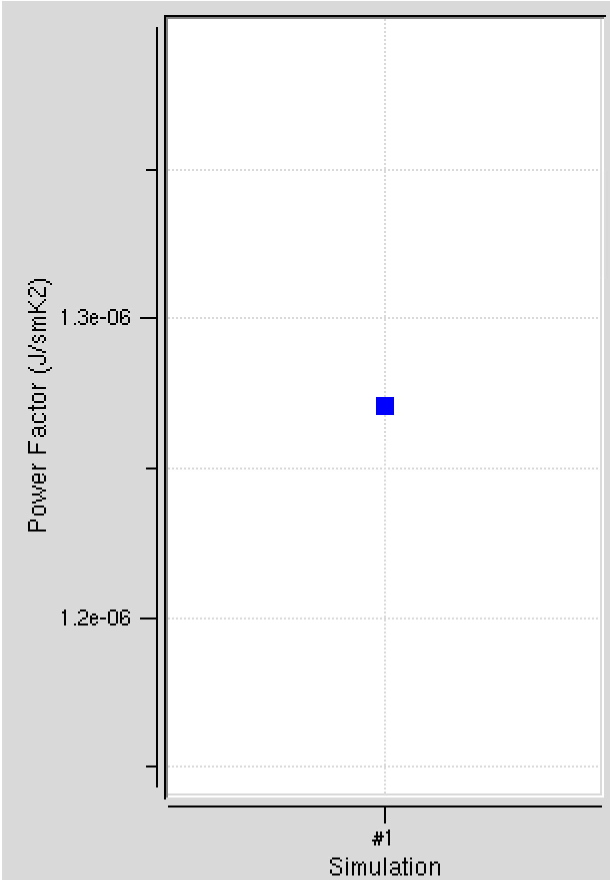

Figure. 25. Illustrates Power Factor (J/smK2) is around 1.27078e-06 J/smK2 at temperature 200K

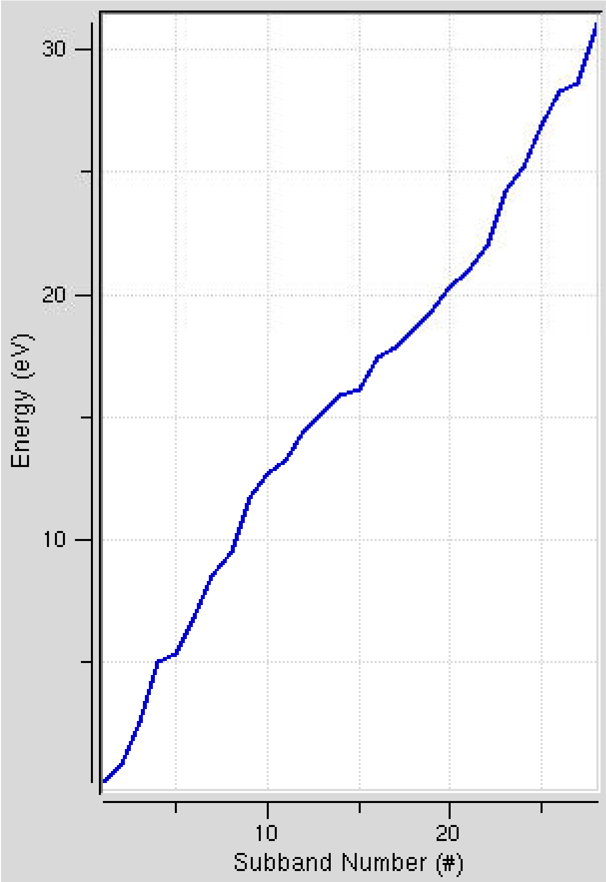

Figure. 26. Illustrates Subband Number (X-axis) and Energy (Y-axis) at temperature 200K

