Initial Sticking Coefficient Attenuation of Gases in Carbon Monoxide Sensing on $Pt_{80}Au_{14}Ti_6$

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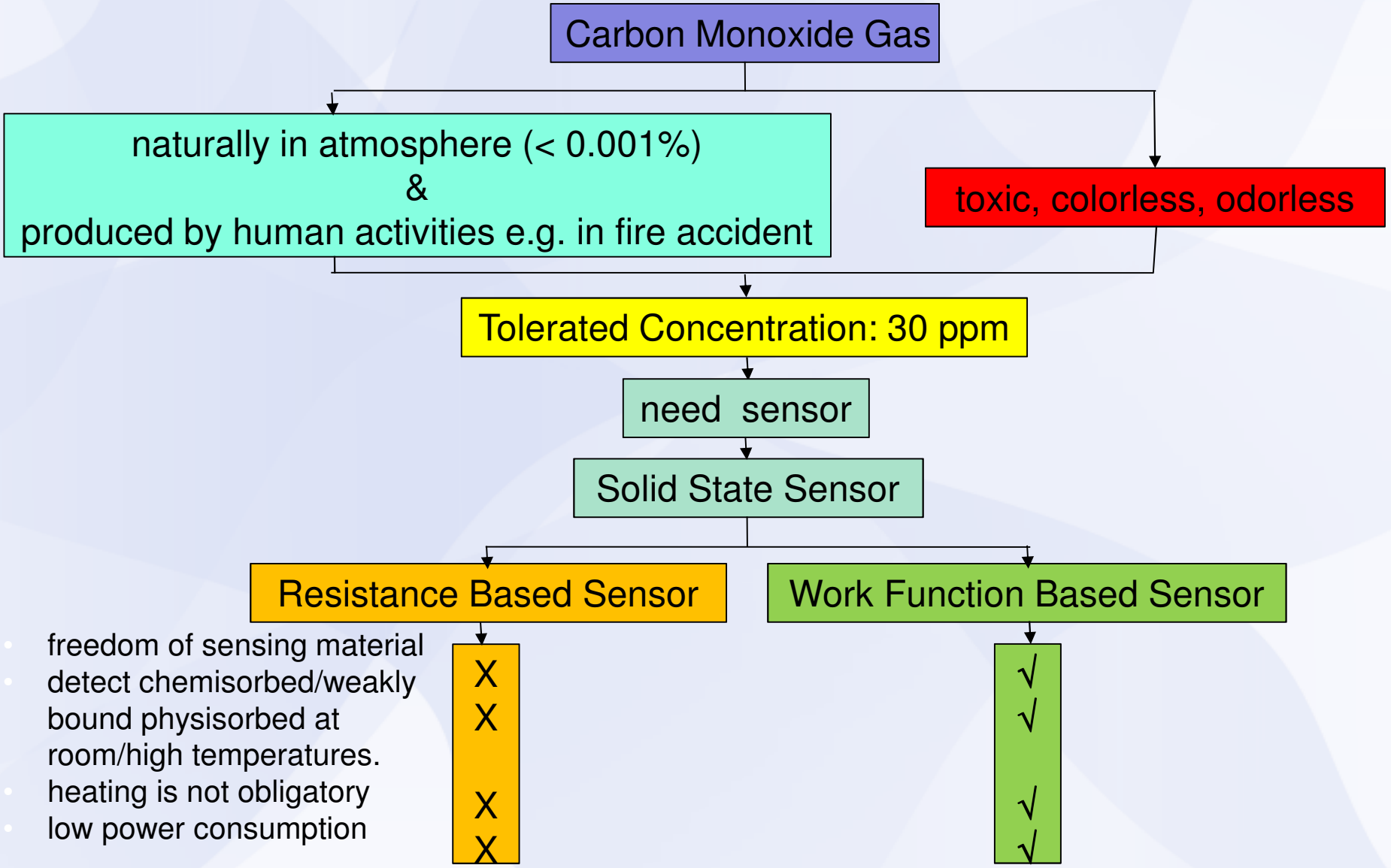
1. Motivation



- freedom of sensing material
- detect chemisorbed/weakly bound physisorbed at room/high temperatures.
- heating is not obligatory
- low power consumption

2. Introduction

$Pt_{80}Au_{14}Ti_{6}$

It was already investigated as CO sensitive layer in normal atmosphere as a work function change based sensor at room temperature.

