

Original Article

# Investigation of Thermal Properties and Mechanical Strength of Polymer: Introducing Silicon Carbide (Sic) and Salt (NaCl) Nano Particles into Poly Styrene

Srinivas Seemala <sup>1</sup>, Ludwig Peetz <sup>2</sup>

<sup>1</sup>*Polymer sciences, Hochschule Kaiserslautern, 66953 Pirmasens, Germany.*

Received: 10 March 2022

Revised: 04 May 2022

Accepted: 16 May 2022

Published: 27 May 2022

**Abstract** - The thermal conductivity of polymers is one of the major technological barriers. Enhancing the thermal conductivity of the polymers is important for daily needs. In this work, we aim to increase the thermal conductivity of the polymer by introducing the Silicon Carbide (SIC) & Salt (NaCl) into the polystyrene (PS) polymer matrix. The effect of salt in the polymer is also investigated. Compounding of these materials using double screw co-rotational extruder to get granules and specimen is prepared by using an injection molding machine, The thermal conductivity is analyzed by using Thermogravimetric Analysis (TGA), the Impact strength is evaluated by Charpy-Impact test, Flexural modulus and Flexural strength are evaluated by 3-point bending test. The results reveal that salt improves thermal conductivity additionally to SIC; after studying internal microstructure, the results reveal that salt forms porosity inside polymer and SIC dispersion is uniform. The results were evaluated by sampling the specimen according to weight percentages. The silicon carbide nanoparticles can be used in injection molding, which leads to maximum design freedom for constructive.

**Keywords** - Compounding, Injection molding, Thermogravimetric analysis (TGA), Microstructure of composite.

## 1. Introduction

A polymer is a substance or material consisting of very large molecules or macromolecules composed of many repeating subunits; polymers are divided according to the molecular structure and chain bonding. We call it thermoplastic or thermosetting plastic. The differences between them are due to structural, thermal, and type of processing [1]. In general, polystyrene is a brittle material that can be processed easily due to its amorphous and nonpolar commodity and good resistance to chemical reactions and electrical conductivity. It has high aromatic content; it is stable to gamma radiation also but has low heat distortion. [2] polystyrene is widely used in many industrial applications, but the poor thermal conductivity of these materials becomes a disadvantage to use in more applications. If the thermal conductivity of polystyrene can be fixed, then it is used in various heat exchangers and electronics industries by maintaining lightweight, corrosive resistance, low cost, and easy processing. To increase the thermal conductivity of polystyrene, there should be a change in aligning the polymer molecular chain, or it should blend with highly thermally conductive fillers. To conduct the heat, these fillers should form an inter-filler network [3], inducing strain and shape change due to polymer molecules wrapping may decrease the thermal conductivity [4]. If in case any water (or) moisture is contained in the polymer, to remove it, we added salt as a medium because it removes any moisture content in the

polymer solution as it disturbs the chain between polymer and water and breaks the bond between them that water molecule ions get attracted to salt ions when enough of salt is added which result in draining of the water from the solution [5] furthermore salt also has a thermal conductivity which is greater than 6  $\text{W/m}\cdot\text{K}$  [6] this also acts as a secondary filler material in polymer to increase thermal conductivity more [7]. To experiment, we have prepared samples firstly by extrusion with a twin-screw co-rotational extruder in which the materials are subjected to dispersive mixing with each other. Then the specimen is prepared by injection molding, and the different specimen is extracted by changing the molds. In this research, we aim to 1) Add the filler material (silicon carbide and salt) to the polystyrene polymer matrix and 2) understand the effects of salt in polymers, 3) test the thermal conductivity value with salt and without salt, 4) check the mechanical strength of the composite

In general, the thermal conductivity of polymers is very low when the polystyrene conductivity measured was 0.17  $\text{W/m}\cdot\text{K}$ . Due to the morphology of the polymer chains, there are many ways to improve the conductivity; one of the ways is adding fillers to the polymer matrix, which has a great influence on conducting. A value of 0.291  $\text{W/m}\cdot\text{K}$  is achieved when 10% of silicon carbide and 10% of salt is added to the polystyrene, as shown in table 1, the result shown for this compounding ratio had inspired to do mechanical testing and



study of the microstructure on how it affects the mechanical properties as shown in Fig 7-10, but there is a decrease in impact strength, flexural modulus, and flexural strength.

