Determination of the band gap of a Semiconductor by Four Probe Set-Up

Experiment No:

Date:

1 Aim

To determine the bandgap of given semiconductor material using four probe method.

2 Apparatus Required

- Sample: Ge crystal

- Oven (heating range up to 200 °C)

- Four probe setup (measuring unit) includes oven controller

- Multi-range digital voltmeter and constant current generator

3 Procedure

- Put the sample on the base plate of the four probe arrangement. Unscrew the pipe holding the four probes, and let the four probes rest in the middle of the sample. Apply very gentle pressure on the probes and tighten the pipe in this position. Check the continuity between the probes for proper electrical contacts. Caution: The Ge crystal is very brittle. Therefore, use only the minimum pressure required for proper electrical contacts.

- Connect the outer pair of the probes (red/black) leads to the constant current power supply and the inner pair (yellow/green) to the probe's voltage terminals.

- Place the four-probe arrangement in the oven and connect the sensor lead to the resistance temperature detectors (RTD) connector on the panel.

- Switch on the mains supply of the four-probe set-up and put the digital panel meter in the current measuring inside. In this position, the LED facing mV will glow and the meter would read the voltage between the probes.

- Now, put the panel of the digital meter inside in voltage. In this position, the mV would glow and the meter would read the voltage between the probes.

- Switch on the temperature controller and adjust the set-temperature. The green LED would light up indicating that the oven is 'ON' and the temperature would start rising. Temperature of the oven in Kelvin is indicated by the digital panel meter (DPM).

- Now, take the voltage reading corresponding to the temperature and tabulate the data starting from 320K to 400K.

4 Formula Used

The resistivity can be determined using the relation

$$\rho = \frac{V \times 2\pi S}{I.G_7(w/s)} \qquad (\text{Ohm. m})$$

Where,

S = Distance between the probes (meter)

V = Potential difference (volt)

I = Current (Ampere)

G_7(w/s) = Correction parameter (meter)

5 Observations – Table 1

Distance between the probes (S) = 2 mm, Thickness of the crystal (w) = 0.5 mm
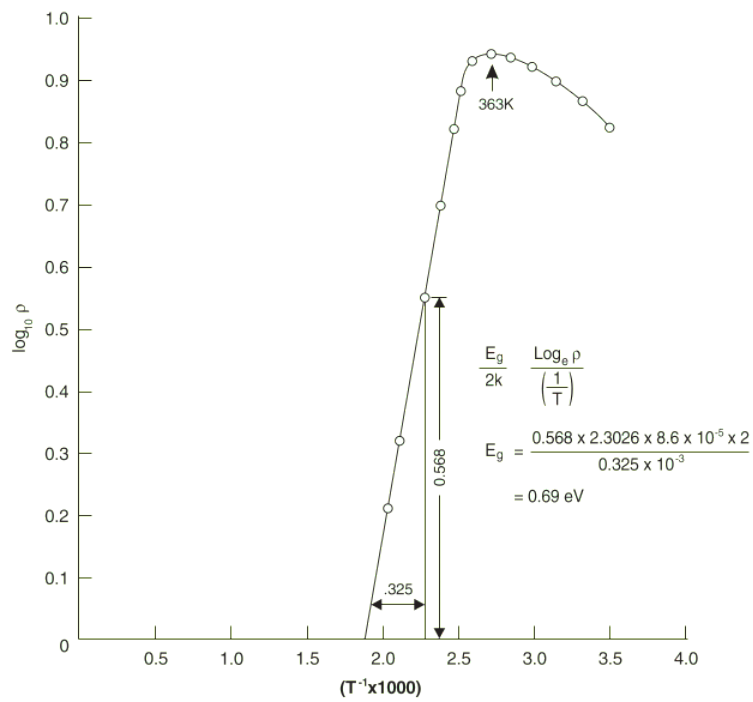Current (I) = mA, Correction parameter G_7 (w/s) = 5.89

FIGURE 1

Model Graph: Resistivity of Ge crystal as a function of temperature

S. No	Temperature (K)	Voltage (V)	ρ (ohm m)	T^{-1} ($\times 10^{-3}$)	Log ρ
1	310				
2	320				
3	330				
4	340				
5	350				
6	360				
7	370				
8	380				
9	390				
10	400				

Result

The bandgap of the semiconductor material (Ge) calculated using Four-Probe method is $E_g = $ eV

Preparation of CuO Nanoparticles by Sol-Gel Method

Experiment No:

Date:

1 Aim

To synthesize copper oxide nanoparticles by sol-gel method and assess the crystalline characteristics with powder XRD pattern.
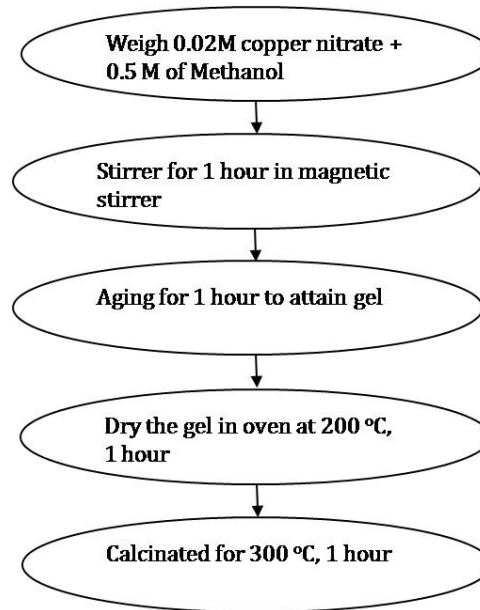
2 Required materials

Copper nitrate ($Cu(NO_3)_2.3H_2O$), methanol (CH_3OH), Beakers, Stirrer, Double distilled water (DD).

3 Procedure

1. 0.02 M of copper nitrate ($Cu(No_3)_2$. $3H_2O$) is taken and made to dissolve in 0.5 M of methanol.