Loss Signal Problem and its Solution

The sensitive layer loses its signal after 24 hours in air and can be refreshed by annealing at 170°C for 10 minutes in air.

Attenuation of Initial Sticking Coefficient

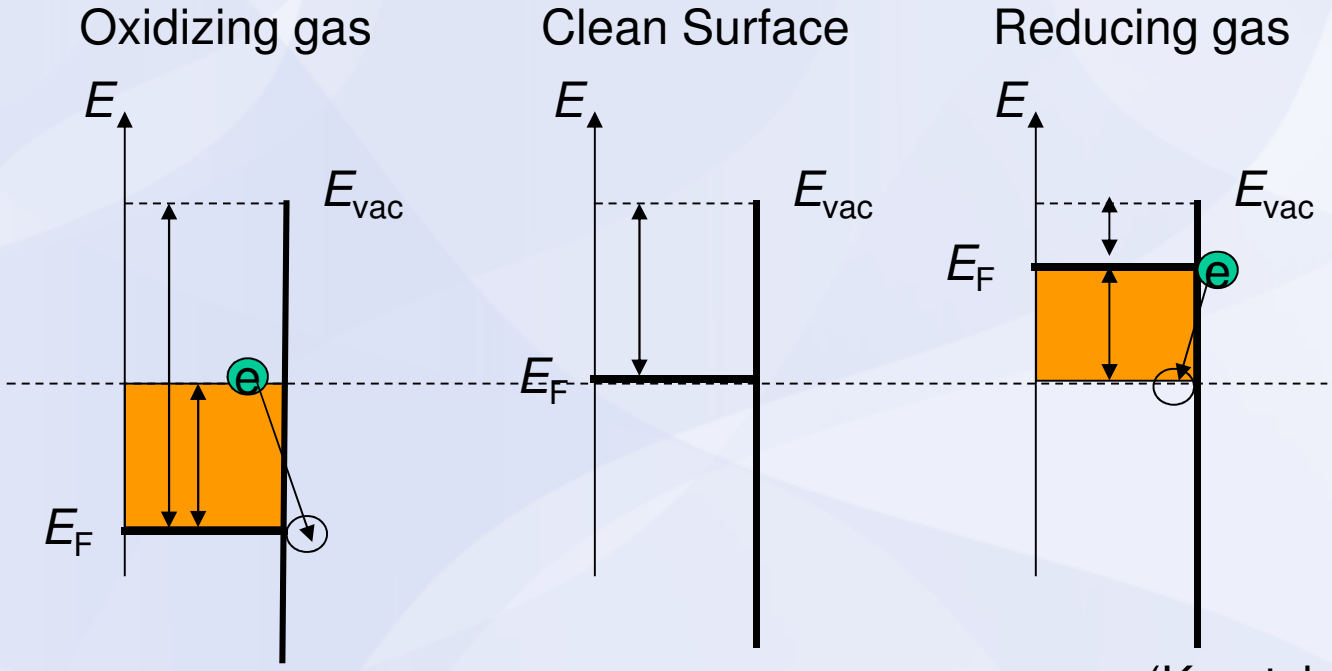
It is suspected causing the loss signal problem.

The Aim of This Research

Finding the attenuation factor of initial sticking coefficient of gases.

3. Basic Theories

Work Function



(Korotchenkov, 2011)

