

## ABSTRAK

### PEMODELAN REAKSI KIMIA ANTARA GAS NO<sub>2</sub> DENGAN Pt<sub>80</sub>Au<sub>14</sub>Ti<sub>6</sub> SEBAGAI SENSOR BERBASISKAN FUNGSI KERJA

Oleh

LIS DWI ANDINI

Telah dilakukan pemodelan reaksi kimia dalam pendeteksian gas NO<sub>2</sub> pada permukaan sensor bahan Pt<sub>80</sub>Au<sub>14</sub>Ti<sub>6</sub> berdasarkan perubahan fungsi kerja ( $\Delta\phi$ ). Penelitian ini bertujuan untuk mengetahui adanya perbandingan nilai *Contact Potential Difference (CPD)* antara hasil eksperimen dengan hasil simulasi. Reaksi kimia pada penelitian ini menggunakan reaksi penyerapan gas NO<sub>2</sub>, penyerapan oksigen dan reaksi antar kedua gas tersebut. Reaksi yang digunakan pada penelitian ini mengandung empat nilai hunian/*coverage* ( $\theta$ ), yaitu hunian/*coverage* ( $\theta_{\text{O}}$ ), hunian/*coverage* ( $\theta_{\text{NO}_2}$ ), hunian/*coverage* ( $\theta_{\text{NO}}$ ) dan hunian/*coverage* ( $\theta_{\text{O}_2}$ ). Simulasi dijalankan dengan menggunakan MATLAB. Penelitian ini berhasil mendapatkan nilai parameter (23 parameter) yang belum didapatkan dari studi literatur. Penelitian ini juga mendapatkan hasil simulasi sinyal sensor gas NO<sub>2</sub> pada bahan Pt<sub>80</sub>Au<sub>14</sub>Ti<sub>6</sub> dengan trend grafik yang mendekati grafik eksperimen. Nilai *CPD* yang dihasilkan dari simulasi masih jauh dibandingkan dengan hasil eksperimen, yaitu sebesar 10 mV dengan nilai *CPD* hasil eksperimen sebesar  $(50 \pm 10)$  mV. Selain itu, penelitian ini juga berhasil mendapatkan perkiraan nilai hunian/*coverage* ( $\theta$ ) untuk gas NO<sub>2</sub>, gas O<sub>2</sub>, gas NO dan atom O secara berturut-turut sebesar  $2,684 \times 10^{-11}$  ML,  $1,048 \times 10^{-11}$  ML,  $1,048 \times 10^{-11}$  ML dan  $4,02 \times 10^{-9}$  ML.

**Kata Kunci :** *CPD*, sensor gas, gas NO<sub>2</sub>, simulasi, perubahan fungsi kerja

## ABSTRACT

### MODELING OF CHEMICAL REACTION BETWEEN NO<sub>2</sub> GAS AND Pt<sub>80</sub>Au<sub>14</sub>Ti<sub>6</sub> AS A SENSOR BASED ON WORK FUNCTION

By

LIS DWI ANDINI

Chemical reactions modeling has been carried out in the detection of NO<sub>2</sub> gas on the surface of the Pt<sub>80</sub>Au<sub>14</sub>Ti<sub>6</sub> material sensor based on the change in work function ( $\Delta\phi$ ). This research aims to determine whether there is a comparison of the *Contact Potential Difference (CPD)* between the experimental results of and the simulation. The chemical reaction in this research uses the NO<sub>2</sub> gas absorption reaction, oxygen absorption and the reaction between the two gases. The reaction used in this study contains four *coverage* ( $\theta$ ), that is *coverage* ( $\theta_O$ ), *coverage* ( $\theta_{NO_2}$ ), *coverage* ( $\theta_{NO}$ ) and *coverage* ( $\theta_{O_2}$ ). The simulation is run using MATLAB. This research can find parameter values (23 parameters) which had not been obtained from literature studies. This research also obtained the simulation results of the NO<sub>2</sub> gas sensor signal on Pt<sub>80</sub>Au<sub>14</sub>Ti<sub>6</sub> material with a trend graph close to the experimental graph. The CPD value resulting from the simulation is still far from the experimental results, which is equal to 10 mV with the CPD by experimental of  $(50 \pm 10)$  mV. In addition, this research also can find an estimate of the *coverage* ( $\theta$ ) for NO<sub>2</sub> gas, O<sub>2</sub> gas, NO gas and O atom respectively of  $2,684 \times 10^{-11}$  ML,  $1,048 \times 10^{-11}$  ML,  $1,048 \times 10^{-11}$  ML and  $4,02 \times 10^{-9}$  ML.

**Keywords :** CPD, gas sensor, NO<sub>2</sub> gas, simulation, work function change