2. To obtain homogeneity the solution is stirred in a magnetic stirrer for 1 hour.

3. The prepared solution is kept for aging for about 1 hour.

4. After aging the gel is made to dry at 200 °C for 1 hour in an oven to remove the absorbed water molecules.

5. Dried powder is then kept at furnace at 300 °C, 1 hour for calcinations.

6. Powder XRD of the synthesized powder is analysed by comparing with JCPDS data to make preliminary identification.

7. Crystalline size for various peaks is estimated by Scherrer formula

Flowchart for synthesis of copper oxide

```
┌─────────────────────────────┐
│ Weigh 0.02M copper nitrate + │
│ 0.5 M of Methanol            │
└─────────────────────────────┘
               │
               ▼
┌─────────────────────────────┐
│ Stirrer for 1 hour in magnetic│
│ stirrer                      │
└─────────────────────────────┘
               │
               ▼
┌─────────────────────────────┐
│ Aging for 1 hour to attain gel│
└─────────────────────────────┘
               │
               ▼
┌─────────────────────────────┐
│ Dry the gel in oven at 200 ℃,│
│ 1 hour                       │
└─────────────────────────────┘
               │
               ▼
┌─────────────────────────────┐
│ Calcinated for 300 ℃, 1 hour │
└─────────────────────────────┘
```

4 Formula Used

The average crystallite size (D) was estimated using Scherrer formula is

$$D = \frac{k\lambda}{\beta Cos\theta}$$

where k is Scherrer constant; λ is wavelength of X-ray used (nm); β is Full-width Half Maximum and θ is diffraction angle.

Table 1: Preliminary Identification by Powder XRD

2θ	(hkl)	Name of the Compound	JCPDS Card No.

Table 2: Estimation of Crystallite Size

Major Peaks	Crystallite Size (nm)
Average Crystallite Size (nm)	

5 Results

Copper oxide nanoparticles were successfully prepared by sol-gel method and the preliminary confirmation was made through powder XRD analysis. Also the average crystallite size was estimated to be _____ nm.

# Preparation of Magnesium Ferrite by Single-Step Combustion Method

Experiment No:

Date:

1 Aim

To prepare magnesium ferrite ($MgFe_2O_4$) spinel structure by combustion method and study its morphological arrangement by SEM analysis.

2 Materials Required

Magnesium nitrate ($Mg(NO_3)_2.6H_2O$), Iron nitrate ($Fe(No_3)_2.9H_2O$), Glycine ($C_2H_5NO_2$), Beakers, Stirrer, Acetone, Double distilled water (DD), Furnace.

Flowchart for synthesis of magnesium ferrite
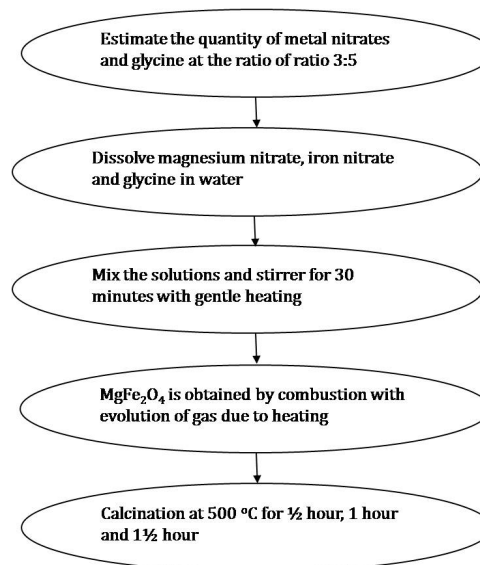
3 Procedure

- Metal nitrates and glycine is taken in the molar ratio of 3:5.

- Weigh appropriate quantity of magnesium nitrate ($Mg(NO_3)_2.6H_2O$), iron nitrate ($Fe(No_3)_2.9H_2O$) and glycine ($C_2H_5NO_2$).

- The precursors are dissolved in double distilled water and made us solution with continuous stirring on magnetic stirrer for half an hour.

- The solutions are mixed together and heated gently on the hot plate until the solution turns into a gel.

- Raw magnesium ferrite ($MgFe_2O_4$) is obtained by single step combustion process with evolution of gas due to heating.

- To remove the excess fuel and nitrates the obtained sample is heated at 500 ºC

- Calcination is carried out at various time (½ hour, 1 hour and 1½ hour).

- Recorded SEM pattern is analysed and the change in textural arrangement as a function of calcination time is studied.

Table 1: Morphological Texture Analysis of Magnesium ferrite.

Reaction Condition	Shape	Size	Comments

4 Results

Magnesium ferrite ($MgFe_2O_4$) with spinel structure was prepared by single-step combustion technique. Also the change in textural arrangements with calcinations time is analysed.

Cell refinement using computer programs

Experiment No:

Date:

1 Aim

To refine and calculate the cell parameters of given crystallographic data file.

2 Motivation

Crystals are the important arena of condensed matter physics and materials science. The properties of the materials are often described based on their crystalline structure. Ideally, crystals are formed by the repeating basic units called 'unit cells', over the three dimensional space. Which means, if you look into a crystal from any direction, it resembles same over the space. This is only in the case of ideal crystals. But practically, due to the experimental limitations, crystals have some defects in their structure. Analysing such a defects are important, especially when we consider the crystal for applications. There are many methods and programs are available to estimate the defects and to refine the crystal structure in literature. Here we use two of such programs to demonstrate the cell refinement process.

3 Basics

3.1 X-ray diffraction

X-ray diffraction (XRD) relies on the dual wave/particle nature of X-rays to obtain information about the structure of crystalline materials. A primary use of the technique is the identification and characterization of compounds based on their diffraction pattern. The dominant effect that occurs when an incident beam of monochromatic X-rays interacts with a target material is scattering of those X-rays from atoms within the tar-

get material. In materials with regular structure (i.e. crystalline), the scattered X-rays undergo constructive and destructive interference. This is the process of diffraction. The diffraction of X-rays by crystals is described by Bragg's Law, $n(\lambda) = 2d.sin(\theta)$. The directions of possible diffractions depend on the size and shape of the unit cell of the material. The intensities of the diffracted waves depend on the kind and arrangement of atoms in the crystal structure.

3.2 Single crystal XRD

Single-crystal X-ray diffraction is a non-destructive analytical technique which provides detailed information about the internal lattice of crystalline substances, including unit cell dimensions, bond-lengths, bond-angles, and details of site-ordering. Directly related is single-crystal refinement, where the data generated from the X-ray analysis is interpreted and refined to obtain the crystal structure.

3.3 Powder XRD

PXRD is primarily used for phase identification of a crystalline material and can provide information on unit cell dimensions. The analyzed material is finely ground, homogenized, and average bulk composition is determined.