Therefore filler concentrations should be low as the concentration increases, and conductivity decreases because it disturbs the crystallization of polymer matrix [8] filler size and thickness matter in influencing the thermal conductivity due to the contact area between polymer matrix and filler, shortening the mean free path of energy carriers. If the filler size is too small, conductivity is low due to large interfacial thermal resistance. If the filler size is too large, conductivity is low due to contact resistance[9]. These ceramic polymer composites (CMC) have excellent specific properties. They are anisotropic and heterogeneous. The material failure in these CMC is caused because it loses its load-carrying capacity, which can reduce the strength and stiffness, and the matrix starts cracking [10]

This review article is arranged as follows. In section 2, we discuss the selection of materials according to their properties and methods for preparing specimens for thermal and mechanical tests, as shown in fig 1, and in section 3, we discuss the test results and study the microstructure as illustrated in Fig (7-10)

## 2. Materials and Methods

### 2.1. Materials

Polystyrene(PS) is an organic polymer made up of styrene monomers manufactured from liquid hydrogen from petroleum. PS will remain in a solid-state at room temperature. Still, PS can be melted above the glass transition temperature [11]. The polystyrene which is used for the experiment is from DENKA STYROL-Singapore, in which glass transition temperature is 100°C, HDT (heat deflection temperature) is 95°C, melting temperature is 270°C, specific gravity is 1.05 g/cm<sup>3</sup> [1] the heat distortion point (rheological properties) of polystyrene is approximately 80°C[12]. Another material used in the experiment is silicon carbide(SiC), a semiconductor material used in high power and high-temperature applications. It acts as an electrical insulator by breaking down the electrical field, and also it has a high thermal conductivity whereas mechanical and chemical properties. It is very hard in nature with young's modulus 424Gpa it does not react with any material at room temperature because it is chemically inert [13] silicon carbide. The bonds between the silicon(Si) atom and the 4 carbon(C) atom are bonded covalently, making it hard to break. This SiC possesses relatively low thermal expansion and resistance to abrasion and corrosion SiC, even at 1650°C, can retain its elastic resistance this property of the material tends to use in a wide range of industrial applications [14] According to the CERABLAST-GERMANY, the physical properties of SiC are hardness:9.0 – 9.5 Mohs, grain size is angular, melting point of Sic is 2300°C, specific gravity: approx 3.2g/cm<sup>3</sup>, Bulk density: approx 1.3-1.5g/cm<sup>3</sup>, According to chemical analysis SiC is 98-99.5% purity with

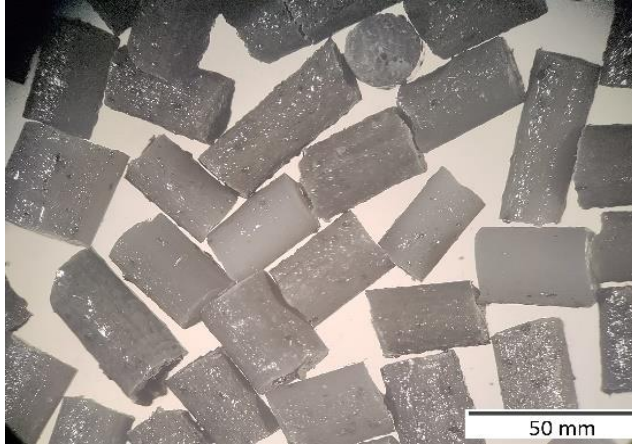
Fe:0.20%, C:0.15%, Magnetic particles:0.07%, size of the Sic particles are 1000-1400µm. Another material which we added is salt. It has many applications in daily life (agriculture, medical & chemical industry) [15] composition of rock salt is from MAXISALT-SPAIN, and these are as follows Sodium Chloride(NaCl):99.9%, Sodium39%, moisture <0.1%, anti-caking agent content measured as Fe(CN)6<9.5 mg/kg and the particle distribution is 3% are < 300 microns,32% are300-500microns,65%are500-1000 microns,0.1%>1000 microns and bulk density measured was 1250kg/m<sup>3</sup> All these are based on dried pure salt