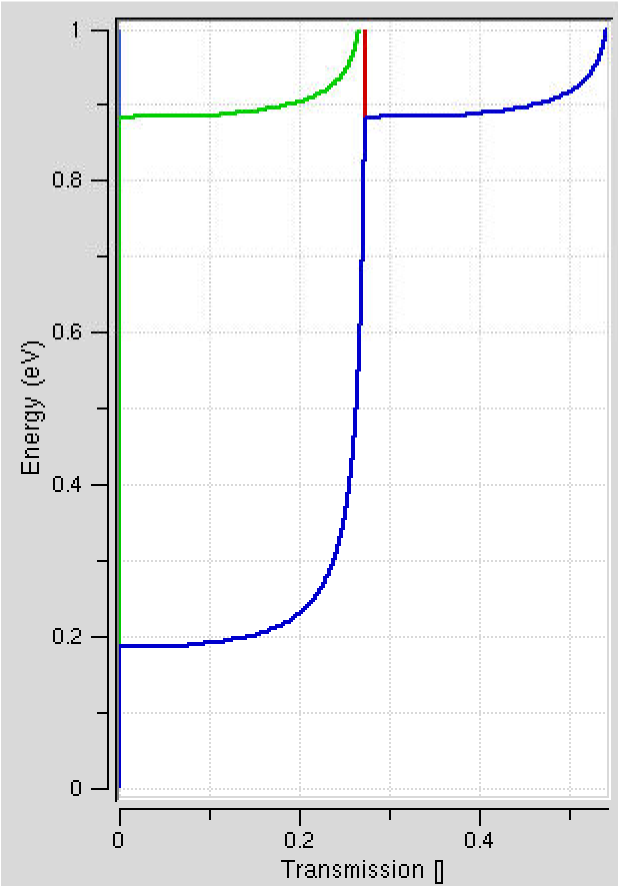

Figure. 27. Illustrates Transmission (X-axis) and Energy (Y-axis) at temperature 200K

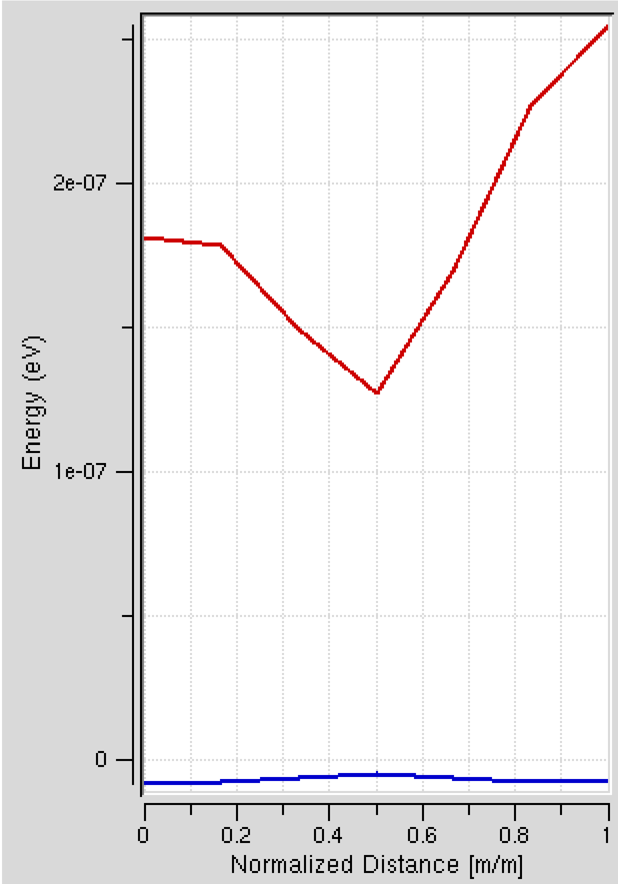

Figure. 28. Illustrates Potential Energy and Normalized Distance (X-axis) and Energy (Y-axis) at temperature 200K