3.4 Crystal structure refinement

The electron density map generated by solution of the phase problem from the single crystal XRD can be seen as a basic structure map. However, the assignment of atoms to different intensity centers is key to understanding the structure. The step of atom assignment is referred to as solving the crystal structure and these resolved structures are given in a 'crystal information file' (cif) for further reference.

4 Method

Eventhough the cif files carries good quality data, they may have slight deviation from the ideal crystals. To analyse such a deviations, crytal refinement programs are used. Here we use two programs for the analysis the single crystal data. The data

file can be downloaded from the crystallographic open database (COD) with information card number. To analyse this structure we need 'Mercury program' - to visualize the crytal structure and to simulate the PXRD data, and 'checkcell package' - for cell refinement.

4.1 Procedure

1. Download the cif file from this page:

   `http://www.crystallography.net/cod`

2. Open the structure in Mercury program and note down its crystall cell parameters.

3. Now from the calculation options, simulate the PXRD data of the given file and save it into a desired folder.

4. Open checkcell program, assign source wavelength and fix 2theta values and enter your simulated data in the given space.

5. Then in the parameter selection page choose the parameters corresponding to your data and proceed to calculation area.

6. Here match your simulated data with theoretical data and calculate the refinement parameters.

5 Observations

5.1 Crystallographic parameters

Identifier		
Formula		
Compound name		
Space group		
Cell lengths	a	
	b	
	c	
Cell angles	α	
	β	
	γ	
Cell volume		

5.2 Simulated PXRD data

2θ	Intensity

5.3 Refinement Data

Cell Parameters	Intial	Refined	Sigma
a			
b			
c			
α			
β			
γ			
Volume			

Mean square deviation of cell parameters = _____

6 Results

The given crystallagraphic data file is refined and the mean square deviation of cell parameters is about _____

Simulation of Vibrational Spectrum by Density Functional Theory Analysis

Experiment No:

Date:

1 Aim

To simulate the vibrational spectrum of carbon dioxide (CO_2), water (H_2O) and methane (CH_4) by density functional theory and to assign its vibrational components.

2 Motivation

Computational materials science involves computational tools for solving materials related problems. There exist different mathematical models for investigating problems at multiple length and time scales which help in understanding evolution of material structures (at different length scales) and how these structures effectively control material properties. With this understanding we can select materials for specific applications and also design advanced materials for new applications. At electronic level, Density Functional Theory (DFT) is a popular computational tool while Molecular Dynamics (MD) and Monte Carlo (MC) methods are considered as preferred tools for atomistic simulations. This experiment is intent to perform some basic steps in computational materials science such as geometry optimization and the simulation of vibratioanl spectrum.

3 Basics

3.1 Density Functional Theory

Quantum chemical wavefunctions can be used derive the complete information about a system. But it is hard to solve the quantum equations as it is. DFT is one

of the available methods, in a simplified form, to solve those equations. In DFT, molecular properties of a many electron system is determined by fucntionals, which is nothing but the spatial distribution electron density. These functionals are pre-implemented in many packages and for the present analysis, DFT implemented in Dalton 2016 is used.

3.2   Basis sets

In DFT, in order to perform the desired calculations, basis sets have to be specified. Basis sets are nothing but mathematical functions that represents electronic wave functions. Present case, 6-31G** basis set, which has the support for the atoms H through Zn is used for the analysis. 6-31G** is a valence double-zeta polarized basis set and it is one of the widely used basis set in DFT calculations.

3.3   Vibrational spectrum

Absorption of energy by specific bonds of the molecule can induce a specific pattern corresponds to particular bonds. These finger prints can be used to confirm the molecular structure.

3.4   Simulation of vibrational spectrum

Vibrations that result in change of dipole moment give rise to IR absorptions. So, the computer program simulates an oscillating electric field of the radiation that couples with the molecular vibration to cause an alternating electric field produced by the changing dipole.

3.5   Types of molecular vibrations

1. *Stretching* (ν) vibrations that alter the bond lengths

2. *Bending or deformation* vibrations that alter the bond angles, (the bond lengths remain unchanged). They can be subdivided into in-plane (δ) and out-of-plane modes (γ). These modes are often referred to as twisting, wagging, and rocking vibration of a fragment.

3. *Torsional vibrations* involve an alternation of the torsion angle. A further division into symmetric (s), antisymmetric (as), and degenerated (e) vibrations are possible.

4 Procedure

1. Login into the system with your credentials.

2. Open Avogadro package and draw the corresponding molecular structure and save it in .mol format

3. Open the saved .mol file (in Avogadro package) and optimize it with UFF algorithm.

4. After optimization, export the structure as Dalton input file.

5. Open .dal file and include commands for geometry optimization.

6. Run the .dal file through command line (> dalton filename.dal).

7. Open the output and copy the last (optimized geometry). Create a new file with commands for vibrational analysis.

8. Run the file and view the output in Gabedit.

9. Note down the frequencies, their intensities and the corresponding vibrations.

5 Input files

5.1 Water

5.1.1 *Geometry optimization*

```
BASIS

6-31G**

Water

----------

Atomtypes=2 Angstrom

Charge=8.0 Atoms=1

O      -0.01310    -0.01860     0.00000

Charge=1.0 Atoms=2

H      -0.29940     0.91860     0.00000

H       0.96590     0.02390     0.00000


**DALTON INPUT

.OPTIMIZE

**WAVE FUNCTION

.DFT

 B3LYP

**END OF INPUT
```

5.1.2 *Vibrational analysis*

```
BASIS

6-31G**

Water

----------

Atomtypes=2 Angstrom Nosymmetry

Charge=8.0 Atoms=1

O

Charge=1.0 Atoms=2

H

H


**DALTON INPUT

.RUN PROPERTIES

**WAVE FUNCTION

.DFT

 B3LYP

**PROPERTIES

.VIBANA

**END OF INPUT
```

5.2 Carbon dioxide

5.2.1 *Geometry optimization*

```
BASIS

6-31G**

Carbon dioxide

----------

Atomtypes=2 Angstrom

Charge=6.0 Atoms=1

C        0.00000     0.00000     0.00000

Charge=8.0 Atoms=2

O       -1.19700     0.00000     0.00000

O        1.19700     0.00000     0.00000


**DALTON INPUT

.OPTIMIZE

**WAVE FUNCTION

.DFT

 B3LYP

**END OF INPUT
```