### 2.2 Methods

#### 2.2.1. Extrusion

For compounding the filler materials into the polystyrene, we have used three feed hoppers double screw co-rotational extruder manufactured by KraussMaffei (ZE 25A x 42D-UTXi-UG) with a screw diameter of 25mm and L/D ratio 42:1 the maximum working temperature of extruder is 400°C with maximum pressure that can be exerted is 350 bars. As co rotational extruder functions with constantly increasing drive power, torque & screw speeds, there are various processing zones(Intake zone, plasticization zone, Melt conveying zone, Distributive mixing zone, Dispersive mixing zone, Pressure build-up zone ) in an extruder each of the processing zones has continuity with each other to process each zone with polymer there is an increasing temperature from the intake zone to the extrusion of the extrudate to adjust the temperature we should know the rheological and thermodynamic properties of the polymer, it is heated through a barrel wall [16] In this experiment virgin polystyrene with moisture is dumped into the main feed hopper and the silicon carbide filled into the secondary feed hopper, Initially, the barrel is heated up to 220°C (Melting point of polystyrene is 270°C) at the intake zone we maintain the temperature of 70°C which should be below the glass transition temperature(Tg of PS=80°C), however at the plasticization zone increase in the temperature above the melting temperature of the polystyrene due to mechanical shearing of polymer. We introduce the PS and SiC into the intake zone according to the volumetric feed rate which depends on the speed of the screw and the speed of the screw depends on the melt properties of the polymer, The melt property of the polystyrene according to the ASTM standard condition is 200°C/5kg (12-16g/10min)[17] we maintained screw speed of 50 rpm and pressure build-the up was 16bar when polymer is passed through different zones, solid particles which are present after melting are melted in kneading blocks(last stage of plasticization zone) with the side feeder at the melt conveying zone we add the salt to the polymer and the ratio of adding the polymer, SiC, Salt as per volume percentages shown in the table 1. the melt mixing mechanism in the twin-screw extruder is dispersive mixing when the polymer is in molten state and dispersion of nanoparticles into polymer matrix through mechanical shearing [18], the extrudate after extrusion is cooled by

treating with cool water and pellets are made by shedding machine as shown in fig 1.



The fraction of filler determines the overall mechanical properties of the composite. It is important to calculate the filler volume fraction in the hybrid composite. We use equations 1 & 2, where  $vf$  is the volume of particles.  $Wf$  is the weight fraction of filler,  $\rho f$  is the density of filler,  $Wm$  is the weight fraction of the polymer matrix,  $\rho m$  is the density of polymer matrix, and  $Wsf$  is the weight factor secondary filler,  $\rho sf$  is the density of the secondary filler.

$$vf = \frac{\frac{Wm}{\rho m}}{\frac{Wf}{\rho f} + \frac{Wm}{\rho m} + \frac{Wsf}{\rho sf}} \quad (1)$$

$$\rho = \rho fvf + \rho mvm + \rho sfvsf \quad (2)$$

Table 1. Compounding ratios in a double screw extruder

The weight fraction of filler	Polystyrene (PS) %	Silicon Carbide (SiC)%	Salt (NaCl) %
Sample 1	95	5	-
Sample 2	95	5	10
Sample 3	90	10	-
Sample 4	90	10	10

Table 2. Volume fraction and densities of the composite

Samples	Volume Fraction%	Densities (g/cm3)
Sample 1	9.8	1.15
Sample 2	9.3	1.37
Sample 3	9.6	1.26
Sample 4	9.1	1.48

