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# To study the phenomena of electric percolation in Carbon Nanotube polymer composite

**Project of Physics of Nano-materials**

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# CNT Polymer composite

## 1.1 Introduction

CNT are known for their extraordinary electrical , mechanical and thermal properties and extremely high aspect ratio as well as low density . CNT gained such an remarkable interest among research because of these surprising properties . These properties make them an ideal reinforcement for making a CNT based polymer composite. The adding of CNT in polymer in small quantities improves the mechanical , thermal and electrical properties . These polymer/CNT composite have wide range of applications in electromagnetic shielding , gas sensing , actuation , etc. Both SWNT's and MWNTs are regarded as promising filler, since they can provide electric percolation at very low concentration. MWNT's based polymer composite also possess better properties than SWNTs based composites. Polymers ranging from conducting polymers such as polyaniline, polypyrrole (PPy), poly(p-phenylenevinylene) to insulating polymers such as polypropylene, polystyrene (PS), polymethylmethacrylate (PMMA) polyvinylalcohol (PVA), epoxy, polycarbonate, polyurethane, polyethylene can be made as host material.

## 1.2 Fabrication of CNT Polymer composite

There are various methods to prepare the polymer composites. Few of the methods have been discussed here :

### 1.2.1 Solvent Casting Method

It is one of the most common method to prepare the CNT polymer composite. In this method the host polymer is first dissolved in suitable solvent. The filler material is dispersed in the solvent by mixing it with the help of magnetic stirrer. We can also use centrifuge process to disperse the filler. After the filler is dispersed in the polymer properly, the solution is allowed to evaporate at room temperature. This method provides quite homogenous dispersion and hence very low threshold can be achieved. This method is only for polymers which are easily soluble in a solvent of low boiling point such as PS, PMMA, PVA and polycarbonate.

### 1.2.2 Melt Processing

This method is for the polymers which are easily dissolve in common solvents. In this method polymer is first mixed with the CNTs mechanically. For better results the mixture is pelletized. The pellet is then put inside an arrangement where it can be heated and composite material is obtained by applying a suitable pressure to the molten mixture. Achieving homogeneous dispersions of nanotubes in melts is generally more difficult than with solutions, and preparation of composite material with high loading of tubes is hard to achieve, due to the high viscosities of the mixtures. This method has been used for polymers such as polyethylene and polypropylene.

### 1.2.3 In-situ Polymerization Method

In this method , a mixture is prepared by dispersing nanotubes in the monomer solution and the resulting mixture is polymerized by standard polymerization methods. Therefore this technique makes the composite fabrication simpler since the monomer polymerization takes place directly on the CNT surface. The important aspect of this method is the potential to graft the polymer onto the CNT surface. Different CNT-polymer composites are prepared using in-situ polymerization are MWNT/PS, MWNT/polyurethane, MWNT/PPy.

## 1.3 Properties of CNT Polymer composite

There are many properties of CNT polymer composite and some of them are listed below:

- **Mechanical Properties:** CNTs significantly enhance the composite's tensile strength, stiffness (Young's modulus), and fracture toughness. The extent of improvement depends on factors like CNT content, aspect ratio (length-to-diameter ratio), and interfacial bonding strength.

- **Electrical Properties:** CNTs can drastically improve the electrical conductivity of the composite. At low CNT loadings, a conductive network can form (percolation), leading to significant conductivity enhancement. The effectiveness depends on CNT type (SWCNT vs. MWCNT) and their dispersion within the matrix.

- **Thermal Properties:** CNTs possess exceptional thermal conductivity. Incorporation of CNTs can improve the composite's thermal conductivity, leading to more efficient heat dissipation.

- **Magnetic Properties:** CNTs are them self are not magnetic but they are change the magnetic properties of polymer matrix and induced a weak magnetic field in the composite and also some studies show that CNTs are align them self as the magnetic field is applied and its cause is still unknown.

# Electrical Percolation of CNT Polymer composite

## 2.1 Introduction

It is very critical concept to study the electrical properties of the CNT polymer composite. Imagine a composite where you have insulating polymer particles scattered throughout. Now, you gradually add conductive CNTs. Initially, the composite remains insulating because the CNTs are isolated and don't form a connected pathway for electricity to flow and as the CNT concentration is reach a limit then there is sudden increase in the conductivity of the composite. At this limit the CNT is connected to each other and make easy pathway for electricity to flow.

## 2.2 Threshold Percolation

It is the minimum weight percent of CNTs the composite after that there is verg high and abrupt change in conductivity of the composite. And we believe that at that change the CNTs are connected to each other and that give an easy passage to the electric current through the insulated polymer matrix.

