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Separating Chemical Signals of Adsorption-Desorption and Diffusive Processes

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***Abstract*— Signal separation at fluctuation-enhanced sensing improves speed, selectivity and sensitivity. We analyze a (symmetrical) two-sensor arrangement with a joint boundary line between the sensors for fluctuation-enhanced sensing. We show a way to separate the adsorption-desorption signal components from the diffusive signal component. Thus the method generates two independent output spectra which double the sensor information for pattern recognition. A two-sensor arrangement with submicron size is modeled by computer simulations, and the key features of the sensing method are demonstrated.**

***Index Terms*— adsorption-desorption, diffusive, chemical separation, fluctuation enhanced sensing**

I. Introduction

FLUCTUATION-ENHANCED sensing (FES) to analyze chemical mixtures was proposed almost a decade ago [1]. It utilizes the omnipresence and great sensitivity of low-frequency conductance fluctuations and conductance 1/*f* noise with regard to structural and environmental changes and inhomogenities/defects in solid state materials [2,3]. In FES we use the stochastic signal component due to the statistical interaction between the chemical agent and the sensor material/structure. Since its introduction [1], the history of FES has shown that this way of sensing is a complex task which includes not only many aspects of sensor development but also advanced signal processing issues [4-10].

The present paper introduces a new method which is able to distinguish between the adsorption-desorption and diffusive fluctuations in FES devices as a result of the surface occupancy of sensors by agent molecules [11,12]. This feature results in a doubling of sensor information and higher speed and/or selectivity.

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II. The New Method

Figure 1 shows a sketch of the two-sensor system [11]. The adsorbed molecules can diffuse freely and the particles can freely enter from one of the sensor surfaces into that of the other sensor. The space occupied by the two zones may be surrounded by a diffusion barrier which limits the diffusion to these subspaces. If there is no diffusion boundary around the whole system, then the particles which leave/enter the system contribute to the adsorption-desorption noise of the given sensor. Other geometries may also be used but they are less simple to fabricate. The time-dependent output signals of the two sensors are stochastic and defined as follows:

$$U_1(t) = KN_1(t) \qquad U_2(t) = KN_2(t) \qquad (1)$$

where K is a calibration constant and $N_1(t)$ and $N_2(t)$ are the instantaneous numbers of molecules over sensor-1 and sensor-2, respectively.

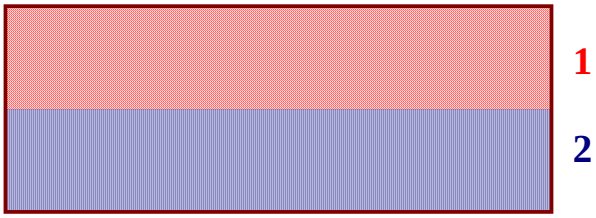

Figure 1. Two-sensor arrangement with enhanced joint boundary. Sensor-1 and sensor-2 share an extended joint boundary to enhance cross-correlations of surface diffusion noise. Particles can absorb/desorb over to the surface and they execute a random walk (diffusion) over the sensor surface and diffuse over the other sensor, too. If there is no diffusion boundary around the whole system, then the particles which leave/enter the system contribute to the adsorption-desorption noise of the given sensor.

The main claims of our study are as follows [1]:

(*i*) The spectrum of $U_1(t) + U_2(t)$ has only absorption-desorption noise. Then the total adsorption-desorption spectrum is

$$S_{12a} = S^{(+)}(f) = S_{1a}(f) + S_{2a}(f) \ , \qquad (2)$$

where $S_{1a}(f)$ and $S_{2a}(f)$ are the adsorption-desorption spectra over sensor-1 and sensor-2, respectively.

(*ii*) The spectrum of $U_1(t) - U_2(t)$ is the sum of absorption and diffusion fluctuations, *i.e.*,

$$S^{(-)}(f) = S_{1a}(f) + S_{2a}(f) + 4S_{1d}(f) \ , \qquad (3)$$

where $S_{1d}(f)$ is the diffusion spectrum over sensor-1 (equal to the diffusion spectrum of sensor-2).

(*iii*) After generating the spectra in (*i*) and (*ii*), the total diffusion fluctuation spectrum can be obtained by a simple subtraction:

$$S_{12d}(f) = 4S_{1d}(f) = S^{(-)}(f) - S^{(+)}(f) \ . \qquad (4)$$

The FES information will be $S_{12a}(f)$ and $S_{12d}(f)$, which are separated adsorption-desorption and diffusion spectra.

