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Development of SiC-FET methanol sensor

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Abstract

A silicon carbide based field effect transistor (SiC-FET) structure was used for methanol sensing. Due to the chemical stability and wide band gap of SiC, these sensors are suitable for applications over a wide temperature range. Two different catalytic metals, Pt and Ir, were tested as gate contacts for detection of methanol. The sensing properties of both Ir gate and Pt gate SiC-FET sensors were investigated in the concentration range 0.3 – 5% of methanol in air and in the temperature range 150–350°C. It was observed that compared to the Ir gate sensor, the Pt gate sensor showed higher sensitivity, faster response and recovery to methanol vapour at comparatively lower temperature, with an optimum around 200°C. Quantum-chemical calculations were used to investigate the MeOH adsorption and to rationalize the observed non-Langmuir behavior of the response functions. The methanol sensing mechanism of the SiC-FET is discussed.

Key words: SiC, FET sensor, Pt, Ir, Methanol, Gas sensor, Solid state sensors

1. Introduction

Carbon dioxide is considered as the most important greenhouse gas, since the increase in carbon dioxide concentration in the atmosphere (at present about 390 ppm) is believed to enhance global warming problems. Conversion of carbon dioxide from large scale industry exhausts, e.g. coal fueled power plants, to useful chemicals and new fuels is one promising way to reduce the problem. Recently research, which focuses on methanol synthesis from CO₂ is published [1-3]. Methanol is a common feed stock for several important chemicals and a potential alternative energy carrier to, e.g., hydrogen. It is also a very useful organic solvent with widespread applications in the manufacturing of colors, dyes, drugs, perfumes, formaldehyde etc. Methanol is toxic and fatal to human beings even in modest concentrations [4]. The wide range of applications of MeOH, its toxicity, and the desirability to be able to fine tune its synthesis under demanding conditions strongly suggest the need of development of reliable and selective methanol sensors.

The gas-sensing properties of nanostructured ZnO thin films to methanol, ethanol and propyl alcohol vapour was studied by Cheng et al. [5]. Arshak and Gaiden [6] investigated the iron and zinc oxide thick film gas sensors to detect methanol, ethanol and propanol in the concentration range of 0–8000 ppm. Neri et al. [7] reported that the addition of Ce^{3+} to Fe_2O_3 increases the response to methanol at low temperature (<350°C). Patel et al. [4] studied an indium tin oxide (ITO) thin film gas sensor for detection of methanol at room temperature. To detect gas molecules at high temperature and in an corrosive environment, the sensor should be hard, robust, chemically inert and

stable even at elevated temperatures. SiC is a wide band gap (3.2 eV) material with break down electric field of $2.2 \cdot 10^6 \text{ V cm}^{-1}$, thermal conductivity 5 W cm⁻¹ K⁻¹ and a melting point ~ 2700°C, that permits its use over a wide temperature range, from RT to above 600°C. Also the extremely good chemical inertness makes it suitable for use in aggressive environments. Since the SiC is commercially available as wafers, so far 100 mm in diameter, mass production of devices enables manufacturing of small and cheap device chips. Gas sensitive field effect devices based on silicon carbide (SiC) with catalytic gate metals are being commercialized by SenSiC AB [8]. Based on the choice of gate material and operation temperature, selectivity to different gas molecules is demonstrated [9].

During gas sensing, the sensor is exposed to methanol molecules that can react with the adsorbed surface oxygen or with the moisture present in air and then decompose to hydrogen atoms on the catalytic gate electrode surface [10-12]. In a study of methanol decomposition over a Pd membrane where the reaction species and products were analyzed by two mass spectrometers, one on each side of the membrane, it was observed that the decomposed hydrogen originated from the methyl group of methanol [10]. This was clarified through the use of deuterium atoms in different positions of the methanol molecule and the following reaction sequences were suggested.

In presence of adsorbed surface oxygen:

 $CH_3OH (g) \rightarrow CH_2OH_{ad} + H_{ad} (methyl),$

 $O_2(g) \rightarrow 2O_{ad}$,

 $CH_2OH_{ad} + O_{ad} \rightarrow 3H_{ad} (methyl) + CO_2 (g),$

 $O_{ad} + H_{ad} \text{ (methyl)} \rightarrow OH_{ad},$

 $OH_{ad} + H_{ad} \text{ (methyl)} \rightarrow H_2O \text{ (g)}$

2H _{ad} (methyl) \rightarrow H₂.