## 2.3 Factor Affecting the Electrical Percolation

There are some factors listed below that affect the electrical percolation in CNT polymer composite:

- **CNT Type:** Single-walled CNTs (SWCNTs) often have a lower percolation threshold compared to multi-walled CNTs (MWCNTs) due to their higher aspect ratio (length-to-diameter ratio) and better conductivity.
- **Dispersion:** Uniform dispersion of CNTs throughout the polymer matrix is essential for achieving a low percolation threshold. Agglomeration of CNTs hinders network formation.
- **Orientation:** Aligned CNTs can form a more efficient conductive network at lower concentration compared to randomly oriented CNTs.
- **Geometry of the System:** The dimensionality (2D or 3D) of the composite and the specific arrangement of the CNTs (random, aligned, etc.) influence the formation of the conductive network.
- **Interactions between CNTs and Polymer:** The interfacial bonding strength and the compatibility between the two material affect the network formation.

## 2.4 Formulation for Electrical conductivity of the CNT Polymer composite

As we see that there are many factor affecting the electrical percolation of the CNT polymer composite and that make very hard to formulate the electrical conductivity. So there is no universally accepted method which account all factors. And in this report we use the Percolation-based Model(Power-law model of percolation theory) formulation for study the given data.

### 2.4.1 Power-law model of Percolation theory

In this model we define the DC electrical conductivity as the function of the weight percent of the CNTs in the composite. And there is power factor is also present. And it has a very good accuracy at near the percolation threshold.

$$\boldsymbol{\sigma_{DC} = \sigma_o(p - p_c)^t} \tag{2.1}$$

where,
$\boldsymbol{\sigma_{DC}}$ is DC conductivity of the composite,
$\boldsymbol{\sigma_o}$ is the scaling coefficient,
$\boldsymbol{p}$ is the weight percent of CNTs in the composite,
$\boldsymbol{p_c}$ is threshold percolation,
$\boldsymbol{t}$ is the critical exponent and its depend upon the degree of formation of percolation network. And due to very small electrical conductivity we apply the logarithm on both side and get the equation

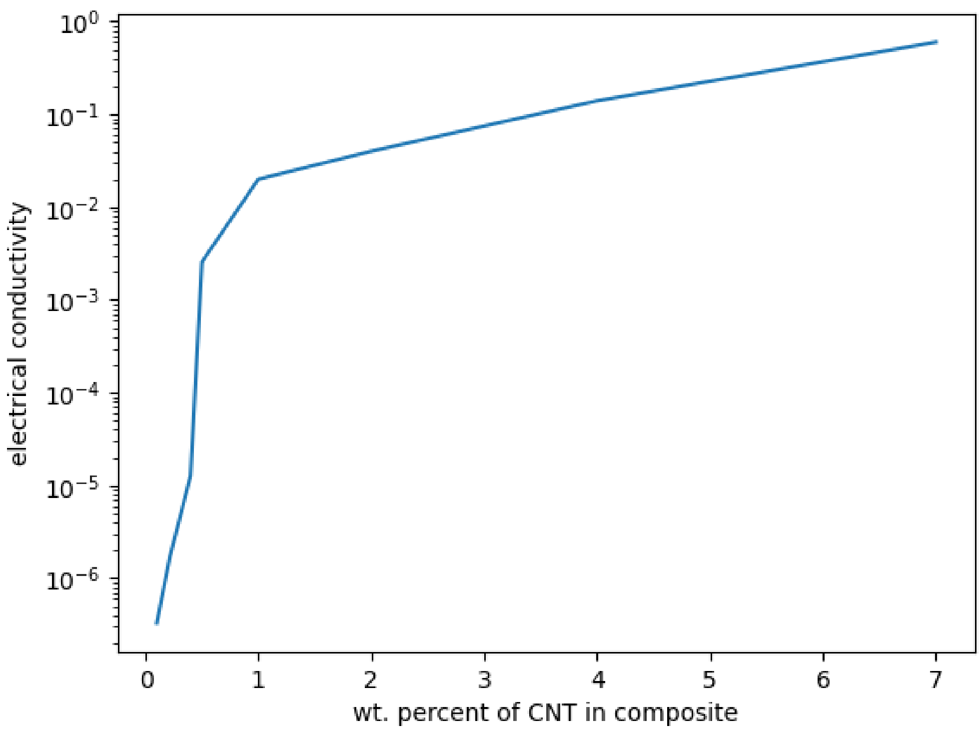
$$\boldsymbol{log(\sigma_{DC}) = log(\sigma_o) + t(log(p - p_c))} \tag{2.2}$$

And both equation (2.1) and (2.2) for fitting the experimental data of CNT polymer composite

# Data and Fittings

## 3.1 Given Data

| Weight percent of CNT in composite $\boldsymbol{p(wt\%)}$ | Electrical Conductivity $\boldsymbol{\sigma_{DC}(m\Omega^{-1})}$ |
|---|---|
| 0.1 | 3.28e-07 |
| 0.22 | 1.76e-06 |
| 0.4 | 1.27e-05 |
| 0.5 | 0.00256 |
| 1 | 0.02 |
| 2 | 0.04 |
| 4 | 0.14 |
| 7 | 0.6 |




Graph between electrical conductivity vs wt% of CNT in composite.

## 3.2 Fitting

### 3.2.1 About

The fitting is done by a custom program made by us. And we write the program in python and use scipy , numpy and matplotlib library/module to do the fitting.