### 2.2.2 Injection Molding

To prepare the test specimen to perform the mechanical and thermal tests, we use injection molding molds to extract the circular and dog bone cross-section specimen using (Arburg-320S), which has a maximum temperature of 400°C screw diameter of 25mm, and an L/D ratio is 24:1. The maximum pressure is 2400bars; in Injection Molding, the granules which are taken from the extrusion will feed into the hopper as the screw rotates and the granules move forward; injection molding cycle consists of mainly 4 stages (Filling, packaging, cooling, and Ejection) when the melted PS is injected into the mold cavity than it passes through the sprue, runner, gate, and cavity [19] with a total cycle time of the 30s and holding time of 6.5s the total volume for the cycle is 0-20%, speed of the screw is 50rpm and pressure is 20bar for the impact and flexural strength samples which has to be extracted from the dog bone. We changed the mold to a circular cross-section designed mold to do the thermal analysis of the material. The advantage of the single screw is the distribution mixing of the particles uniformly [18]. In this process, we use a cold runner system, so when the part cools down, we remove the part after each cycle; for the thermal analysis, we have extracted 4 cylindrical samples as per the table 1, and for the impact and flexural strength test we have extracted 10 samples of each type with a total of 40 samples as shown in Fig 1.

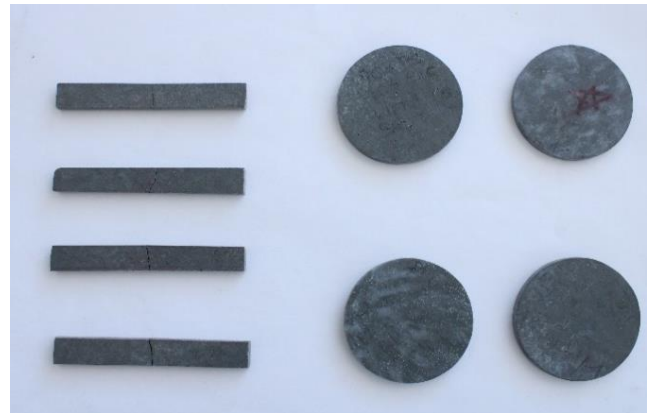


Fig. 1 samples used for thermal conductivity test and mechanical tests

### 2.2.3. Thermal conductivity test

The material's property (or) ability to conduct the defined quantity of heat per unit area and thickness in a period when there is a temperature difference in each face (or) side. To perform the thermal conductivity test, we have used a cylindrical shape testing sample with diameters 45mm and 25mm thick placed between the heat source and heat sink as per Fig 1; before performing the test, calibrating the device to reach a steady-state condition with known thermal conductivity steel bar (15.9w/m\*K) is used, we will heat the source with a known power input (Voltage= 20W and electrical current=0.27A) and when the steady-state distribution is achieved there is a temperature drop across the length which is measured by the temperature sensors it takes up to 1hour to reach this state. For measuring the temperature,

thermocouple sensors are used with small wire diameter and low conductivity material wires due to their accuracy and also heat loss due to thermocouple is less than 1% [20]

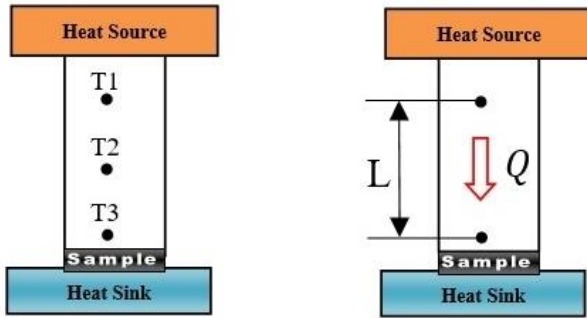


Fig. 2 Apparatus for testing thermal conductivity

From Fig 1. In the heat source, the heat supplied is 60°C, and the heat sink is maintained at 20°C. The length (L) between T1 & T2 is 85mm, and Q is the heat flow in a steady-state condition. To minimize the heat loss due to convection and radiation, we experimented in a vacuum with radiation shields. We keep the samples as shown in fig 1. As per the ISO 8302, the testing procedure was performed, and the conductivity value of polystyrene was measured was 0.17 W/m·K. And the following thermal conductivity values for each sample are obtained as fig 4.