In presence of moisture, the following reactions are possible:

$$CH_3OH + H_2O \rightarrow 6H^+ + 6e^- + CO_2$$

$$6\mathrm{H}^+ + 6\mathrm{e}^- \rightarrow 3\mathrm{H}_2$$

However, another possibility is the decomposition of methanol to formaldehyde and formic acid by reacting with the chemisorbed oxygen on the oxide surface [4, 13].

 $CH_3OH + O_{ad} \rightarrow HCOH + H_2O + e_{ad}$

 $CH_3OH + O_2^- \rightarrow HCOOH + H_2O + e^-$

This shows that there are quite many possible adsorbed species including hydrogen atoms or ions on the catalytic metal surfaces and some of them may spill over to the exposed oxide in the porous film. A discussion about the detection mechanism of the methanol sensor is found in the Discussion and Future work section.

In this communication, highly sensitive and fast response Pt gate SiC-FET sensors are reported for methanol detection at elevated temperatures. For comparison, the same set of experiments were carried out for Ir gate SiC-FET sensors. The adsorption of methanol was in addition investigated by quantum-chemical computations. Selectivity and cross-sensitivity to some gases and stability of both sensors are also reported.

2. Experimental

The MISiC transistor device was designed by SenSiC AB [8] and processed from 4H– SiC wafers by ACREO AB [14], see schematic picture in Fig. 1. The Ohmic contacts to drain, source and the backside of the SiC substrate consist of 50 nm Ni, subjected to rapid thermal annealing in Ar at 950°C for 10 min and thereafter 50 nm TaSi_x + 400 nm Pt was deposited on top of the Ni. The Pt layer is necessary as an oxygen diffusion barrier for high temperature operation, while the TaSi_x serves as adhesion layer between Ni and Pt. The different catalytic gate materials (Ir, Pt) of about 20 nm thickness were deposited by sputtering at high pressure which creates porous films [9].



Fig. 1. (a) Schematic diagram of the sensor structure and (b) the mounting of the SiC-FET sensor.

The sensor measurements were performed at a constant source to drain current of 100 μ A, taking the drain to source/gate voltage as the sensor signal. The sampling rate used for all the measurements was 1 s⁻¹. The gases used were dry and of 99.99% purity. The sensors were tested for their responses to different concentrations of methanol (0.3% to 5%) in 10% O₂ mixed with N₂ as the carrier gas at different temperatures ranging from 150°C to 350°C in steps of 50, in order to evaluate the sensitivity profile vs. temperature.

The methanol was produced by blowing the carrier gas through liquid methanol (synthetic grade purity) at room temperature in a gas washing bottle, assuming that the carrier gas got saturated by methanol. The MeOH containing gas was then mixed in various proportions with the main carrier gas flow, and this procedure did not allow concentration lower than 0.3 %. The tested concentration range of the methanol is 0.3%-5%. The carrier gas composition, $10\% O_2$ in N₂, is typical for diesel exhausts and flue gases. It should be noted that according to our experience, there is usually no difference in the sensor response to test gases containing 10% or $20\% O_2$ in N₂. The exposure to the test gas was performed during 3 min and recovery in carrier gas was allowed for 3 min. The selectivity and cross sensitivity of the sensors were studied for hydrogen and propene.

3. Results

We studied the sensing characteristics with different methanol concentrations in 10 or 20% O₂ in N₂ as carrier gas. The response is defined as the change in voltage in presence of methanol to the voltage in air at constant current and is expressed as $\Delta V = (V_a - V_g)$ where V_a is the voltage in air, and V_g is the voltage in presence of methanol gas. The response time of the sensor was calculated as the time to reach the sensor response to 90% of its saturation value on exposure to sensing gas mixed with 10 or 20% O₂ in N₂, and the recovery time was calculated as the time corresponding to the decrease of the sensor response by 90% of its saturation value in the carrier gas [15, 16].

Methanol response vs. temperature characteristics for both Ir and Pt gate FET sensors were plotted from the repeated cycle transient response at different temperatures and are shown in Fig. 2. The operation temperature corresponding to maximum response was 250°C for the Ir gate sensor and 200°C for the Pt gate sensor. The magnitude of the gas response was also found to be quite high for the latter sensor with a maximum of about 2 V. The lower temperature for maximum response as well as the higher value of the response of Pt sensors as compared to Ir sensors was also observed for other gases (H₂,

 NH_3 , CO, NO/ NO_2 ,

C₃H₆) in ref. [9].