5.2.2 *Vibrational analysis*

```
BASIS

6-31G**

Carbon dioxide

----------

Atomtypes=2 Angstrom Nosymmetry

Charge=6.0 Atoms=1

C

Charge=8.0 Atoms=2

O

O


**DALTON INPUT

.RUN PROPERTIES

**WAVE FUNCTION

.DFT

 B3LYP

**PROPERTIES

.VIBANA

**END OF INPUT
```

5.3 Methane

5.3.1 *Geometry optimization*

```
BASIS

6-31G**

Methane

----------

Atomtypes=2 Angstrom

Charge=6.0 Atoms=1

C       0.00002    0.00002   -0.00000

Charge=1.0 Atoms=4

H      -0.36405   -0.51484    0.89178

H       1.09222    0.00001    0.00000

H      -0.36403    1.02976    0.00000

H      -0.36405   -0.51484   -0.89178


**DALTON INPUT

.OPTIMIZE

**WAVE FUNCTION

.DFT

 B3LYP

**END OF INPUT
```

5.3.2 *Vibrational analysis*

```
BASIS
6-31G**
Methane
----------
Atomtypes=2 Angstrom Nosymmetry
Charge=6.0 Atoms=1
C
Charge=1.0 Atoms=4
H
H
H
H

**DALTON INPUT
.RUN PROPERTIES
**WAVE FUNCTION
.DFT
 B3LYP
**PROPERTIES
.VIBANA
**END OF INPUT
```

6 Observations

6.1 Water

6.1.1 *Optimized geometry*

Atom	x	y	z
O			
H			
H			

6.1.2 *Vibrations*

S. No	Frequency	Intensity	Assignment
1.			
2.			
3.			

6.2 Carbon dioxide

6.2.1 *Optimized geometry*

Atom	x	y	z
C			
O			
O			

6.2.2 *Vibrations*

S. No	Frequency	Intensity	Assignment
1.			
2.			
3.			

6.3 Methane

6.3.1 *Optimized geometry*

Atom	x	y	z
C			
H			
H			
H			
H			

6.3.2 *Vibrations*

S. No	Frequency	Intensity	Assignment
1.			
2.			
3.			
4.			

7 Results

Vibrational spectra of the given molecules are simulated and their molecular vibrational components are assigned.

Determination of dipole moment, linear polarizability, and energy gap of ZnO nanoclusters using semiempirical method

Experiment No:

Date:

1 Aim:

1. To determine the dipole moment, linear polarizability and energy gap of five ZnO nanoclusters of different point groups and different energies, using semiempirical PM7 method.

2. To analyse the variation of dipole moment, linear polarizability and energy gap with respect to molecular energy.

2 Requirements:

Avogadro software to draw molecules and to create the input geometries, MOPAC2016 package for geometry optimization and polarizability calculation, Gabedit package for HOMO, LUMO calculation.

3 Theory:

3.1 Semiempirical Formalism

Molecular properties vary with respect to the molecular energy and often same molecules of different point groups possess different molecular energy. In this experiment five different ZnO nanoclusters of different point groups are considered for the analysis. Since it would take much time to simulate the properties of moleculae on *ab initio* and DFT level theories semiempirical formalism is used for the analysis. In

semiempirical algorithms, experimental and accurate theoretical data are substituted to the current molecule and the optimization process is normalized to get good qulaity results in a short span of time. The molecules are pre-optimized using universal force field theory (UFF) in order to get a resonable structure.

3.2 PM6 Algorithm

In this experiment Parametrization Model Number 7 (PM7) is used for the calculations. It is a successor of PM3 model and based on *Neglect of Differential Diatomic Overlap* integral approximation and uses two Gaussian functions for the core repulsion function. This method supports all the elements in the periodic table and included hydrogen bond correction in its core function. So, highly correlated materials like transition metals can be studied with good accuracy.

3.3 Transition Dipole Moment (μ)

Transition dipole moment is a type of electric dipole moment denotes a transition from intial state to final state ($m \to n$). In mathematical terms it is a complex vector quantity and its direction gives the polarization of the transition, which determines how the system will interact with an electromagnetic wave of a given polarization and its square of the magnitude gives the strength of the interaction due to the distribution of charge within the system.

3.4 Linear Polarizability (α)

Polarizability is one of basic properties of materials and it gives the ability of a material to form instaneous dipoles. It is used as an estimation for the dynamical response of a bound system to external fields and can be used to interpret the electronic structure of molecular systems.

3.5 Energy Gap (eV)

In molecular chemistry, energy gap corresponds to the energy difference between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital

(LUMO). Since a molecule may possesses different energy levels, HOMO and LUMO are often termed as frontier orbitals and their energy difference gets major concern. Energy gap can be used to predict the optical and electrical properties of materials and further can be used to predict the stregth and stability of a particular transition metal complex.

4 Procedure:

1. Draw the molecules as given in **Figure 1** using avogadro package.

2. Pre-optimize them with UFF algorithm using the same package.

3. Create the MOPAC input file and edit it with necessary parameters.

4. Submit the job to MOPAC package and edit the generated .arc output file for polarizability calculations.

5. Use .aux file in Gabedit and calculate the HOMO, LUMO and E_g values.

6. Note down the values and plot the variation of dipole moment, linear polarizability and energy gap with respect to molecular energy (*See sample graph. Three similar graphs to be plotted.*)
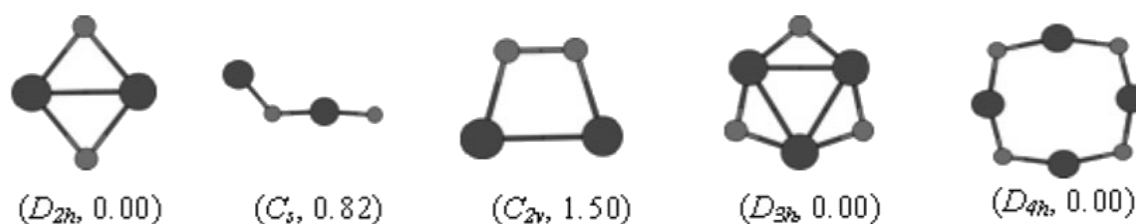