2.2.4. Bending Test (3-point)

The tendency of the material to resist bending moment is called flexural modulus. In this testing method, we determine the flexural deformation of the sample when the force is applied in the middle of the sample. The bottom face of the specimen is subjected to tensile stress, and the upper face is subjected to compressive stress. According to the ISO178 dimensions of the sample are length=80mm, width=10mm, and thickness=4mm; we performed the test on machine Zwick Roell at room temperature with preload of 0.1MPa, crosshead speed of 1.5mm/min, Normal polystyrene flexural strength measured was 67Mpa, and Flexural Modulus is 2300Mpa, and a minimum of 4 tests were performed for each average sample value reported in fig 3 & 4

2.2.5. Impact strength Test

We have conducted the Impact test on the ISO179 to study the temperature-dependent ductile-brittle transition. It is a high strain rate test, which measures the energy absorbed by the specimen during breaking under impact load. Firstly, calibrate the device by the potential energy of the pendulum before and after impact by calculating the initial and final location of the pendulum. The test was performed at ambient

room temperature with hammer velocity of 2.900 m/sec, hammer weight of 0.9510kg, Impact energy is 3.99 joules, dimensions of samples are length=55mm, width=10mm, and thickness=10mm. A Ran-Ray advanced universal pendulum impact tester was used. A minimum of 4 tests were performed for each sample, and the average values are reported in Fig 5

2.2.6. Optical Microscopic Test

To create the samples for the microscopic test, we used epoxy resin according to the ratio, and the hardener was mixed and stirred carefully. The samples were examined with an OLYMPUS BX40 microscope

3. Results and Discussion

To know the thermal conductivity, they are methods in theoretical and empirical has proposed earlier in this research. We have conducted a low concentration of the filler nanoparticles in the polymer and the influence of salt in the polymer. Increasing the thermal conductivity include not only filler concentration but also filler network

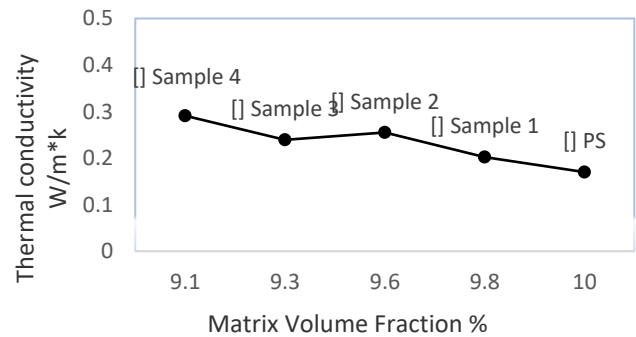


Fig. 3 Thermal conductivities of samples

These test results are evaluated when the temperature distribution along the direction of heat flow is linear. As per the values of sample 4, when the filler concentration increases, conductive chains arise and increase the conductivity by improving the crystallization of the matrix if a further increase of filler concentrations disturbs the crystallization of the matrix and reduces the thermal conductivity. The rate of heat flow depends on the probability of particles in contact, thus producing the path of low resistance to conduct heat flow in case of conductivity value of samples 2 & 4 increases slightly when compared with samples 1 & 3 due to the addition of salt as it fits the polymer matrix tightly by filling the vacancies and acts as a bridge between matrix and filler. All the experiment is carried out without heat loss. For the functional design and application of composite material, it is important to know the mechanical properties of the composite.

