学 位 論 文 概 要

題　目　Difference in adsorption mechanisms for polar and non-polar organic molecules in multi-walled carbon nanotubes-based gas sensors

（多層カーボンナノチューブを基にしたガスセンサーにおける極性有機分子と非極性有機分子の吸着機構の違い）

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Gas sensors are used in various applications, including environmental monitoring, industrial process control, and medical diagnosis. In 1991, Japanese scientist Iijima observed multi-walled carbon nanotubes (MWCNTs) using a tunneling electron microscope, and since then, carbon nanotubes (CNTs) have attracted significant attention as a potential material for gas sensors due to their higher sensitivity, faster response time, and a wider range of detectable concentrations.

In Chapter 1, I introduction part, I mainly introduced the background of this research about the gas sensor, it was found that nowadays it is still in high demand for the gas sensor which can detect gas concentration more accurately and faster, and also can work under various temperatures with less energy consumption.

In Chapter 2 paper review part, I mainly introduced the synthesis of CNT, the development of CNT gas sensors, and the application of CNT gas sensors.

Chapter 3 is the motivation and objective of this research, as introduced in Chapter 1 and Chapter 2, the potential of CNTs to be used in gas sensors has led to a surge of research in this area. However, the related research to understand the underlying mechanisms of CNT-based gas is still not well studied yet. Therefore, our total objective is to investigate the different adsorption mechanisms between polar and non-polar organic molecules in multi-walled carbon nanotube-based gas sensors.

Chapter 4 is the experimental part, in this chapter, I discussed the procedure of producing gas sensors based on MWCNTs (multiwall carbon nanotubes). Specifically, it will include the preparation of the MWCNTs solution (Chapter 4.1), the synthesis of the MWCNTs paper (Chapter 4.2), and the structure, conductivity, and homogeneity analysis of the resulting material (Chapter 4.3). It is important to note that our primary objective is to develop high-quality gas sensors using MWCNTs as the primary material, and the information presented in this chapter will help us achieve this goal by providing a detailed understanding of the processes involved in producing MWCNTs-based gas sensors.

In Chapter 5, a preliminary study of the adsorption of polar organic chemicals is discussed. And experiments will be conducted to assess the sensitivity of the MWCNT paper gas sensor. The preparation of the gas sensors (Chapter 5.2) and the Langmuir Adsorption Isotherm Model will be introduced (Chapter 5.3), and the results of sensitivity and Langmuir Adsorption Model fitting will be presented. The response and recovery time of the gas sensor will also be discussed, as well as the reproducibility of gases, which is an important characteristic of a gas sensor (Chapter 5.4).

In Chapter 6, I investigated the adsorption behavior of non-polar organic chemicals to carbon nanotubes. To better understand the adsorption behavior of non-polar molecules, I selected benzene and hexane as the target non-polar organic chemicals in this study. I observed step-like sensitivity behavior when I used the MWCNT paper gas sensor to detect the vapors of these chemicals, which is distinct from the behavior observed for polar molecules. Based on the IUPAC isotherm model and the relatively weak interaction between the surface of the MWCNT paper gas sensor and the non-polar gas molecules, I infer that this adsorption behavior can be fit by Type VI isotherm model.

In Chapter 7, I discussed the mechanism behind the different adsorption behavior of polar and non-polar molecules. Based on my model results, I proposed two hypotheses for the adsorption mechanism of these molecules: a line parallel structure, in which the molecules are arranged in the same plane parallel to the graphene, and a sandwich structure, in which the second layer of molecules is located on top of the first layer that has been adsorbed onto the surface of graphene. To prove these hypotheses, I used Gaussian 16 software to calculate the total energy of each possible structure. Results indicate that non-polar molecules are adsorbed by graphene in a sandwich structure, with the second layer of molecules located on top of one another, while polar molecules showed one-layer adsorption in a parallel structure.

Conclusions of this research are given in Chapter 8. It can be concluded that this research includes the fabrication of a gas sensor using MWCNT paper and the analysis of the different behavior towards various vapors of polar and non-polar organic chemicals. It shows that the Langmuir adsorption isotherm model fits well with polar molecules, while the Type VI isotherm fits well with non-polar molecules. In addition, the total energy calculated by Gaussian 16 indicates different adsorption mechanisms for polar and non-polar molecules, one-layer adsorption and two-layer adsorption, respectively.