Chapter 4
GAS Sensor Modelling and Simulation

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ABSTRACT

Both graphene and CNTs experience changes in their electrical conductance when exposed to different gases (such as CO2, NO2, and NH3), and they are, therefore, ideal candidates for sensing/measuring applications. In this research, a set of novel gas sensor models employing Field Effect Transistor structure using these materials have been proposed. In the suggested models, different physical properties such as conductance, capacitance, drift velocity, carrier concentration, and the current-voltage (I-V) characteristics of graphene/CNTs have been employed to model the sensing mechanism. An Artificial Neural Network model has also been developed for the special case of a CNT gas sensor exposed to NH3 to provide a platform to check the accuracy of the models. The performance of the models has been compared with published experimental data which shows a satisfactory agreement.

INTRODUCTION

It is a known fact that every physical phenomenon needs a mathematical representation to allow for an in depth study of the general characteristics and behaviour in real conditions. More importantly, since the experimental study of some phenomena are costly, hazardous, time and energy consuming or due to many other restrictive reasons, the need to develop mathematical models with which one can predict the actual behaviour and characteristics of different physical properties, chemical properties, etc. is inevitable. Therefore, to study the electrical properties of graphene and carbon nanotubes when employed in metal oxide semiconductor field effect transistor (MOSFET) based gas sensors, a set of mathematical models have been proposed and developed for different electrical properties. These include conductance,
capacitance, and carrier concentration as well as drift velocity. The modelling procedure has used an initial assumption of the direct proportionality of the gate voltage with gas concentration and temperature.

A single model has also been proposed for CNT based gas sensor utilizing an artificial neural network algorithm to provide a benchmark for comparison with the analytical model for the sake of validation and in order to check the plausibility and viability of the model. Both models will later on be compared with the experimental results from previous experiments by other researchers. The steps taken to develop both models have been presented in the following sections after which the results and the comparative study come.

**ANALYTICAL CONDUCTANCE MODEL OF GRAPHENE BASED CO₂ GAS SENSOR**

In this study, a new model for the gas sensor based on the gradient of GNR conductance as a function of gas concentration has been provided and a FET based structure as a modelling platform is suggested. Lastly, the proposed model is evaluated through a comparison study between model and experimental result. The graphene gas sensor is able to operate under ambient conditions and at room temperature. For different concentrations of carbon dioxide (CO₂) adsorbed on graphene surface, changes in the device conductance have been reported (Yoon et al. 2011). By increasing CO₂ concentration gas from 10 to 100 ppm, the conductance of the graphene gas sensor rises. This sensor benefits from advantages such as fast response time, high sensitivity, low power consumption and short recovery time (Yoon et al. 2011). Since the mid-20th century, CO₂ and other greenhouse gases emissions have increased daily due to the increasing industrial activities. This phenomenon is known as global warming which is caused by the increase of the average temperature of near-surface air as well as oceans on earth. By monitoring and subsequently decreasing CO₂ emissions released by fuel combustion in vehicle engines and burning coal in power plants, the greenhouse gas concentration is expected to decrease. This can illustrate the need for developing low-cost, highly sensitive, adjustable sensors that can be employed to monitor and control the CO₂ concentration in industrial exhaust gases.

With the aim of enhancing the sensing performance, numerous attempts have been made to develop and improve gas sensors. In this study the modelling of features of a CO₂ gas sensor based on graphene application has been carried out. The sensing characteristics of the gas sensor have also been evaluated during its operation on different temperature and concentration values. Efforts were made to determine whether graphene is a viable candidate to be used in a wide range of sensory applications (Bradley 2012, Wei et al. 2012).

The underlying operational principle for MOSFET (Figure 1) is based on the flow of electrons between source and drain electrodes which is controlled by the gate voltage. The efficiency of electron transport is the important quantity which has been defined as conductance (Hwang et al. 2013, Wouter Olthuis 2007).

According to the Landauer formula, graphene conductance, \( G \), is proportional to the carrier transmission probability from one electrode (source) to another (drain) (Datta 1997) equated as:

\[
G = \frac{2q^2}{h} T
\]  

(1)
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