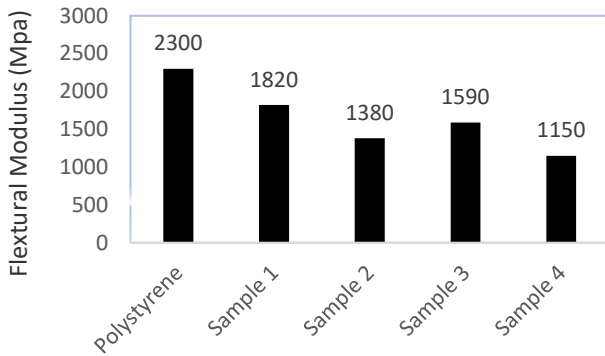


Fig. 4 Flexural Modulus of the samples

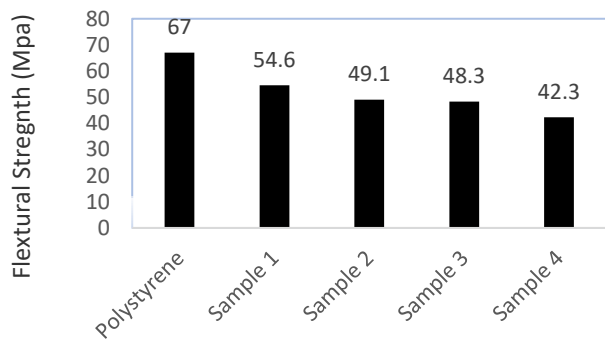


Fig. 5 Flexural Strength of the samples

Flexural modulus and Flexural strength determine the maximum stress and tendency to oppose the composite's bending moment, which is used to know the product application suitability and longevity. In general, the filler should add stiffness to the composite. Still, when compared with the normal polystyrene to sample 4, there is a decrease in the flexural strength and modulus due to the addition of filler particles when compared with the same composition of samples with the sample (1 & 2) & (3 & 4) there is not much difference between them.

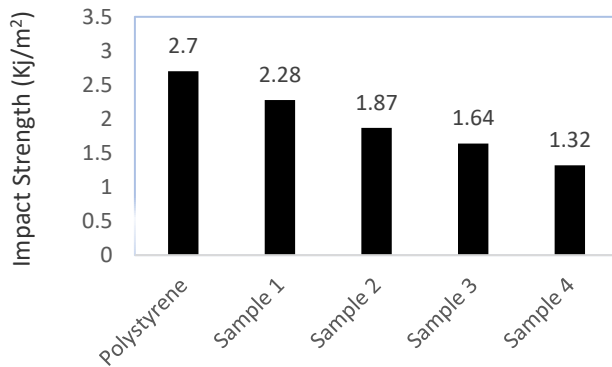


Fig. 6 Impact Strength of Samples

Generally, material properties depend on the matrix properties and less on the filler as the matrix transfers stress distribution and crack propagation by providing an alternative route in brittle failure. The samples' assessment shows a decrease in the impact values due to the addition of fillers and weak bonding between the fillers and the matrix.

**Microscopic Structure**

To determine the effective properties of the composite, it is important to know the microstructure. When there is a larger filler concentration, the accumulation of the particle becomes large. Thermal conductivity and other mechanical properties depend on filler concentration and filler shape and size.