In this work we computer simulate adsorption/desorption processes on nanoscale sensors (such as gateless MOSFETs) as a representation of the system depicted in Fig. 1 and, as a demonstration, we use this computer simulated data to verify the accuracy of equations (2)-(4).

III. Demonstration by Computer Simulations

In this simplified demonstration, the system in Fig. 1 is simulated by two types of particles. One type is doing only diffusion and the other type is doing only absorption. There are two time-domain simulation data, representing $U_1(t) + U_2(t)$ and $U_1(t) - U_2(t)$. Each of these time-domain data consists of 1,048,576 points. The Welch spectrum method is applied for computing the Power Spectral Density patterns of the two time domain data (a window size of 8192 is applied, using Hamming window).

- $S^{(+)}(f)$ corresponds to the spectrum of $U_1(t) + U_2(t)$ and has only absorption-desorption noise.
- $S^{(-)}(f)$ corresponds to the spectrum of $U_1(t) - U_2(t)$ and is the sum of absorption and diffusion fluctuations.
- The extracted diffusion fluctuation spectrum then is obtained by $S^{(-)}(f) - S^{(+)}(f)$.

Figure 2 shows that the extracted spectrum $S^{(-)}(f) - S^{(+)}(f)$ is very close in value and shape to the actual diffusion fluctuation spectrum. A least-squares approach yields a coefficient value of 1.0031.

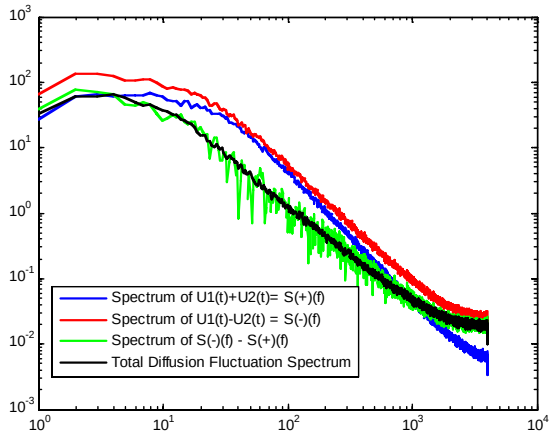

Figure 2. $S^{(-)}(f) - S^{(+)}(f)$ = 1.0031 x the actual diffusion fluctuation spectrum. There is a 0.3 % error as a result of strong "background noise" caused by the absorption-desorption noise.

Figure 3 shows that the spectrum $S^{(+)}(f)$ is very close in value and shape to the real absorption-desorption spectrum (after multiplication with the computed least-squares coefficient). A least-squares approach yields a coefficient value of 1.9825.

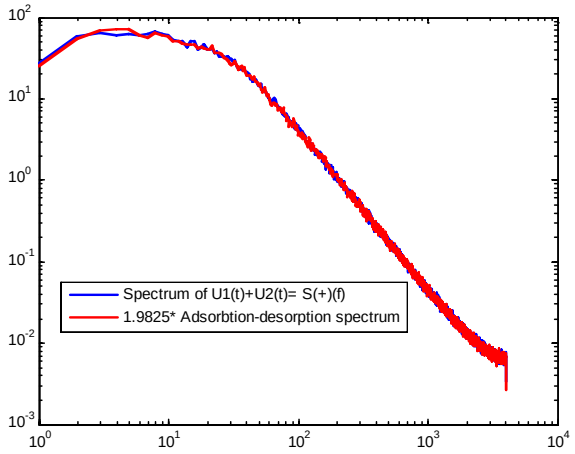

Figure 3. $S^{(+)}(f)$ = 1.9825 x the absorption-desorption spectrum. This is less than 2 % error as the result of strong "background noise" caused by the diffusion noise.

IV. Conclusion

The new method utilizes the joint presence of surface diffusion and adsorption-desorption in submicron-size fluctuation-enhanced sensors. In the classical way, the joint presence of the two noises would be distractive and reduce the sensory information. By using the new method, the sensory information is doubled and the output is enhanced by two independent types of patterns. The method has a potential in field effect transistor sensor arrangements and similar surface-active structures, such as micro-surface-acoustic-wave (SAW) sensors.

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