Fig. 2. Response vs. temperature characteristics of Ir gate and Pt gate SiC-FET sensors for methanol in 10% O_2 / N_2

Fig. 3 displays the transient signals for the sensors at different concentrations of methanol (0.3%, 0.43%, 0.57%, 0.71%, 0.84%, 0.98%, 1.11%, 1.23%, 1.36%, 1.95%, 2.5%, 3, 3.46%, 3.88%, 4.28%, 4.65% and 5%) and at the respective maximum operation

temperature, showing the expected increase in the response with increasing methanol concentrations. Especially for the Pt sensor, the signal to methanol behavior was very stable with minimum drift in the base line, while the Ir sensor needs longer recovery time in order to fully return to the baseline. Figure 2 indicates that for Ir an operation temperature of 350°C would also be possible and would likely increase the speed of response. This will be further investigated in future studies.



Fig. 3. Transient signal characteristics at different concentration of methanol in 10% O_2/N_2 for (a) Ir gate and (b) Pt gate SiC-FET sensors.

Fig. 4 shows the change in response versus methanol concentration for both samples. For the Ir gate sensor, the response increases almost linearly with increasing concentration, that is Ir shows a large dynamic range of at least 0 - 5% for detection of methanol. The Pt gate FET sensor shows an almost linear increase of the response for lower methanol concentrations, and then the slope of the curve decreases and the response reaches saturation at higher concentrations. Neither the Ir nor the Pt sensor response curve could be fitted by the Langmuir isotherm, which indicates that the sensing process probably cannot be reduced to a simple adsorption-desorption phenomenon, as further discussed below.



Fig. 4. Response vs. methanol concentration (carrier gas: $10\%O_2 / N_2$) characteristics of Ir gate and Pt gate SiC-FET sensors.

To investigate the interaction of MeOH with Pt and Ir further, quantum-chemical calculations were carried out. The Gaussian03 [17] program was used to perform density functional theory B3LYP/LanL2MB [18-20] computations for metal particles with various degrees of MeOH coverage, as shown in Fig. 5. A 14-atom Pt or Ir cluster was employed as a compromise between cluster size and computational speed. Methanol was found to adsorb to the surface via its oxygen atom at a distance of about 2 Å for both Pt and Ir. At the Pt cluster, the adsorption energy of a single MeOH molecule is 235 kJ/mol. But when the surface of the particle is covered with multiple adsorbates to form approximately half (5 MeOH) and full (14) monolayers the adsorption energy decreased to 193 kJ per mol MeOH. For the Ir particle the trend is found to be the same, although MeOH binds somewhat stronger to Ir than to Pt, e.g. 290 kJ/mol for a single adsorbate, which decreased to 143 kJ per mol MeOH (14 monolayers). One of the prerequisites for the Langmuir isotherm to apply is that the adsorption energy per adsorbate should be independent of coverage, which from the calculations is not the case and thus could be the explanation for the observed non-Langmuir behavior of the response curves.



Fig. 5. Platinum clusters with various amount of MeOH adsorbates from quantumchemical calculations. a) single adsorbate, b) 5 adsorbates and c) 14 adsorbates.

Table 1 presents the response, the response time and recovery time of both sensors. A minimum in the response time of 2.5 s and a recovery time of 9 s was observed for the Pt gate sensor at 1% methanol concentration, while the corresponding minima for the Ir sensor were 3 s and 22 s for 5% MeOH. The stability of the sensors was tested through subjecting the sensors to 3 min pulses of 0.3% methanol in carrier gas with 3 min outgassing repeated with 1 hour in between for a total of 5 hours at their maximum operation temperature, see Figs. 6. It is clear from the figures that, although the response is higher for the Pt gate sensor, in this study the Ir gate sensor shows better stability.

sensors at different methanol concentrations in $10\% O_2 / N_2$ as carrier gas corresponding to their optimum operating temperature Type of Operating Methanol Response Response Recovery

Table 1. Response, response time and recovery time of Ir gate and Pt gate SiC-FET

Type of sensor	Operating temperature (0C)	Methanol concentration (%)	Response voltage (mV)	Response time (s)	Recovery time (s)
Iridium gate FET sensor	250	0.3	124	5	64
		1	208	4	46
		5	472	3	22
Ptatinum gate FET sensor	200	0.3	221	4	37
		1	1058	2.5	9
		5	2103	2	21

To study the selectivity of the sensors both were exposed to hydrogen (0.05%, 0.1%, and 0.15%) and propene (0.02%, 0.03%, and 0.04%) mixed with the carrier gas of 10% oxygen in nitrogen. The corresponding transient signal characteristics of both sensors are given in Figs. 7 and 8. The response for different concentrations of hydrogen and propene at maximum operating temperatures for methanol are given in Table 2. For



Fig. 6. Stability study of (a) Ir gate and (b) Pt gate SiC-FET sensors with 0.3% methanol pulses in $10\% O_2$ in N_2 as the carrier gas.

