Polyacetylene: A Thorough Analysis of Synthesis and Applications of Conducting Polymer

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Abstract

A prevalent belief is that polyacetylene serves as a prototype for the conjugated organic polymer class. The films are chemically doped with p- or n-halogen derivatives or alkali metals, respectively, following polymerization. The Schottky barrier, heterojunction, and junction between severely doped polyacetylene and an inorganic semiconductor are reviewed in relation to their electrical and photovoltaic properties. Utilizing quantum chemical theory and ultraviolet photoelectron spectra obtained during the earliest stages of aluminium deposition on oxygen-free films of trans-polyacetylene oligomers, the subject of chemical interactions at the aluminum-polyacetylene interface has been addressed. There was found to be a strong interaction between the metal and the polyene chain, leading to the reduction of the π -electron conjugation along the chain and the production of covalent aluminum–carbon bonds. Nonetheless, there is still a significant amount of delocalization in π -levels.

Exceptionally good electrical properties of polymeric devices employing polyacetylene as the active semiconductor ingredient, such as Schottky diodes, MIS diodes, and MIS field-effect transistor architectures. In that instance, a precursor polymer that could be processed in a solution gave rise to the polymer. One of the main drawbacks of employing polyacetylene is the strict requirements regarding oxygen exclusion. Because polyacetylene is so reactive, the device will quickly fail if the environment is not carefully regulated. Additional barriers to polyacetylene's application as an electronic material include its high gap density, poor photoconductivity, low chemical stability against heat oxidation, and inadequate preparation repeatability. A future objective would be to combine the excellent electric properties of the polyacetylene device with the excellent processing properties of other available doped and undoped conjugated polymers (e.g., PPy, polythiophene), poly(p-phenylene vinylene) (PPV), polyaniline (PAni), and and their derivatives.

Keywords: Polyacetylene; Conducting polymer; Application; Optoelectronics properties

I. Introduction

Prior to the discovery of conducting polymers (conjugate polymers), polymers were thought to be electrical insulators; however, these organic polymers have special electrical and optical properties that are comparable to those of inorganic semiconductors (Nezakati et al., 2018). The electrical and optical properties of a conjugated carbon chain are attributed to the highly delocalized, polarised, and electron-dense π bonds. The chain is composed of alternating single and double bonds. Polyacetylene (PA), polyaniline (PANI), polypyrrole (PPy), polythiophene (PTH), poly(para-phenylene) (PPP), poly(-phenylenevinylene) (PPV), and polyfuran (PF) are examples of typical conducting polymers (Fig. 1).



Fig. 1: Structural illustration of different conducting polymers (DOI: 10.1039/d0ra07800j, RSC Advances).

The first polymer to conduct electricity, PA was created by Shirakawa inadvertently in the middle of the 1970s (Shirakawa, 2001). With the repeating unit $(C_2H_2)_n$, it is an organic polymer. A quick burst of research activity focused on finding novel CPs resulted from the development of highly conducting PA. The excellent electrical conductivity of these polymers has drawn significant attention to the application of organic compounds in microelectronics. Conducting polyacetylene was studied as a result of the discovery of $(SN)_x$ sulphur nitride metal, an inorganic substance that demonstrated increased electrical conductivity when doped with bromine. This material was found by physicist Alan J. Heeger and scientist Alan G. MacDiarmid. A Nobel Prize in 2000 was given for this research, which showed that polyacetylene doped with bromine possesses conductivity that is a million times higher than that of pure polyacetylene (Heeger, 2001). There was minimal evidence indicating that a precisely replaced polyacetylene molecule would exhibit superconductivity of 10^5 S/cm or more (Hatano et al., 1961). The topochemical polymerization of diacetylenes yields polydiacetylene (Yamamoto et al., 1980).

SYNTHESIS OF POLYACETYLENE

The Nobel Prize was given for the development and improvement of conductivity using polyacetylene doping (Marsh, 2001). The compounds derived from polyacetylene have multifunctional properties. Some of its characteristics, such as chiral recognition, electrical conductivity, photoconductivity, and liquid crystal qualities, can be investigated in more detail. A linear polyene chain makes up the primary chain of polyacetylene. It is malleable and can be ornamented with pendant groups, meaning that a foreign molecule can be substituted for the hydrogen atoms in the alternating carbon to create a mono- or disubstituted polyacetylene (**Fig. 2**) (Liu et al., 2010).