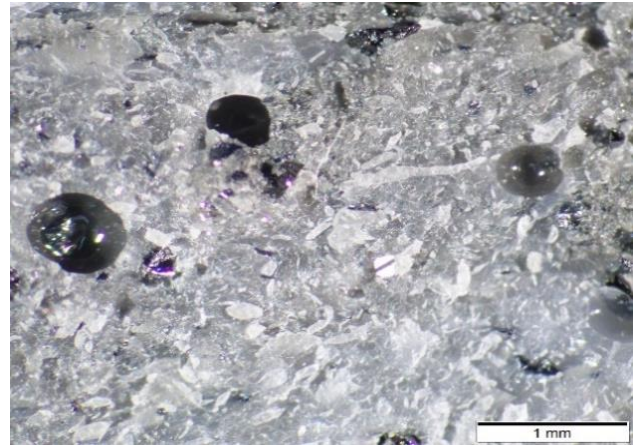


Fig. 7 Microscopic structure of the sample

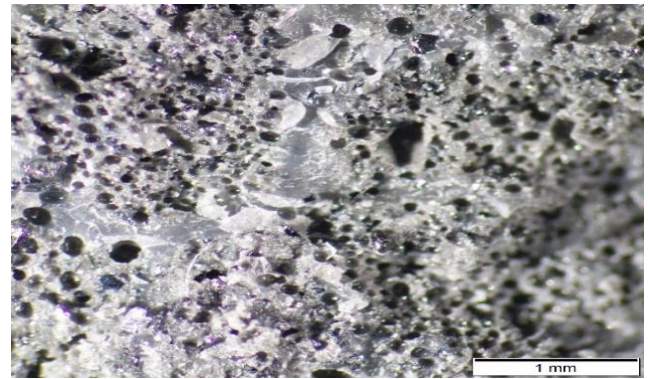


Fig. 8 Microscopic structure of sample 2

When comparing sample 1 to sample 2, there are many voids formed inside the polymer matrix when salt is added, which decreases the mechanical properties when seen in fig 6. there is uniform dispersion of particles. However, negligible voids formed. The interfacial area around the filler induces stress concentration when the load is applied, resulting in breakage. According to fig 9 and 10, the same effects are observed voids are formed in sample 4 when salt is added, but in the sample 1&3, the dispersion is uniform, and no flakes were observed; ceramic particles are induced into the polymer matrix effectively, and conducted the heat through it.



Fig. 9 Microscopic Structure of sample 3

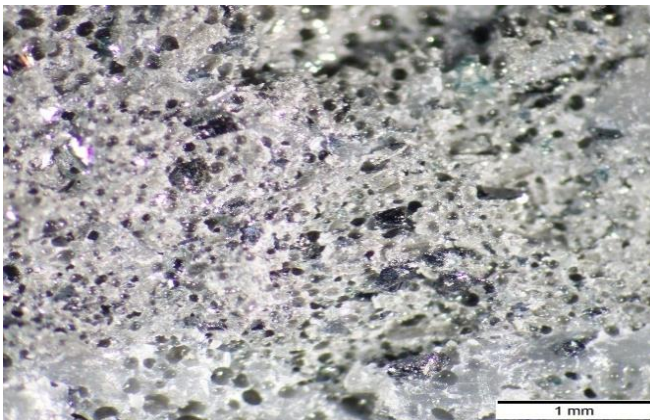


Fig. 10 Microscopic Structure of Sample 4

#### 4. Conclusion

As the thermal conductivity increases by adding salt by 10% and filler material by 10%, there is a 172% increase in the composite compared with polystyrene. From a comparison of the sample (1&2) and (3&4), it states that if salt is added by 10%, it increases the conductivity by 25% because the nature of salt is that it increases the conductivity by increasing the temperature when the mechanical properties are concerned there is a decrease in the impact strength when compared with normal polystyrene was 16% and between the samples are (18% to 20%) decrease. Flexural modulus and flexural strength compared with polystyrene were decreased by 20%, but when compared between all the samples, they are (20% to 25%). The increase of the filler concentration tends to rearrange the polymer matrix as the salt increases thermal conductivity but decreases the mechanical properties due to weak bonding. When the microscopic structure of the composite was studied, adding salt generated porosity. This effect is due to the melting of salt (or) elimination of the water molecules. A high number of pores result in easy crack propagation and material failure. Preferably adding salt by (5-10%) depending on the need to increase the conductivity. Where the stress concentration on the material is less, further investigations are needed to study the effect of salt in a polymer.