$(D_{2h}, 0.00)$ $(C_s, 0.82)$ $(C_{2v}, 1.50)$ $(D_{3h}, 0.00)$ $(D_{4h}, 0.00)$

FIGURE 1

ZnO nanoclusters of different point groups and energy

5 Input Comments:

1. **Molecular Charge:** `CHARGES`

2. **Geometry Optimization:** `LET CHARGE=N PM7 AUX GNORM=10` (substitute N with the above value)

3. **Polarizability Calculation:** `LET CHARGE=-N PM7 POLAR`

6 Observations:

Tabulation:

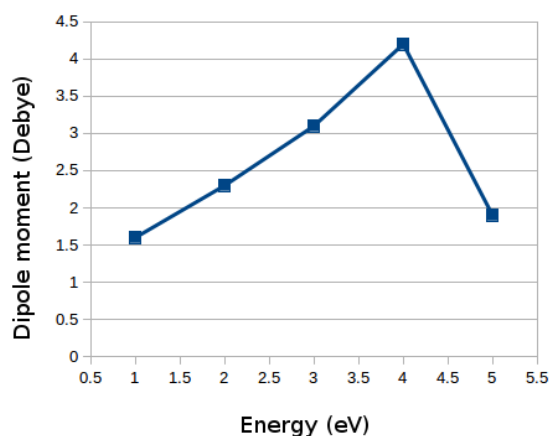| Point group	Energy ((eV))	μ (($Debye$))	α (a.u.)	E_g (eV)
D$_{2h}$				
C$_s$				
C$_{2v}$				
D$_{4h}$				

Sample Graph:

FIGURE 2

Variation of dipole moment with respect to molecular energy

7 Results:

The dipole moment, linear polarizability and energy gap of ZnO nanoclusters of different point groups and different energies are calculated and their variation with respect to energy is plotted.

Determination of Planck's constant by Photoelectric Effect

Experiment No:

Date:

1 Aim

To determine the Planck's constant and work function of a metal by demonstrating photo electric effect.

2 Apparatus

The present experimental set-up comprises of a tungsten light source with five different colour filters, a Caesium-type vacuum phototube, a built-in power supply and a current multiplier. The base of the phototube is built into a dark room and infront of it a receptor (pipe) is installed to mount filters.

3 Procedure

- Plug in and switch on the apparatus using the red button at the bottom right corner of the set up.

- Before the lamp is switched on, put the toggle switch in current mode and check that the dark current is zero.

- Turn on the lamp source. Set the light intensity near to maximum. Note that the intensity should be such that the value of current should not exceed the display range. In case it happens, reduce the intensity.

- Insert one of the five specified filters into the drawtube of the receptor.

- Now, set the voltage direction switch to '-ve' polarity. Adjust the voltage knob at minimum and current multiplier at X 0.001. Vary the voltage and record the current till the value of current becomes 0. Use the display mode switch to record the values of voltage each time.

- Repeat the above two steps for all the filters provided.

- Fill up the observation tables and draw necessary plots. Determine the values of Planck's constant and work function of the metal used in the phototube.

4 Formulas and constants

1. Standard Planck's constant = 6.626 x 10^{-34}Js

2. Frequency of light $\nu = c/\lambda$, where c is the velocity of light in vacuum (3 x 10^8m/s)and λ is the wavelength of light.

3. Charge of the electron (e) =1.602 x 10^{-19}C

4. Linear regression formula: y = mx + c

5. Slope=b/a= Δv / ΔV_0

6. The linear fit of the experimental data in graph resembles V_0= (h/e)ν - Φ.

(a) So, h/e = Slope, and h = Slope xe and

(b) The intercept of the graph equals to work function (Φ) of the metal

7. 'h' Error % = (6.626-h(calc))/6.626) x 100 %

Table 1: Specification of filters

Colour	Blue	Green	Yellow	Orange	Red
Wavelength (nm) Frequency (Hz)	460	500	540	570	635

Table 2: Stopping Potential

Colour	Blue	Green	Yellow	Orange	Red
Frequency (Hz) Stopping potential (V_0)					

Graph Results
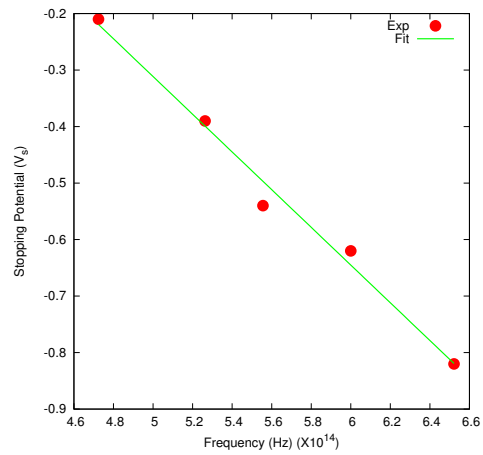
1.   Calculated Planck's constant value h=

2.   'h' Error % =

3.   Calculated working function of the metal=

Determination of the wavelength of laser and refractive index of the given materials – using He-Ne laser

Experiment No:

Date:

1 Aim

- To determine the wavelength of the Helium-Neon laser using diffraction pattern.

- To determine the refractive index of given material using Helium-Neon laser

2 Apparatus

He-Ne laser, Screen, a meter scale, millimeter graph paper, a plate of transparent material, graduated turn table, a photo detector with inducting instrument

Formula

The wavelength of the laser is, $\lambda = \frac{d}{2Z} \left[\frac{Y_m - Y}{M} \right]$

Where

d=diffraction grating width

Z_o=distance between the grating element and the diffraction pattern are obtained on the screen ($\times 10^{-2}$)

M=order of the fringes

λ=wavelength of He-Ne laser to be determined

Y_o- distance between the first diffraction pattern and central diffraction pattern

Y_m-distance between the central pattern and n^{th} order pattern

3 Procedure

(i) **Determination of the wavelength of the laser :**

This experiment was first demonstrated by shadow using a ruler. Initially the scale must be engraved. The Vernier calliper is placed on the horizontal table and the laser is in alignment such that the unexpected beam is incident at the grating angle as shown in the figure 1. The diffraction pattern is observed at a distance of 3 to 4 meter from the scale. The beam can be aligned so that the diffraction pattern is at its best as shown in figure 1.