$$\Phi = E_{\mathrm{F}} - E_{\mathrm{vac}}$$

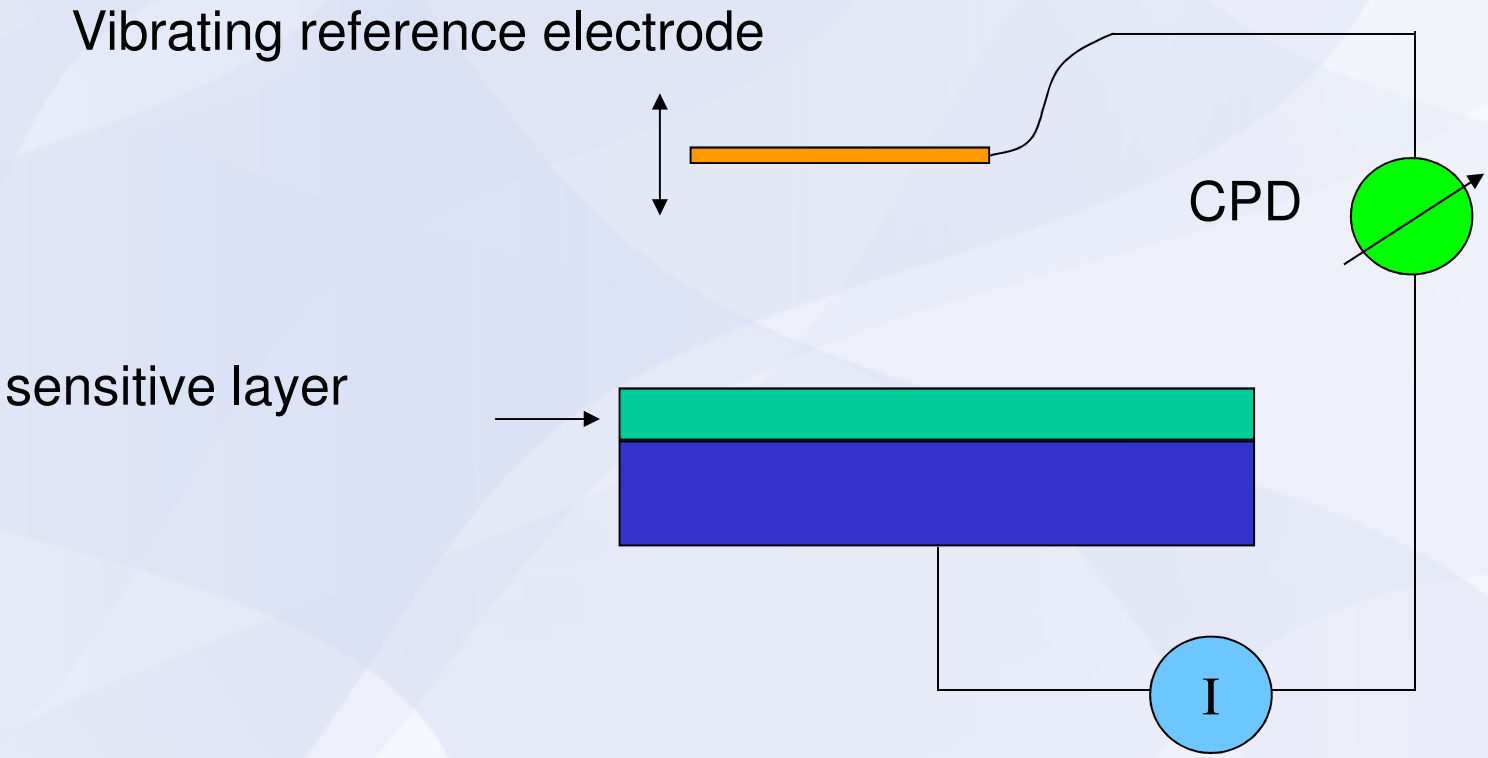
$$\Delta\Phi = E_{\mathrm{F}}^{\mathrm{new}} - E_{\mathrm{F}}^{\mathrm{old}}$$

where:

Φ	: work function (eV)
E_{vac}	: vacuum energy level (eV)
E_{F}	: Fermi energy level (eV)
$\Delta\Phi$	: work function change (eV)

