Simulation of $Pt_{80}Au_{14}Ti_6$ Work Function Change-Based Sensor of H_2 Gas

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Abstract	Chemical reactions simulation in detecting hydrogen gas (H-2) on Pt80Au14Ti6 sensor surface based on work function change (Delta phi) has been conducted. The simulation result is compared with laboratory results of detecting H-2 gas. Three chemical reactions contained three coverages, H coverage (theta(H)), O coverage (theta(O)), and H2O coverage (theta(H2O)). The simulation was run using MATLAB. This research can find the reaction parameter values such as the Arrhenius coefficient of H2O forming reaction on Pt (upsilon(f3Pt)), H2O forming reaction on Au (upsilon(f3Au)), i.e., H2O dissociation on Au (upsilon(f3Au)), O-2 desorption on Ti (upsilon(d2Ti)), H2O forming reaction on Ti (upsilon(f3Ti)), and H2O dissociation on Ti (upsilon(f3Ti)), i.e., 7.5x10(14) s(-1), 9.85x10(15) s(-1), 3.25x10(15) s(-1), 7.11x10(15) s(-1), 3.425x10(15) s(-1) and 2.725x10(15) s(-1), respectively. The simulation results also have the same trend as the laboratory results. However, the contact potential difference (CPD) simulation result, i.e., -240 mV, is not the same as the laboratory result, (-297 +/- 9) mV. In addition, this simulation also obtained approximation coverage for atoms/molecules on PT80Au14Ti6 surface, i.e., theta(H) = 0.665154 Mono Layer (ML); theta(O) = 1.5621x 10-6 ML; and theta(H2O) = 5.41676 x10(-5) ML.
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