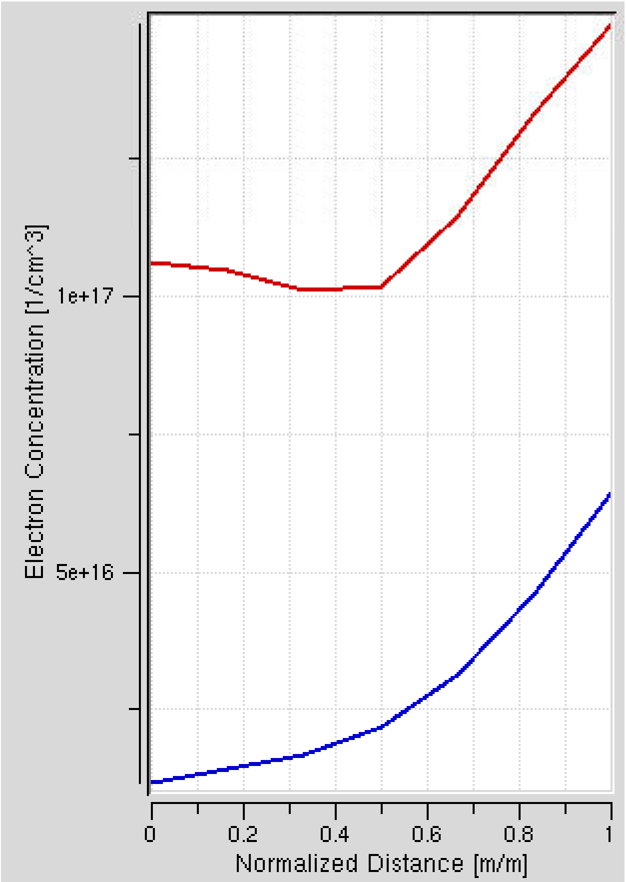

Figure. 29. Illustrates Electron Density and Normalized Distance (X-axis) and Electron Concentration (Y-axis) at temperature 200K

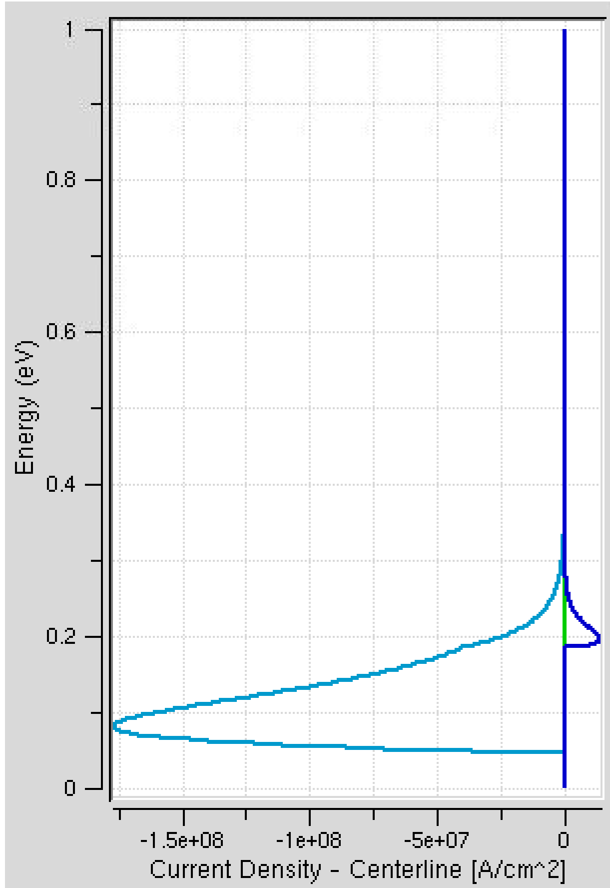

Figure. 30. Illustrates Current Density and Current Density (X-axis) and Energy (Y-axis) at temperature 200K