3. Basic Theories, cont.

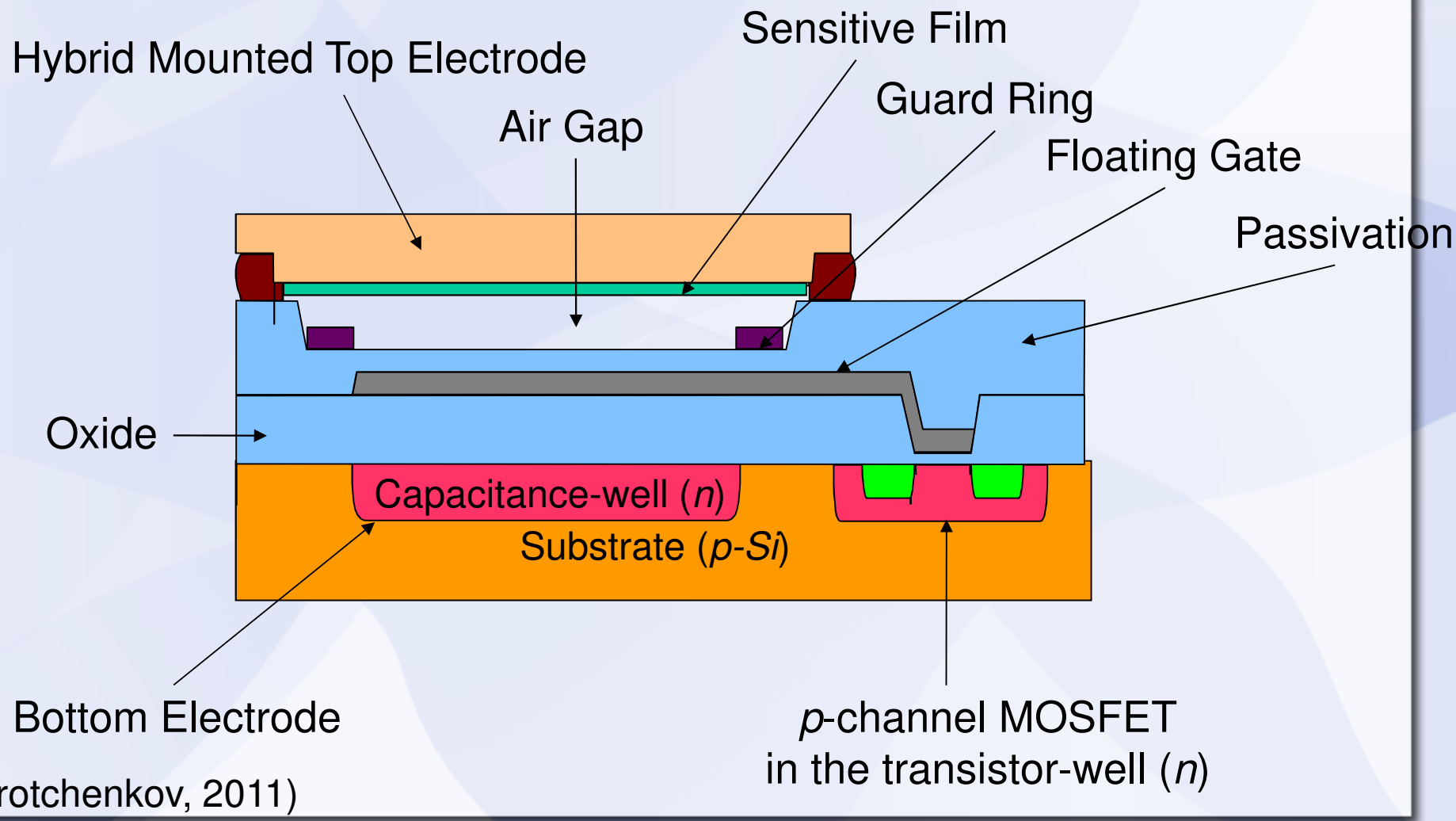
Kelvin Probe



(Korotchenkov, 2011)