Fig. 2: Formation of monosubstituted and disubstituted polyacetylene (DOI: 10.1039/d0ra07800j, RSC Advances).

A variety of techniques were used to create conducting polymers, such as the inclusion method, the solid state method, the vapour phase synthesis, hydrothermal, solvothermal, template-assisted, electrospinning, self-assembly, and photochemical techniques (Charles, 1995; MacDiarmid et al., 2001; Tang et al., 2009; Park et al., 2016). In their pure form, conducting polymers often have poor optical and electrical conductivity; however, doping them with the right substances can give them exceptional qualities. The conductivity of polyacetylene is in the range of 10^5 Scm^{-1} , but as the doping level increases, it rises dramatically to 10^2 to 10^3 Scm^{-1} (Bredas and Street, 1985). Its properties also change depending on the type of dopant material, giving it tunable properties such as electrochemical or optical mechanical properties, etc (Hakansson et al., 2006; Le et al., 2017). Polyacetylene can be synthesised using a variety of techniques, including precursor-assisted

synthesis, non-catalytic polymerization, catalytic polymerization of other polymers, and catalytic polymerization. Ziegler–Natta or Luttinger catalysts are examples of the types of catalysts used in the synthesis of the catalytic polymerization process. Acetylene polymerization yields vinyl acetylene and polyacetylene oligomers such as cyclooctatetraene. Zeigler-Natta catalysts are highly selective and soluble in organic solvents, making them one of the many catalysts available for the synthesis of polyacetylene. They result in extremely crystalline free-standing films of polyacetylene on the wall of the reaction flask on which the catalyst is coated (Fig. 3), combining both $Ti(0-n-C_4H_9)_4$ and $(C_2H_5)_3A1$ (Ito et al., 1974).



Fig. 3: Synthesis of polyacetylene using a Ziegler–Natta catalyst (DOI: 10.1039/d0ra07800j, RSC Advances).

Polyacetylene is also prepared using luttinger catalysts, which are composed of a complex of a group [VIII] metal, such as nickel chloride, and a hybrid reducing agent. With no oligomer residue, these catalysts generate high molecular weight polyacetylene (Fig. 4). In contrast to a Ziegler-Natta catalyst, a Luttinger catalyst employs hydrophilic solvents for catalytic action, such as acetonitrile or water-ethanol tetrahydrofuran (THF). Nevertheless, compared to a Zeigler-Natta catalyst, it has reduced catalytic activity, and the products these catalysts create have nearly identical chemical and physical properties (Luttinger and Colthup, 1962).



Fig. 4: Synthesis of polyacetylene using a Luttinger catalyst (DOI: 10.1039/d0ra07800j, RSC Advances).

Non-catalytic polymerization includes the electrochemical polymerization of acetylene. Electrochemical synthesis is defined as the anodic oxidation of a monomer precursor on an inert metal surface in the presence of appropriate electrolytes. For synthesis, a variety of electrochemical methods have been employed, including galvanostatic charge discharging, potentiostatic, cyclic voltammetry, and galvanostatic charge discharging. The primary benefit of this method is that it enables the direct deposition of a polymer film on metal, and by adjusting the electrochemical parameters, we can easily regulate the thickness of the film (Chen and Shy, 1985). One example of synthesising polyacetylene without the use of an acetylene monomer is the ring-opening polymerization of 1,3,5,7-cyclooctatetraene with a metathesis catalyst, W[OCH(CH₂Cl)₂]nCl₆-n(C₂H₅)₂AlCl (n = 2 or 3), as reported by Korshak et al. (1985). There have also been reports of light-induced synthesis of the conjugated system, in which polyacetylene is produced by irradiating acetylene gas with UV light (Simionescu and Percec, 1982).

APPLICATIONS

1. Due to its exceptionally high electrical conductivity, doped polyacetylene can be employed as an electrode material in lightweight rechargeable batteries or in electrical wiring.

2. The concentration of glucose can be detected using a sensor made of tri-iodide-oxidized polyacetylene.

3. Chemical sensors, electro-magnetic shielding, antistatic coatings, corrosion inhibitors, and other products are made with them.

4. Additionally, they find application in small-sized electrical devices including lasers, light-emitting diodes (LEDs), and polymer-based transitions.

5. They are utilised for coatings that absorb microwaves, especially those that absorb radar and are applied to stealth aircraft.

6. They shield copper from oxidation and hinder its solderability, which is why printed circuit boards are made with them.

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