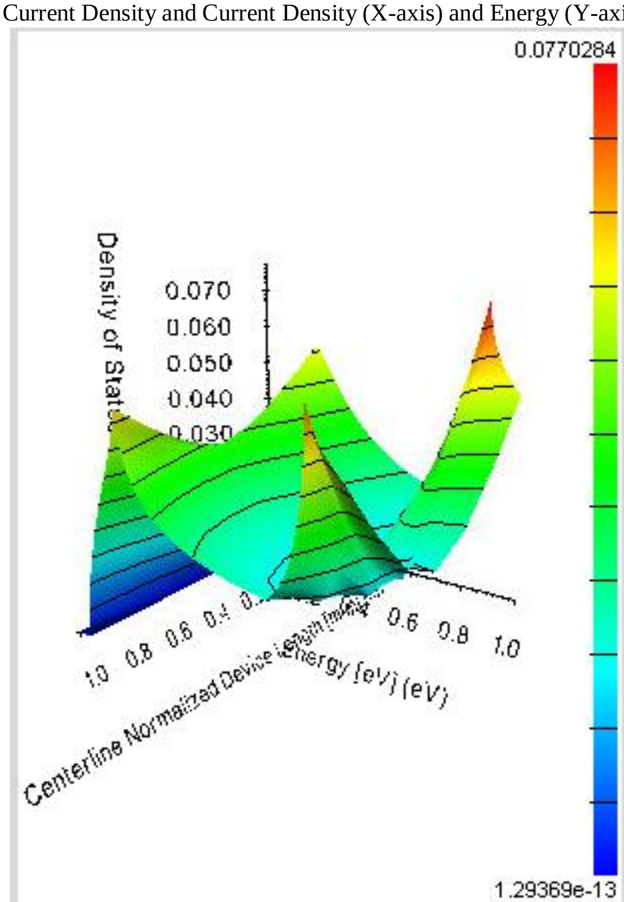

Figure. 31. Illustrates Density of States and its graphical representation at temperature 200K

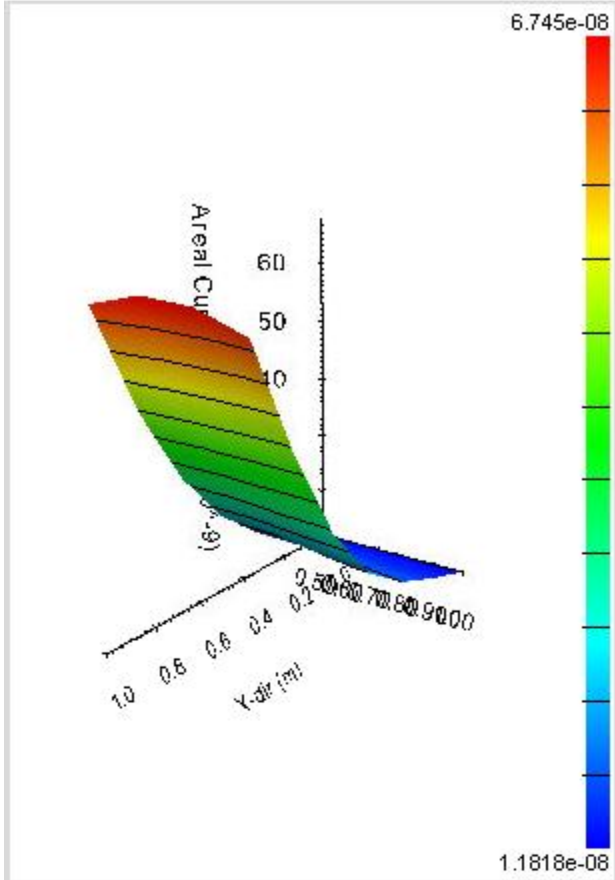

Figure. 32. Illustrates Areal Current and its graphical representation at temperature 200K

TABLE 5
SIMULATION NOTES FOR TEMPERATURE GRADIENT OF 200K

Sl No:	Source Parameters	Values
1	Temperature	300K
2	Temperature Gradient	200K
3	Silicone Doping	1e+18/cm3
4	Germanium Doping	1e+18/cm3
5	Substrate concentration Si(x) Ge (1-x)	1
6	Material 1	Silicon
7	Material 2	Germanium
8	Material 1 Horizontal Thickness	0.2nm
9	Material 1 Vertical Thickness	0.2nm
10	Material 2 Horizontal Thickness	0.2nm
11	Material 2 Vertical Thickness	0.2nm

TABLE 6
SIMULATION NOTES FOR TEMPERATURE GRADIENT OF 200K
ADVANCED PARAMETERS

Sl No:	Advanced Parameters	Values
1	Base Number of Energy Integration Steps	600
2	Poisson Self-Consistent Method	Anderson Mixing
3	Simple Mixing Parameter	0.2
4	Anderson Mixing Parameter (w):	10
5	Number of Previous Terms	5
6	Energy AMR	on
7	Energy AMR Maximum Divisions	5
8	Material 1 Horizontal Thickness	0.2nm
9	Material 1 Vertical Thickness	0.2nm
10	Material 2 Horizontal Thickness	0.2nm
11	Material 2 Vertical Thickness	0.2nm

