Chapter 37
Modeling, Design, and Applications of the Gas Sensors Based on Graphene and Carbon Nanotubes

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ABSTRACT

Gas sensing continues attracting research communities due to its potential applications in the sectors military, industrial and commercial. A special emphasis is placed on the use of carbon nanomaterials such as carbon nanotubes and graphene, as sensing materials. The chapter will be divided as follows: In the first part, a description of the main topologies and materials (carbon nanomaterials plus polymers, metals, ceramics or combinations between these groups) used to fabricate gas sensors based on graphene and carbon nanotubes that are operated by conductance or resistance electrical, is realized. Next, different mathematical models that can be used to simulate gas sensors based on these materials are presented. In the third part, the impact of the graphene and carbon nanotubes on gas sensors is exemplified with technical advances achieved until now. Finally, it is provided a prospective analysis on the role of the gas sensors based on carbon nanomaterials in the next decades.

INTRODUCTION

Gas sensing continues attracting research communities due to its potential applications such as detecting air pollutants, determining the toxic gas leakage in facilities, monitoring and quantifying in specific gas generation during chemical reactions of interest, etc. In nowadays, gas sensors are fabricated using a multitude of materials in accordance with the global research effort reported in the scientific literature in last decades. Today's modern world requires the sensing at ultra-low concentration of gases, which have led to the necessity of developing ultrasensitive and ultrafast electronic sensors. Different types of gas sensors can be developed using distinct principles such: optical, magnetic, thermal, acoustic,

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and electrical. Electrical gas sensors transduce the interaction between the gas molecules and sensing materials as a change in the electrical conductance or electrical resistance. The main parameters to be controlled by designers of gas sensors consist into five different technical aspects: selectivity, sensitivity, stability, recovery time, and response time. In addition, it is desirable that concentrations by below of parts of million can be detected, to achieve the better gas sensor. Among all possible materials to fabricate gas sensors, carbon nanomaterials such as carbon nanotubes and graphene represent the better option to develop the sensing that allow fulfills the aforementioned requirements. Carbon nanomaterials with semiconducting behavior are sensitive to the surrounding environment thanks to their capacity of absorption of gas molecules, which modifies the current flowing through of the sensing material as a function of the applied voltage between a pair of electrodes. Graphene and carbon nanotubes present exceptional properties: electrical, chemical, electrochemical and optical; these qualities make them ideal candidates for use in gas sensors. Moreover, nanostructured materials offer a huge number of expectations to enhance and modulate the properties of the gas sensing, by providing properties such as defined structure, high chemical stability, high surface area and a good thermal conductivity. The combination of polymers, metals or ceramic materials with carbon nanomaterials for the preparation of gas sensors has led to novel areas of research, due to their excellent sensitivity and selectivity to specific gases, thanks to large surface-area-to-volume ratio found in nanomaterials such as carbon nanotubes and graphene. In the case of polymers, these materials can be assembled either by polymer-wrapped carbon materials, placing layer-by-layer of polymer and carbon materials, as composite materials based on polymer, and carbon nanomaterials, as well as molecularly imprinted polymers (MIPs) with carbon nanomaterials. The use of polymers not only improves the dispersion of the carbon nanomaterials in them, but also enhances redox behavior and biocompatibility, and provides additional properties such as photoelectric or swelling capacity. In the case of ceramic materials, they use chemical linkages such as functional groups between carbon nanomaterials and materials such as clay, nitrides, and metal oxides, to achieve a composite material with good properties to be used in gas sensors. Carbon nanomaterials and metal oxide nanoparticles are combined to increase the selectivity and reduce the response and recovery times of the gas sensors. Various transition metals (Pt and Au) can be embedded in carbon nanomaterials for creating functional structures to be used as sensing material in gas sensors. The synergistic combination of metal nanoparticles and carbon nanomaterials modulates the electron properties of carbon nanomaterials, leading to enhancement of selectivity and sensitivity in gas sensors. The use of mathematical models, for predicting the behavior of the gas sensors based on carbon nanotubes and graphene before that they are fabricated in the industry at large quantities, allow realizing comparisons between theoretical results with those obtained from the experimental works of other researchers around the world. In recent years, some researchers have developed mathematical approaches based on algorithms of artificial neural network (ANN), support vector regression (SVR) as well as analytical modeling to simulate the behavior of gas sensors based on carbon nanomaterials. The main purpose of this chapter consists in discussing the more recent advances on the modeling, design and applications of the gas sensors based on carbon nanomaterials, since these materials will facilitate the outstanding development of the next-generation of gas sensors in concentrations below the level of parts per million (ppm), that is, parts per billion (ppb) or even parts per trillion (ppt), in the future decades. The chapter will be divided as follows: In the first part, a description of the main topologies and materials (carbon nanomaterials plus polymers, metals, ceramics or combinations between these groups) used to fabricate gas sensors based on graphene and carbon nanotubes that work by means of electrical conductance or electrical resistance is realized. Next, different mathematical models that can be used to simulate gas sensors based on these materials are

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