3. Basic Theories, cont.

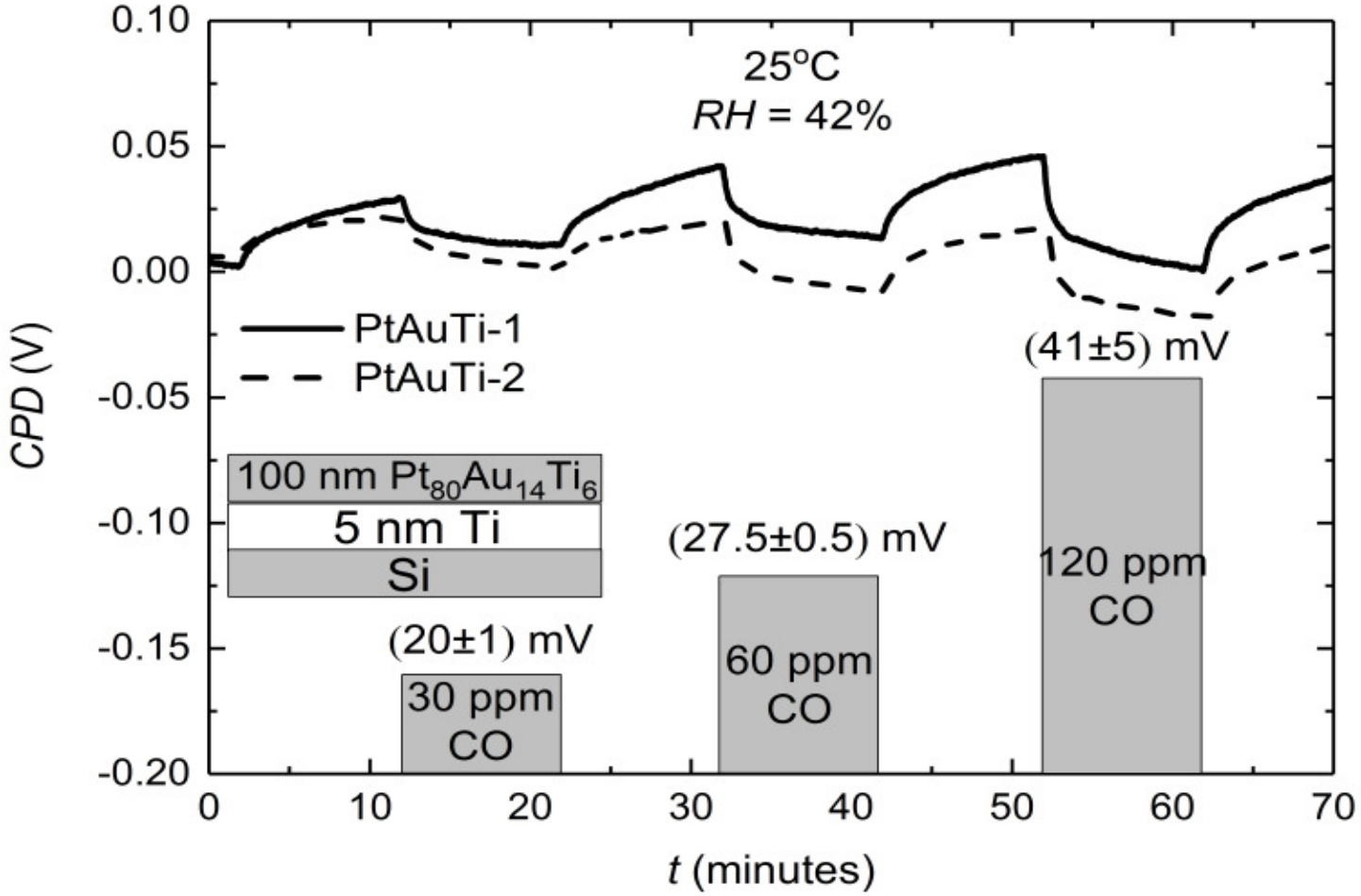
Floating Gate Field Effect Transistor (FG-FET)



(Korotchenkov, 2011)

3. Basic Theories, cont.

$Pt_{80}Au_{14}Ti_6$



3. Basic Theories, cont.

Adsorption, Reaction, Dissociation and Desorption

Surface Coverage Change Rate of:

1. Adsorption Process

$$\frac{d\Theta}{dt} = \frac{S_0 (1-\Theta)^2 P}{\sigma\sqrt{2\pi mkT}} \exp\left(-\frac{E_a}{kT}\right)$$

2. AB as product of A and B

$$\frac{d\Theta_{AB}}{dt} = \upsilon_r \exp\left(-\frac{E_r}{kT}\right)\Theta_A\Theta_B$$

3. A as dissociation of AB

$$\frac{d\Theta_A}{dt} = \upsilon_{diss} \exp\left(-\frac{E_{diss}}{kT}\right)\Theta_{AB}$$

4. Desorption Process

$$\frac{d\Theta}{dt} = \upsilon_d \exp\left(-\frac{E_d}{kT}\right)\Theta$$

where

S_0 : initial sticking coefficient of gas
Θ : coverage of gas on the sample surface (ML)
P : partial pressure of gas (Pa)
σ : surface atom densiy of the layer (atoms/m2)
m : mass of gas molecule (kg)
k : Boltzmann constant = 1.38×10^{-23} J/K
T : temperature (K)
E : activation energy (J)
υ : frequency of reaction (s^{-1})

3. Basic Theories, cont.

Reaction Mechanism Model

- Adapting from Water Gas Shift Reaction (WGSR)
- State of the art: 18 reactions were filtered from 60 of WGSRs by Callaghan.
- This research: Callaghan's reactions + 2 of WGSRs + 1 new reaction = 21 reactions.
- Every reaction: forward and reverse reactions.
- One way reaction: reaction energy parameter and Arrhenius coefficient.
- Every material: 42 energy parameters and Arrhenius coefficient.