The pattern arises due to diffraction at the engraving on the scale and governed by the grating equation

d sin(-sinθ m) = mλ

Where m is the diffraction order and d is the grating constant. For m=0, the beam is specularly reflected. The grating equation is expressed in terms of angle α and β in the form

d (cosα-cosβ)=mλ

Where, $\pi/2$-i and β_m=$\pi/2$-0

The distance between the region of distance of the rule and the screen is Zo. The diffraction spots are taken to lie along Y-axis and the position of Mth spot is represented by Y$_m$.

For zeroth order $\alpha = \beta_o$. Therefore

$\cos\beta_m = [1-(Y_m/Z_o)^2]^{1/2} = 1-1/2\ Y_m^2/Z_o^2$

Similarly,

$\cos \alpha = \cos \beta_o = 1-1/2,\ Y_o^2/Z_o^2$

Therefore

$\cos \alpha - \cos \beta_m = \left(\frac{Y_m^2 - Y_o^2}{2Z^2} \right)$

The wavelength of light is given by

$\lambda = d/2Z^2 \cdot \frac{Y_m^2 - Y_o^2}{M}$

Here the distance are measured from the horizontal plane by making purpose the position of the direct beam on the screen and the distance of various diffraction spots are measured from this position and later reduced to the position midway between the direct beam and secularly reflected beam positions. This distance can be measured on millimetre graph paper pasted on the screen. The distance Zo can be measured with a scale.

Table 1: Wavelength of laser

S.No	Order of fringes (m)	Y_m ($\times 10^{-2}$m)	Y^2_m ($\times 10^{-4}$ m)	Y^2_m- Y^2_o ($\times 10^{-4}$ m)	$\frac{Y^2_m - Y^2_o}{M}$ ($\times 10^{-4}$ m)

(i) **To determine the refractive index of the given material using Helium – Neon laser :**

The plate of transparent material is mounted on the turn-table such that the plane of incidence is horizontal as in figure 2. In front a spectrometer with the eye-piece replaced by a photo-detector will be appropriate. The output of laser should be bare its vector is confined to horizontal plane. As goniometer is rotated the intensity of reflected beam keeps on decreasing first reached almost zero value and then increases again. The angle at which the irradiance reaches almost zero is the Brewster angle.

The refractive index of the plate will be obtained from

$\mu = \tan \theta_\beta$

Where

θ_β– Brewster's angle (degree)

Table 2: Refractive index of the material.

S.No	Transparent material	Main scale meter ($\times 10^{-2}$)	Vernier scale (division)	$\mu = \tan \theta_\beta$

Results

- The wavelength of the He-Ne laser is found out by diffraction method

λ=--------------- nm

Z_o =------------m

- The refractive index of the different transparent materials is determined by measuring the Brewster's angle

    The refractive index of

I) Glass = --------------

II) Mica = --------------

Determination of dispersion relation for mono-atomic and diatomic lattices

Experiment No:

Date:

1 Aim

- To study the dispersion relation for mono atomic and diatomic lattices.

- To determine the cut-off frequency for the corresponding lattices.

2 Apparatus

Lattice dynamics kit and CRO operating in XY mode

3 Description of the kit

1. Switch positions: Low (LO) in the frequency range 0.8 – 8.9 kHz and High (HI) in the frequency range 8.7 – 91 kHz (There might be slight variation depending on the individual kits)

2. Toggle Switches for mono-atomic and di-atomic modes

3. An amplitude controller and two variable resistor (R1 and R2)

4 Procedure

1. Connect the horizontal (H) and vertical (V) lines of the kit to the X and Y of the CRO (should be in XY mode)

2. Adjust the amplitude, R1 and R2 knobs to the maximum value (maximum turn on the clock-wise direction) and toggle the switch LO

3. Choose 'Mono-atomic' lattice switch, adjust TTP to minimum and then switch on the kit and CRO

4. Lissajous figures of line/circle/ellipsoid can be achieved

5. Vary R2 slightly to approach nearly circle pattern in CRO

6. Vary the TTP values and determine the frequencies corresponding to phase diiferences

7. After the maximum LO frequency, adjust TTp to minimum and continue the experiment by toggle HI switch

8. Repeat the same for di-atomic lattices

Table 1: Mono-atomic and Di-atomic Lattices

S. No	CRO Pattern	$N(\theta)$	$(\theta = \frac{N(\theta)}{10})$	Obs Frequency (kHz)	Calc. Frequency (kHz)

5 Calculations

In the given kit, L = 1mH, C = 0.047 μF, C_1 = 0.147 μF

Mono-atomic Lattices: The dispersion relation for mono-atomic lattice can be given as,

$$\omega^2 = \frac{2}{\text{LC}}(1 - \cos\theta)$$

6 Di-atomic Lattices

The dispersion relation for diatomic lattice can be written as,

$$\omega^2 = \frac{1}{L}[\frac{1}{C} + \frac{1}{C_1}] \pm \frac{1}{L}[(\frac{1}{C} + \frac{1}{C_1})^2 - \frac{4\sin^2\theta}{CC_1}]^{\frac{1}{2}}$$

Substitute and the L and C, C_1, values in the corresponding equations and calculate the values for mono-atomic and di-atomic lattices.

$$\frac{1}{L}[\frac{1}{C} + \frac{1}{C_1}] \pm \frac{1}{L}[(\frac{1}{C} + \frac{1}{C_1})^2 - \frac{4\sin^2\theta}{CC_1}]$$

7 Result

The dispersion curves for the mono-atomic and di-atomic lattices are drawn.

Determination of Hall Coefficient

Experiment No:

Date:

1 Aim

To measure the Hall voltage of the given semiconductor sample and to estimate the Hall coefficient, carrier charge density and carrier mobility.

2 Apparatus Required

- Hall probe (Ge Crystal)

- Hall effect Set-up

- Electromagnet

- Constant current power supply

- Digital Gauss meter

3 Theory

The Hall effect is basic to solid-state physics and an important diagnostic tool for the characterization of materials - particularly semiconductors. It provides a direct determination of both the sign of the charge carriers, e.g. electron or holes, and their density in a given sample. The objectives of this experiment are to demonstrate the effects of a magnetic field (B) on a current carrying conductor (semiconductor/metal). If a current carrying conductor is placed in a magnetic field oriented perpendicular to the direction of the current, a voltage is developed across the conductor in a direction perpendicular to both the magnetic field and the direction of the current. This effect is known as the Hall effect.