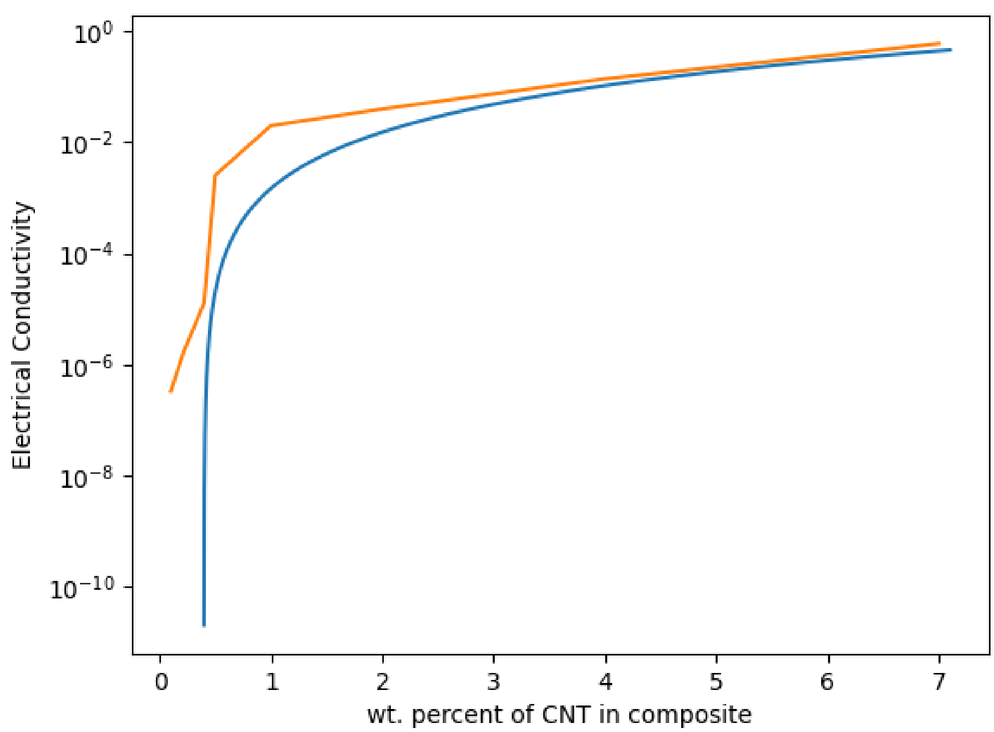
### 3.2.2 Initial Values

And the initial values are :
Scaling Factor, $\boldsymbol{\sigma_o} = \mathbf{0.0003}$ with bound $\mathbf{(0, 0.01)}$,
Threshold percolation, $\boldsymbol{p_c} = \mathbf{0.5}$ with bound $\mathbf{(0.40.6)}$,
Critical exponent, $\boldsymbol{t} = \mathbf{3}$ with bound $\mathbf{(1.6, 4)}$

### 3.2.3 Fitted Values

Scaling Factor, $\boldsymbol{\sigma_o} = \mathbf{0.0049851}$,
Threshold percolation, $\boldsymbol{p_c} = \mathbf{0.4}$,
Critical exponent, $\boldsymbol{t} = \mathbf{2.38165834}$

### 3.2.4 Graph




Blue is Fitted data and orange is given data

### 3.2.5 Source Code

```
from scipy.optimize import curve_fit
import numpy as np
import matplotlib.pyplot as plt

# Function that we use to fit the data
def func(x,sigma,pc,t):
    return np.log10(sigma) + t*np.log10(x+pc)

# Function that we use to generate the graph
def func1(x,sigma,pc,t):
    return sigma*(x-pc)**t

# opening file that having entries greater than threshold percolation
# because for other entries value inside log is negative that not work
with open('data.txt',"r") as file:
    data = file.readlines()

# Here we extract the data from the file entries write into list /array
x,y,logy = [],[],[]
for line in data:
    x.append(float(line.split(";")[0]))
    y.append(float(line.split(";")[1]))
    logy.append(float(line.split(";")[2]))

# here we fit the curve using the initial value and bounds
popt,pov = curve_fit(func,x,logy,p0=[0.0003,0.5,3],bounds=((0,0.4,1.6),(0.01,0.6,4)))

print(popt) # -> [0.00498501 0.4        2.38165834]

# here the full data file is present for plot the graph
with open('datafull.txt',"r") as file:
    data = file.readlines()
x,y,logy = [],[],[]
for line in data:
    x.append(float(line.split(";")[0]))
    y.append(float(line.split(";")[1]))
    logy.append(float(line.split(";")[2]))

# here we generate the value of conductivity from fitted data
```

```
x_fit , y_fit = [] , []
x_int = (x[-1])/10000
for i in range(-10,10000):
    x_fit.append(x[0]+i*x_int)
    y_fit.append(func1(x_fit[-1],popt[0],popt[1],popt[2]))

# here plotting the both graphs
plt.plot(x_fit,y_fit)
plt.plot(x,y)
plt.xlabel("wt. percent of CNT in composite")
plt.ylabel("Electrical Conductivity")
plt.yscale('log')
plt.show()
```

"percolation.py"

# References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