Example:

1. $CO^{(g)} + S \rightleftharpoons CO^{(s)}$
4. $CO^{(s)} + O^{(s)} \rightleftharpoons CO_2{}^{(s)}$

9 coupled differential equations.

$$\frac{d\Theta_{CO}}{dt} = r_{f1}F_{CO} - r_{f4}\,\Theta_{CO}\Theta_O + r_{r4}\,\Theta_{CO2} \Rightarrow \Theta_{CO}, \Theta_O, \text{etc.} \Rightarrow \Phi \Rightarrow CPD$$

$$F_x = (1-\Theta_x)^n \frac{P}{\sigma\sqrt{2\pi mkT}}$$

$$r_{\text{f or r, N}} = \upsilon_{\text{f or r, N}} \exp\left(-\frac{E_{\text{f or r, N}}}{kT}\right)$$

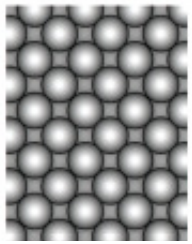
4. Results and Discussions

Attenuation Factor (f_{adj1}) of Initial Sticking Coefficient

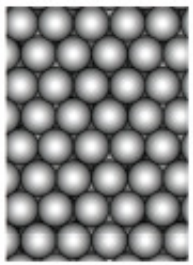
Loss Signal Problem

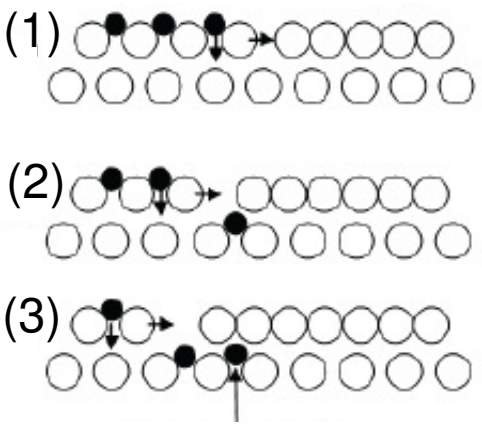
Reports:
Oxygen can diffuse in Pt

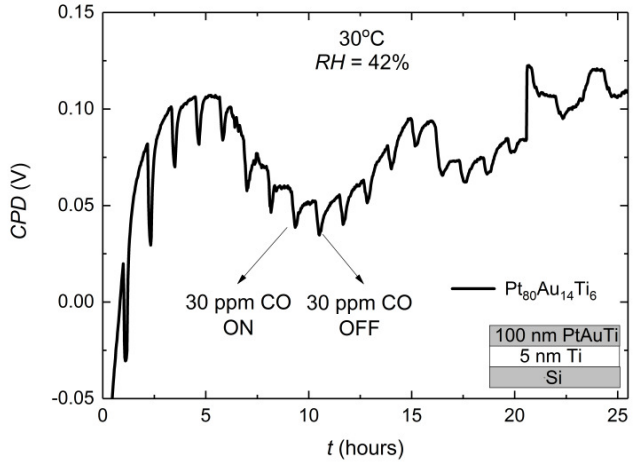
Pt(100)(1x1)

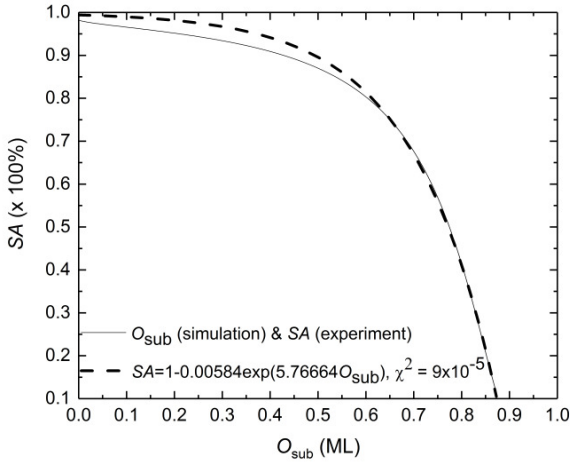


hex-Pt(100)