4 Procedure

- Connect the red coloured contacts of the Hall probe to the terminals marked 'Voltage' and green coloured contacts to terminals marked 'Current'.

- Switch 'ON' the Hall effect set-up and check that the adjustment current is in zero.

- Switch over the display to voltage side. There may be some voltage reading even outside the magnetic field. This is due to imperfect alignment of the four contacts of the Hall probe and is generally known as the 'Zero field Potential'. In case its value is comparable to the Hall Voltage it should be adjusted to a minimum possible (for Hall Probe (Ge) only). In all cases, this error should be subtracted from the Hall Voltage reading.

- Now place the probe in the magnetic field and switch on the electromagnet power supply and adjust the current to the desired value. Rotate the Hall probe till it become perpendicular to magnetic field. Hall voltage will be maximum in this adjustment.

- Measure Hall voltage for both the directions of the current and magnetic field (i.e. four observations for a particular value of current and magnetic field).

- Measure the Hall voltage as a function of current keeping the magnetic field constant. Plot a graph.

- Measure the Hall voltage as a function of magnetic field keeping a suitable value of current as constant. Plot a graph.

5 Formula Used

With the help of this experiment we can calculate the following terms of the given semiconductor. The value of Hall coefficient can be calculated using the relation

$$R = \frac{V_H.d}{I.H} \tag{1}$$

where, V_H is the Hall voltage (volt), d is the sample thickness (metre), I is the current (ampere) and H is the magnetic field (Gauss).
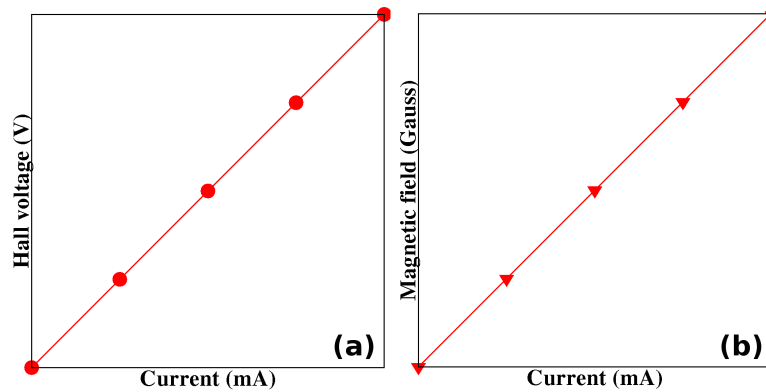
FIGURE 1

Graph: (a) Current in Hall voltage and (b) Current in the magnetic field

Calculate charge carrier density from the relation

$$R = \frac{1}{n.q}; n = \frac{1}{R.q} \qquad (2)$$

where q is the electron charge (q = 1.6×10^{-19} Coulomb)

Calculate carrier mobility, using the formula

$$\mu_n(\text{or } \mu_p) = R\sigma$$

Where, μ_n is the mobility of charge carrier (electrons), μ_p is the mobility of charge carrier (holes) and σ is the conductivity of Ge semiconductor sample and it is about 0.1 coulomb volt^{-1} sec^{-1} cm^{-1} at room temperature.

6 Observations – Table 1

Current Vs. Hall Voltage

d=1.5 mm, Constant magnetic field at 0.5 A of coil current is Hz =--------------------
-Gauss

Current (mA)	Hall Voltage (mV)	Mean H ($\times 10^{-3}$ volts)
	Current	Magnetic field
	H1	H2
0.5		
1.0		
1.5		
2.0		

Observations – Table 2

1.0			
1.5			
2.0			

7 Result

Hall parameters for as given semiconductor sample is measured and its

- Hall coefficient (R) is

- Carrier density (n) is

- Carrier mobility (μ) is

Measurement of Thickness of Polymeric Thin Films using Air Wedge Technique

Experiment No:

Date:

1 Aim

- To deposit thin films of polyvinyl alcohol (PVA) by dip coating method.

- To estimate the thickness of the deposited thin films using air wedge technique.

2 Apparatus Required

For thin film deposition

- Glass beakers

- polyvinyl alcohol (PVA)

- double distilled water

- microscopic glass slides

For thickness measurement

- Travelling microscope

- Optically plane glass plates

- Sodium vapour lamp

- Sample mounter

- Scale

3 Theory

The monochromatic light incident normally on the air wedge will be divided into two parts by the wave amplitude-division method. One part is reflected at the upper glass surface OP and the other part passes to the lower glass surface OP' where it undergoes a further reflection upon striking that surface. Since this reflection is from an optically denser (higher refractive index) medium (glass) to a lower optical density medium (air), the reflected light waves will be phase shifted by 180° (this is equivalent to an additional optical path difference of $\lambda/2$ between the two upper and lower reflected beams). Due to the overlapping (interference) of the two reflected light beams, bright and dark straight fringes are observed in the traveling microscopes' field of view.

The fringe at point A is formed by interfering light ray, reflected off the upper glass surface OP, with the one reflected from the lower glass plate which suffered a 180° – phase shift in addition to traversing double the distance AA' when it propagates back and forth. If the total phase shift equals odd multiples of the half the light wavelength, then a dark interference fringe will be formed. On the other hand, the interference fringe will be bright whenever the total phase shift equals even multiples of the light wavelengths used. The next interference fringe formed at point B is due to the increase of air-wedge width by an amount of half the light wavelength (the distance BC in the figure 1).

