A study on SERS sensor for the identification and spatial distribution visualization of the VOC gas

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論 文 名　：A study on SERS sensor for the identification and spatial distribution visualization of the VOC gas

（表面増強ラマン散乱センサを用いた VOC ガスの識別と空間分布の可視化に関する研究）

区　　分　：甲

論　文　内　容　の　要　旨

The main origins of volatile organic compounds (VOC) in the air include human production and activities, as well as natural processes. Monitoring and controlling VOC can reduce emissions caused by human activities, thereby maintaining environmental quality and safeguarding human health. Gas sensor technology, as an online detection method, has been widely utilized for the detection and identification of VOC gases. Simultaneously, upon identifying the types of gases, visualizing their spatial distribution allows for the search of gas sources and facilitates understanding the information within the gas sources. Gas sensors based on the principles of Surface enhanced Raman scattering (SERS) offer rapid response, molecular-level detection sensitivity, specific identification based on molecular structure, and high-resolution visualization capabilities.

Hence, the aim of this research is to develop a SERS gas sensing platform capable of identifying multiple VOC and visualizing the spatial distribution of gases. This dissertation comprises five chapters outlined as follows:

In Chapter 1, the study's background was introduced. The introduction and gas sensor technologies related to VOC were depicted. Moreover, the detection principles and fabrication methods of SERS sensors were explained.

In Chapter 2, the SERS sensor with high intensity, modified with hydrophilic materials, was utilized to detect ultra-low concentrations of geosmin in aqueous solutions. Gas was generated from a heated geosmin aqueous solution using a bubbling method. Upon contact with the cooler surface of the sensor, the high-temperature gas condensed into mist, enabling the collection of geosmin SERS spectra. With our ultra-high sensitivity detection system, a response ranges from 10 ppt to 10 ppb geosmin in ultrapure water was confirmed. Additionally, detection of 100 ppt geosmin in tap water was achievable.

In Chapter 3, a multiple SERS gas sensor matrix via spin-coating functional polymer was proposed to enhance gas recognition capability. Polymer films were fabricated using Poly(acrylic acid), Poly(methyl methacrylate), and Polydimethylsiloxane. The high design flexibility of a two-layer film was achieved using the layer-by-layer method with two one-layer films. SERS gas sensor coated with different polymer films exhibited distinct affinity to target gases. The principal com-ponent analysis algorithm was employed to further cluster gas molecules in a two-dimensional graph. The three target gases—phenethyl alcohol, acetophenone, and anethole—were effectively distinguished when analyzing the characteristic variables in the response matrix, which combined gas responses obtained from sensors coated with three one-layer and three two-layer films.

In Chapter 4, a SERS sensor array was developed to visualize the spatial distribution of gas evaporating from an odor source. The SERS sensor array was placed on the odor source and scanned by a home-made detection system to acquire the SERS spectra matrix of the odor gas. The intensities of the characteristic peaks from the collected spectra were utilized to generate a heatmap graph. After noise reduction processing of the heatmap graph, the localization of the odor source became distinctly identifiable in the resultant graph. Additionally, the size of the odor source could be determined using the visualization result. Moreover, this method was employed to visualize the spatial distribution of two distinct odor sources. To recognize between these two odor sources, the non-negative matrix factorization algorithm was utilized to decompose the obtained SERS spectra matrix, extracting feature and concentration information at each spot on the sensor array. The feature information was used to identify the odor source, while the concentration information facilitated the generation of the heatmap image. Gaussian fitting was applied to process the image for localizing the odor source. Consequently, the localizations of these two odor sources were identified and visualized using a single heatmap image.

In Chapter 5, the experimental results were summarized, and the future prospects of this dissertation were presented.