

Role of Pz Orbital in n-Doped and p-Doped Conducting Polyaniline

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Abstract - In this materialistic era, huge amount of amazing material is available. Conducting polymers are being counted among them. Conductive polymers are, the polymers that conduct electricity. Such compounds possess two types of conductivity in the form of solid state or semiconductors and in the form of solution or complexes with metal. The biggest benefit of conductive polymers is their ability to be processed, mainly by dispersion. Conductive polymers are generally not thermoplastics, i.e., they are not thermally formed. But, like insulating polymers, they are organic materials. The electrical conduction is classified into ionic conduction and electronic conduction, based on whether the charge carriers are ions or electrons. Ionic conduction occurs in polymers which contain ionic groups or to which ionic materials have been added. They can offer high electrical conductivity but do not show similar mechanical properties to other commercially available polymers. The electrical properties can be fine-tuned using the methods of organic synthesis and by advanced spreading techniques.

Keywords: Polyaniline, n-doping, p-doping, Pz -orbital

I. INTRODUCTION

The conductivity of such insulating materials such as polymers is the result of several processes. For example, in traditional polymers such as polyethylenes, polyvinyl pyrrolidone and polyacetylene the valence electrons are bound in sp^3 hybridized covalent bonds. Such "sigma-bonding electrons" have low mobility and do not contribute to the electrical conductivity of the material. In these materials absorption and adsorption of water plays a dominant role because water may act as a source of ions, as high dielectric impurity or as a local structure modifier. However, in conjugated materials, like polyacetylene the situation is completely different. Conducting polymers have backbones of contiguous sp^2 hybridized carbon centers. One valence electron on each center resides in a pz orbital, which is orthogonal to the other three sigma-bonds. All the pz orbitals combine with each other to a molecule wide delocalized set of orbitals. The electrons in these delocalized orbitals have high mobility when the material is "doped" by oxidation, which removes some of these delocalized electrons. Thus, the conjugated p-orbitals form a one-dimensional electronic band, and the electrons within this band become mobile when it is partially emptied. In amorphous polymers it can also occur due to the drift of defects on the application of an electric field. Though the phenomenon is best understood only in alkali halides, the process has been invoked to explain the high field and high temperature effects in organic molecular solids^{21, 22} and polymers²³.

II. MATERIALS AND METHODS

Complex formation of polymeric material with zinc or lithium is carried out with polymers such as polyaniline and polyethyl aniline to convert the insulating polymeric material as conducting complex metric material. In polymeric material crystals have a perfectly regular arrangement of atoms and molecules, while amorphous materials have a completely random arrangement. To use these polymeric material polyaniline and polyethyl aniline as conducting electrode, doping of the same material is brought about. Sulphate or chloride salts of polymers are taken for this purpose. Oxidation with halogen (or p-doping) and reduction with alkali metal (called n-doping), processes are carried out.

Table: Conductance of Polyaniline (PANI) observed before and after doping

Serial No.	Sample	Conductance (mhos cm ⁻¹)	Type of doping
1.	Polyaniline	0.398 X10 ⁻³	Without doping
2.	Polyaniline	5.83 X 10 ⁻⁷	n-doping
3.	Polyaniline	9.4 X 10 ⁻⁵	p-doping

III. DISCUSSION

The conductivity depends on the number of charge carriers (number of electrons) in the material and their mobility. In a metal it is assumed that all the outer electrons are free to carry charge and the impedance to flow of charge is mainly due to the electrons "bumping" in to each other. Insulators however have tightly bound electrons so that nearly no electron flow occurs so they offer high resistance to charge flow. So for conductance free electrons are needed. Three simple carbon compounds are diamond, graphite and polyacetylene. They may be regarded as three- two- and one-dimensional forms of carbon materials Diamond, which contains only σ bonds, is an insulator and its high symmetry gives it isotropic properties. Graphite and acetylene both have mobile electrons and are, when doped, highly anisotropic metallic conductors. How can plastic become conductive? Plastics are polymers, molecules that form long chains, repeating themselves. In becoming electrically conductive, a polymer has to imitate a metal, that is, its electrons need to be free to move and not bound to the atoms. Polyacetylene is the simplest possible conjugated polymer. It is obtained by polymerization of acetylene. Two conditions to become conductive 2-The second condition is that the plastic has to be disturbed either by removing electrons from (oxidation), or inserting them into (reduction), the material. The process is known as Doping.

IV. SURVEY OF LITERATURE

Subsequent doping of the conducting polymers will result in a saturation of the conductivity at values around 0.1–10 kS/cm for different polymers^{4,5}. Highest values reported up to now are for the conductivity of stretch oriented polyacetylene with confirmed values of about 80 kS/cm⁶. Although the pi-electrons in polyacetylene are delocalized along the chain, pristine polyacetylene is not a metal^{7,8}. Polyacetylene has alternating single and double bonds which have lengths of 1.44 and 1.36 Å, respectively^{9,10,11}. After doping, the bond alteration is diminished in conductivity increases. Non-doping increases in conductivity can also be accomplished in a field effect transistor and by irradiation. Some materials also exhibit negative differential resistance and voltage-controlled "switching" analogous to that seen in inorganic amorphous semiconductors¹². Despite intensive research, the relationship between morphology, chain structure and conductivity is still poorly understood which are largely amorphous. Due to their poor processability, conductive polymers have few large-scale applications¹³. They have promise in antistatic materials² and they have been incorporated into commercial displays and batteries, but there have had limitations due to the manufacturing costs, material inconsistencies, toxicity, poor solubility in solvents, and inability to directly melt process^{14, 15}. Literature suggests they are also promising in organic solar cells, printing electronic circuits, organic light-emitting diodes, actuators, electrochromism, super capacitors, chemical sensors and biosensors, flexible transparent displays, electromagnetic shielding and possibly replacement for the popular transparent conductor indium tin oxide. Another use is for microwave-absorbent coatings, particularly radar absorbent coatings on stealth aircraft. Conducting polymers^{16, 17, 18} are rapidly gaining attraction in new applications with increasingly process able materials with better electrical and physical properties and lower costs. The new nanostructure forms of conducting polymers particularly augment this field with their higher surface area and better dispersability. With the availability of stable and reproducible dispersions, Polyaniline is widely used for printed circuit board manufacturing in the final finish, for protecting copper from corrosion and preventing its solder ability^{3, 19, 20}.

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