1. **Title of the Project:**
   Electrical and Gas Sensing Studies of Polymer Nanocomposite
   (Ref. No. 42S_BE_2762)

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4. **Key words**
   Conducting polymer, Polypyrrole, gas-sensor

5. **Introduction**

   During the last 5 years, polymers have gained tremendous recognition in the field of artificial sensor in the goal of mimicking natural sense organs. Better selectivity and rapid measurements have been achieved by replacing classical sensor materials with polymers involving nano technology and exploiting either the intrinsic or extrinsic functions of polymers. Semiconductors, semiconducting metal oxides, solid electrolytes, ionic membranes, and organic semiconductors have been the classical
materials for sensor devices. The emission of gaseous pollutants such as sulfur oxide, nitrogen oxide and toxic gases from related industries has become a serious environmental concern. Sensors are needed to detect and measure the concentration of such gaseous pollutants. In fact analytical gas sensors offer a promising and inexpensive solution to problems related to hazardous gases in the environment. Both intrinsically conducting polymers and non-conducting polymers are used in sensor devices.

6. Objectives

The following objectives were set and executed:

- To synthesize base polymer: Polypyrrole
- To synthesize Metal oxide nanoparticles: Copper Oxide
- To prepare nanocomposite films of different ratios of polypyrrole doped with CuO
- To fabricate a gas sensing apparatus
- To perform gas sensing studies
- To perform electrical studies.

7. Methodology

For the synthesis of Polypyrrole, pyrrole (C₅H₅N) is the main raw material used along with Ammonium Per Sulfate((NH₄)₂S₂O₈) as an oxidizing agent. Methanol, Ethanol, Ferric chloride anhydrous, m-cresol, Cupric acetate monohydrate, sodium hydroxide are used.

Pyrrole was synthesized by chemical oxidation. Aqueous solution of 0.1M Pyrrole(50mL) was mixed with oxidizing agent 0.1M FeCl₃ solution. It was kept in ice bath for 3hrs with continuous stirring for the polymerization to occur. Later the solution was filtered and dried in oven at 60°C.

Boil the copper acetate monohydrate solution and add glacial acetic mixture and stir the solution. Add 6M NaOH which makes the soln turn black. Cool and centrifuge the mixture. Filter and precipitate the mixture with distilled water and absolute ethano. Calcined the resultant to obtain dry powder of CuO nanoparticles.

The obtained PPy was blended with CuO nanoparticles by varying the weight percent of CuO. And three different composites of 10, 30 and 50 wt% PPy/CuO were prepared. The blended mixture was dissolved in m-cresol and stirred for 24 hrs to get a uniform solution. This solution was casted on glass plates and kept for drying.
A circular aluminum disc of diameter 4.9 cm and height 12 cm was casted on the circular discs making volume of cylinder up to 226.28 ml was fabricated. Copper wires were used as electrodes in contact with the films. The gas was injected through the syringe to this insulated sensing device. The prepared film was mounted on the metal surface which is in contact with the electrodes. The change in resistance was noted.

8. Results and Conclusion

- The nanocomposites films were characterized by FTIR and XRD.
- The oxidizing agent FeCl$_3$ gives better result when ethanol is used as solvent.
- Synthesized PPy powder dissolves in m-cresol only after grinding operation.
- The nanocomposite films were prepared by varying the weight % of CuO. The films prepared were uniform and prepared for 10, 30 and 50 wt% of PPy/CuO.
- The FTIR results of PPy and CuO were found to be in good agreement with literature values.
- In FTIR spectra, the incorporation of CuO leads to the shift of some bands of PPy.
- The XRD pattern of PPy showed that the polymer is in an amorphous state, and hence there are no sharp peaks observed in the diffraction pattern. But the pattern showed the broad, amorphous diffraction peak at approximately $2\theta = 20-30^\circ$.
- The XRD pattern of the nano copper oxide showed the diffraction peaks indicating the formation of monoclinic phase of CuO and the values were found to be in good agreement with literature values (JCPDS file no. 48-1548).
- The size of CuO NPs were determined by using Scherrer’s formula and average diameter came out to be less than 90 nm.
- The electrical studies of polymer nanocomposites were studied. And the I-V graph showed that the current versus voltage characteristics are asymmetric and nonlinear for forward direction of applied voltage.
- The non-linear behavior is due to the influence of Polypyrrole on surface and vacancy states of nanocrystalline copper oxide particles.
- The current density versus voltage graph showed that the cut-in voltage (or knee voltage) for PPy/CuO composite is 125 V.
- The gas sensing studies showed the films can sense gas like NH$_3$ at room temperature.
Better response was obtained for gas at higher wt% of PPy/CuO composite i.e. for 50 wt% with the lowest response time making it suitable film for NH$_3$ gas sensing application.

9. **Scope for Future Work**

- Gas sensing studies can be extended for other gases such as H$_2$S, NO$_2$ etc.
- Concentration of the gases can be varied and studied.
- Gas sensing can be studied at higher temperatures.