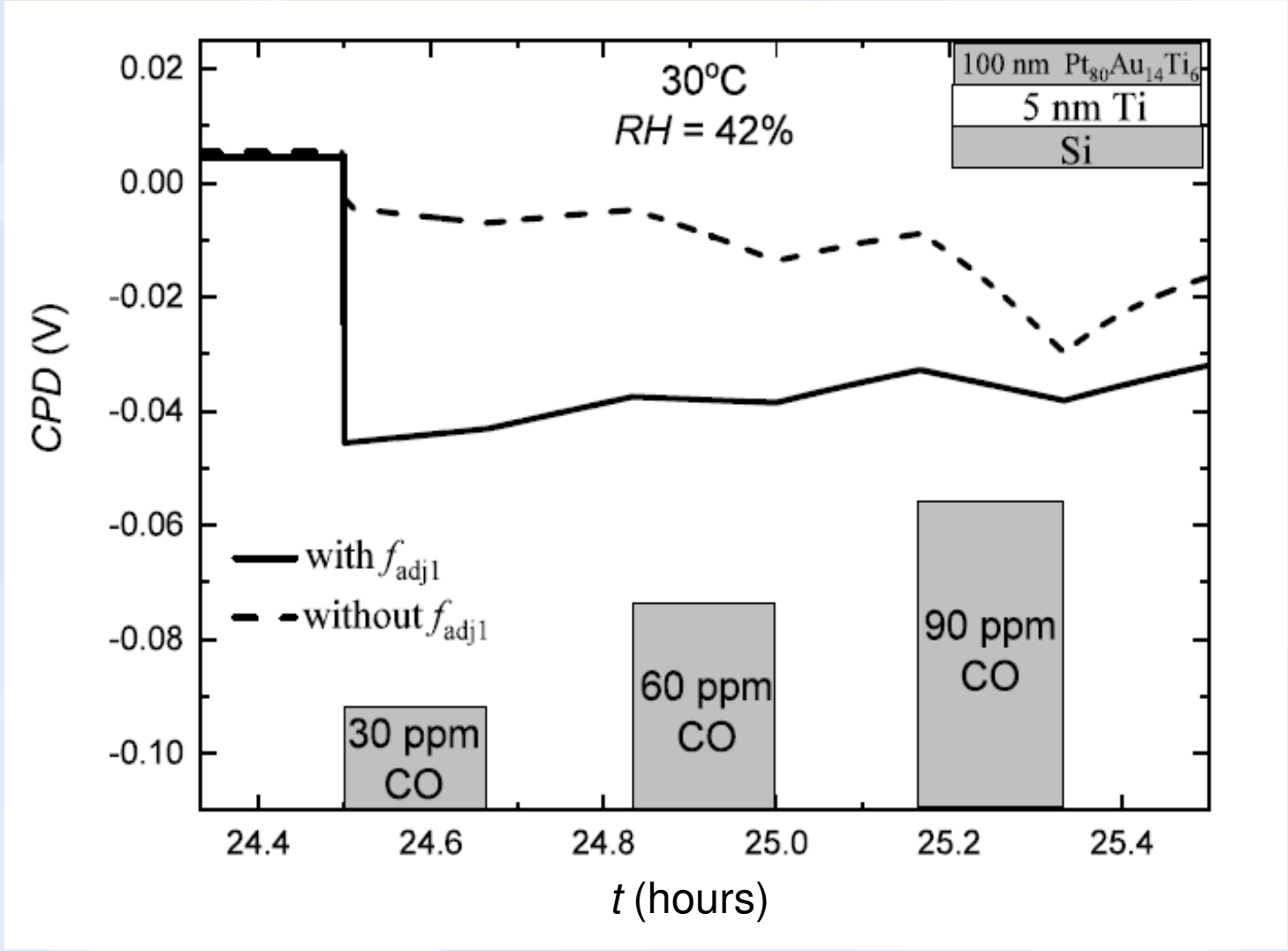




$$f_{adj1}=1-0.00585\exp(5.76664O_{sub})$$

4. Results and Discussions, cont.

Simulation with/without Attenuation Factor (f_{adj1})



6. Conclusion & Acknowledgement

Conclusion

1.The Reaction Mechanism Model is in agreement with the experiment results.
2.Initial Sticking Coefficient should be adjusted with the attenuation factor.
3.Attenuation factor of the Initial Sticking Coefficient is f_{adj1}=1-0.00585exp(5.76664O_{sub}).

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Thank You for Your Attention

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