4.2 Observations

Below are the observations that are noted for 200K for nanocrystalline composites
1. Seeback Coefficient is around 703.625 µV/K
2. Electrical Conductivity is around 2.56678 A/Vm
3. Power Factor is around 1.27078e-06 J/smK2
4. Subband Plot is noted
5. Transmission Plot is noted
6. Potential Energy is plotted and its low peak value is around 1.27195e-07eV @ 0.5
7. Electron Density is plotted and filled electrons are 1.01949e+17 @ 0.5 (red color) and free electrons are 2.16621e+16 @ 0.5 (blue color)
8. Current Density is plotted and Drain Current Subband is 0.0784641eV @ -1.77063e+08 (light blue color) and Source Current Total is 0.196995eV @ 1.36106e+07 (dark blue color)
9. Density of States is plotted
10. Areal Current density is plotted

5. RESULTS

In this article what isclaimedare

1. Seeback Coefficient of Nanocrystalline composites are 484.4 µV/K for temperature 10K, 570.843 µV/K for 100K and 703.625 µV/K for 200K
2. Electrical Conductivity of Nanocrystalline composites are 58.8823 A/Vm for temperature 10K, 16.0819 A/Vm for 100K and 2.56678 A/Vm for 200K
3. Power Factor of Nanocrystalline composites are 1.38163e-05 J/smK2 for temperature 10K, 5.24066e-06 J/smK2 for 100K and 1.27078e-06 J/smK2 for 200K
4. Subband plots remains similar but not same for all the three temperatures
5. Transmission plots remains similar but not same for all the three temperatures
6. Electron Density of Nanocrystalline composites are filled electrons are 5.25883e+16 @ 0.5 (red color) and free electrons are 5.04261e+16 @ 0.5 (blue color) for 10K temperatures
7. Electron Density of Nanocrystalline composites are filled electrons are 6.50548e+16 @ 0.5 (red color) and free electrons are 3.45178e+16 @ 0.5 (blue color) for 100K temperatures
8. Electron Density of Nanocrystalline composites are filled electrons are 1.01949e+17 @ 0.5 (red color) and free electrons are 2.16621e+16 @ 0.5 (blue color) for 200K temperatures
9. Current Density of Nanocrystalline composites for Drain Current Subband is 0.190317eV @ -2.81537e+08 (light blue color) and Source Current Total is 0.193656eV @ 2.15539e+08 (dark blue color)
10. Current Density of Nanocrystalline composites for Drain Current Subband is 0.165275eV @ -2.03707e+8 (light blue color) and Source Current Total is 0.195326eV @ 6.47464e+07 (dark blue color)
11. Current Density of Nanocrystalline composites for Drain Current Subband is 0.0784641eV @ -1.77063e+08 (light blue color) and Source Current Total is 0.196995eV @ 1.36106e+07 (dark blue color)
12. Density of States of Nanocrystalline composites changes drastically for three different temperatures
13. Areal Current Density of Nanocrystalline composites changes for three different temperatures

6. Conclusion

To conclude, below are the observations made for Thermoelectric Power Factor for 10K, 100K and 200K temperature gradients in Nanocrystalline Composites based on the results. However, only three temperature gradients were made. If more samples were taken the results would have been much better and temperature gradients in Nanocrystalline Composites would have been better understood:
1. Seeback Coefficient are increasing in nanocrystalline composites with an increase in temperature
2. Electrical Conductivity is decreasing in nanocrystalline composites with an increase in temperature
3. Power Factor is decreasing in nanocrystalline composites with an increase in temperature
4. Increase in Temperature for 10K, 100K and 200K does not affect too much on subband and transmission plots but care is necessary that the angle made by it may be different.
5. In Electron Density filled electrons are increasing and free electrons are decreasing with an increase in temperature of 10K, 100K and 200K
6. In Current Density, points are taken at different positions hence there is a change in both drain current and as well as source current. But based on the graphs drain current is increasing drastically and source current is decreasing drastically with an increase in temperature of 10K, 100K and 200K
7. Density of States of Nanocrystalline composites changes drastically for three different temperatures
8. Areal Current Density of Nanocrystalline composites changes for three different temperatures

7. Conflicts of interest

There is no conflicts of interest as per author’s point of view.

8. Acknowledgment

Author would like to thank Prof. Navarun Gupta, Prof. Hassan Bajwa, Prof. Linfeng Zhang and Prof. Hmurcik for their academic support. Author also thanks anonymous reviewers for their comments.

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10. BIOGRAPHY

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