If α is the wedge angle in degrees, then from the triangle ABC, it is apparently that

$$\frac{BC}{AC} = \frac{BC}{A'C'} = \frac{\lambda/2}{\beta} = \frac{\lambda}{2\beta} \tag{1}$$

where β represents the distance between two successive (dark or bright) fringes. In the triangle OPP'

$$tan(\alpha) = \frac{PP'}{OP'} = \frac{t}{l} \tag{2}$$

where t = PP' represents the width of the thin films and OP = l is the separation between the inner edge of the thin films and line of contact of the two glass plates.

$$\frac{t}{\lambda} = \frac{l}{2\beta} \tag{3}$$

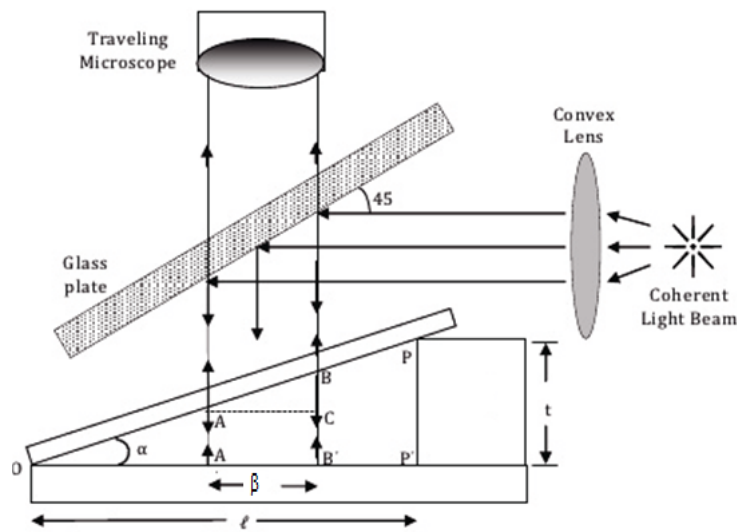$$t = \frac{\lambda l}{2\beta} \tag{4}$$

FIGURE 1

The air wedge formed between two glass plates, illumination of the wedge by monochromatic light and collection of reflected rays by the objective of the telescope

4 Procedure

Step 1: A convex lens is used to get a parallel light beam emerging from the monochromatic light source (typically the monochromatic sodium light λ_{average} = 589.3 nm). This parallel light beam is to be making 45° angle of incidence with a horizontally oriented 45° angle, half-silvered glass plate. The light rays reflected off this plate will perpendicularly incident on the lower thick glass plate of the air-wedge.

Step 2: The traveling microscope is then focused until getting the lower thick glass plate of the air-wedge at the focal plane of the traveling microscope's eyepiece. Doing so, a distinct interference pattern should become viewable.

Step 3: The distance between a suitable numbers of dark (or bright) fringes is measured using the traveling microscope Vernier and the width of the dark of bright fringe is deduced by dividing the measured distance on the number of fringes. The measurement is then recorded in a suitable table.

Step 4: Step 3 is repeated for a number of times and the average of such measurements is evaluated.

Step 5: Using a micrometer Vernier, the distance *l* is measured.

Step 6: Finally, the thickness of the thin films t is estimated by applying the formula 1.

Least Count for Travelling Microscope

Least Count (LC) = Value of 1 Main Scale Division (MSD)/ Number of divisions in the Vernier

20 MSD = 1 cm

Value of 1 MSD = 1/20 cm = 0.05 cm

Number of divisions in the vernier = 50

LC = 0.05/50= 0.001 cm

Formula Used

Thickness of the dip coated polymeric thin films

$$t = \frac{\lambda l}{2\beta} \tag{5}$$

t = thickness of the coated thin films

λ = wavelength of the sodium vapour light

l = is the separation between the inner edge of the thin films and line of

contact of the two glass plates

β = fringe width

To determine the fringe width (β)

LC = 0.001 cm *TR = MSR + (VSC $\times$ LC)

Order of fringes	Microscope Reading MSR (10^{-2} m)	Fringe width (β) (10^{-2} m) VSC (div)

Mean = ------------------- 10^{-2} m

5 Results

- The PVA thin films were deposited by dip coating method

- The thickness of the films is calculated as --------- μm

Synthesis of CdO Nanoparticles by Microwave Assisted Wet Chemical Method

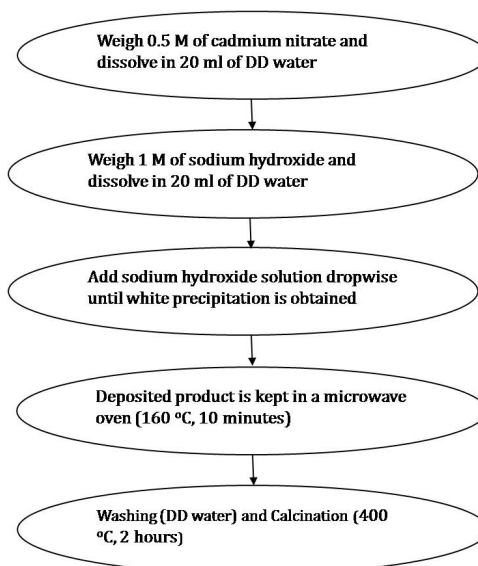**Experiment No:**

Date:

Aim

To synthesize CdO nanoparticles by microwave assisted wet chemical method and study its molecular structure by FTIR analysis.

1 Required materials

Cadmium nitrate ($Cd(NO_3)_2.4H_2O$), sodium hydroxide (NaOH), Beakers, Stirrer, Acetone, Double distilled water (DD), Microwave oven.

Flowchart for synthesis of cadmium oxide

2 Procedure

- Beakers are cleaned with double distilled water and rinsed with acetone to dry the water molecules.

- 0.5 M of Cadmium nitrate [Cd $(NO_3)_2$.$4H_2O$] and 1 M of sodium hydroxide (NaOH) is taken as a precursor.

- Cd $(NO_3)_2$.$4H_2O$ is dissolved in 20 ml of double distilled water. The solution is kept for stirring using magnetic stirrer for 10 minutes at room temperature.

- NaOH is separately dissolved in 20 ml of DD and stirred for 10 minutes at room temperature.

- The prepared NaOH solution is slowly added to the cadmium solution on constant stirring. Cadmium hydroxide forms themselves as white precipitation and gets deposited at the bottom of the beaker.

- The deposited product is washed with DD to remove the impurities and kept in a microwave oven for irradiation at 160 ºC for about 10 minutes.

- The product is grinded well and calcinated at 400 ºC, 2 hours in a furnace.

- FTIR spectrum of synthesized product is analysed and various vibrational peaks are assigned to confirm the molecular structure.

Table 1: Vibrational Mode Assignments with FTIR

Vibrational Peaks	Assignments

3 Result

Cadmium oxide nanoparticles were prepared by microwave assisted wet chemical method and their molecular structure was analysed by FTIR analysis.

3 Result