#### References

- [1] H. F. Brinson und L. C. Brinson, Polymer engineering science and viscoelasticity: An introduction. New York: Springer, (2008).
- [2] V. R. Sastri, Commodity Thermoplastics in Plastics in Medical Devices, Elsevier, (2010) 73–119. [CrossRef]
- [3] C. Huang, X. Qian und R. Yang, Thermal conductivity of polymers and polymer nanocomposites, Materials Science and Engineering: R: Reports, 132 (2018) 1–22. DOI: 10.1016/j.mser.2018.06.002. [CrossRef]
- [4] Explore properties of Polymer teachers-guide-jiggle-gels [CrossRef]
- [5] Thermal conductivity of salt, metal, and semiconducting melts, Phys. Stat. Sol. (a), 4(3) (1971) A15-A21. DOI: 10.1002/pssa.2210040348. [CrossRef]
- [6] Y. Ueki, N. Fujita, M. Kawai, and M. Shibahara, Thermal conductivity of molten salt-based nanofluid, AIP Advances, 7(5) (2017) S. 55117. DOI: 10.1063/1.4984770. [CrossRef]
- [7] Y. Ueki, N. Fujita, M. Kawai, and M. Shibahara, Thermal conductivity of molten salt-based nanofluid, AIP Advances, 7(5) (2017) S. 55117. DOI: 10.1063/1.4984770. [CrossRef]
- [8] M. Bozlar, D. He, J. Bai, Y. Chalopin, N. Mingo und S. Volz, Carbon nanotube microarchitectures for enhanced thermal conduction at an ultralow mass fraction in polymer composites (eng), Advanced Materials (Deerfield Beach, Fla.), 22(14) (2010) S. 1654–1658. DOI: 10.1002/adma.200901955. [CrossRef]
- [9] S. Yu, S. Yang, and M. Cho, Analysis of thermal conductivity of polymeric nanocomposites under mechanical loading, Journal of Applied Physics, 114(21) (2013) S. 213503. DOI: 10.1063/1.4834575. [CrossRef]
- [10] S. Gholizadeh, A Review of Impact Behaviour In Composite Materials, (2022).[CrossRef]
- [11] G. R. Koerner, Y. G. Hsuan und R. M. Koerner, The durability of geosynthetics in Geosynthetics in Civil Engineering, Elsevier, (2007) 36–65. DOI: 10.1533/9781845692490.1.36.[CrossRef]
- [12] B. Maxwell und L. F. Rahm, Rheological Properties of Polystyrene below 80° C, Ind. Eng. Chem., 41(9) (1949) S. 1988–1993. DOI: 10.1021/ie50477a036. [CrossRef]
- [13] S. E. Sadow and A. Agarwal, Hg., Advances in silicon carbide processing and applications. Boston, London: Artech House, (2004).
- [14] J. D. Selvam, I. Dinaharan und R. S. Rai, Matrix and Reinforcement Materials for Metal Matrix Composites in Encyclopedia of Materials: Composites, Elsevier, (2021) S. 615–639. DOI: 10.1016/B978-0-12-803581-8.11890-9 [CrossRef]
- [15] Uses of Salt Chart, Ind. Eng. Chem., 15(9) (1923) S. 971. DOI: 10.1021/ie50165a052. [CrossRef]
- [16] R. Rudolf, „General Overview of the Compounding Process: Tasks, Selected Applications, and Process Zones in Co-Rotating Twin-

Screw Extruder, K. Kohlgrüber, Hg., München: Carl Hanser Verlag GmbH & Co. KG, (2007) S. 57–89.  
doi: 10.3139/9783446433410.004. [CrossRef]

- [17] L. McKeen, Introduction to the Physical, Mechanical, and Thermal Properties of Plastics and Elastomers in The Effect of Sterilization on Plastics and Elastomers, Elsevier, (2012) S. 57–84. DOI: 10.1016/B978-1-4557-2598-4.00003-4. [CrossRef]
- [18] International Academic Printing Co. Ltd., J. Chem. Eng. Jpn. 44(11) (2011) 831-839.[CrossRef]
- [19] R. Zheng, R. I. Tanner und X.-J. Fan, Injection molding: Integration of theory and modeling methods. Berlin, Heidelberg: Springer, (2011).
- [20] D. Zhao, X. Qian, X. Gu, S. A. Jajja und R. Yang, Measurement Techniques for Thermal Conductivity and Interfacial Thermal Conductance of Bulk and Thin Film Materials, Journal of Electronic Packaging, 138(4) (2016) Art. no. 040802. DOI: 10.1115/1.4034605. [CrossRef]