0.05% hydrogen concentration the response is shown to be quite high, 220 mV for Ir gate and 845 mV for Pt gate sensor, but for the 0.04% propene concentration it is only 45

mV for Ir gate and 25 mV for Pt gate sensor, which corresponds well to earlier measurements, e.g. in Ref. [9]. Therefore it can be concluded that both sensors are highly sensitive for hydrogen but not sensitive for propene at the operation temperatures used in this investigation.

Table 2. Selectivity and cross sensitivity studies. Response of Ir gate and Pt gate SiC-FET sensors at different concentrations of hydrogen, propene and mixtures of these gases with methanol in 10% O_2 / N_2 as carrier gas at the chosen operation temperature for methanol detection.

Test gas	Concentration	Response Ir 250°C	Response Pt 200°C
	(%)	(mV)	(mV)
H ₂	0.05	222	846
H ₂	0.1	517	1239
H ₂	0.15	913	1519
Propene	0.02	39	18
Propene	0.03	42	23
Propene	0.04	43	25
Methanol (before	0.3	104	97
H ₂)			
Methanol + H ₂	0.3 + 0.02	187	522
(Cross sensitivity)			
Methanol (before	0.3	103	112
propene)			
Mehtanol +	0.3 + 0.02	112	114
propene			
(Cross sensitivity)			

Cross sensitivity studies using hydrogen and propene were also carried out for both Ir and Pt gate sensors. The corresponding transient signal characteristics are shown



Fig. 7. The response of (a) Ir gate and (b) Pt gate SiC-FET sensors to hydrogen.



Fig. 8. Response of (a) Ir gate and (b) Pt gate SiC-FET sensors to propene.

in Figs. 9 and 10. Here the first three pulses are for 0.3% methanol only and the following pulses are for 0.3% methanol mixed with 0.02% hydrogen and 0.02% propene respectively, with 10% O_2 mixed with N_2 as carrier gas in all cases. Table 2 also presents



Fig. 9. Cross sensitivity study of (a) Ir gate and (b) Pt gate SiC-FET sensors between methanol and hydrogen.



Fig. 10. Cross sensitivity study of (a) Ir gate and (b) Pt gate SiC-FET sensors between methanol and propene.

the response to methanol with hydrogen or propene present in the gas mixture. The response increases from 105 to 185 mV for the Ir gate sensor, and from 95 to 520 mV for the Pt gate sensor when hydrogen was mixed with methanol. However, the response

increases from 105 to 110 mV for the Ir gate sensor, and from 110 to 115 mV for Pt gate sensor when propene was mixed with methanol. Thus both sensors show large cross sensitivity for hydrogen but not for propene at the chosen operation temperatures for the methanol detection.

4. Discussion and Future work

As stated in the introduction, the large number of applications of methanol, e.g. as a liquid fuel produced from the conversion of CO_2 , as well as its toxicity justifies the development of a methanol sensor. The work performed in this study show an interesting complex behavior for methanol detection by SiC-FET sensors, which is different for Pt and Ir gates.

The investigation of the methanol sensitivity of Pt and Ir gate SiC-FET devices was obvious as a starting point since these sensors are the most characterized for this type of gas sensors [9, 21]. The high concentration of the tested methanol originates from practical circumstances, since for this introductory study we choose to produce methanol molecules from the well-known method of blowing air through methanol in a gas washing bottle. On the other hand, the high concentration also introduced the interesting extremely high response of the Pt gate sensor, for which we can only speculate about the reason. It can be assumed that part of the response is due to hydrogen atoms decomposed from methanol, which are detected as OH groups formed on the insulator surface in the normal way for hydrogen containing gases by these sensors [22]. A theoretical value for the saturated hydrogen response for a thick film sensor is about 800 mV and for a porous

film about 200 mV adds to the response from consumption of oxygen ions adsorbed on the insulator surface by the hydrogen [23, 24]. The transistor devices used as sensors provide some amplification through the transistor gain (transconductance), still a response of 2 V has to include also detection of more species. This could be decomposition products of methanol adsorbed on top of OH groups or at other sites on the insulator surface and / or at the metal – insulator border. It should be pointed out that field effect sensors do not detect resistivity change in the catalytic gate material like in Refs. [4-7], but charging effects of the gate area. The size of the response and the recovery time for, e.g., 1% methanol revealed in Table 1 is another indication that different detection mechanisms are involved in the case of Pt and Ir at the rather high concentrations of methanol investigated here.

The difference in stability of the response of Pt and Ir gate sensors is mainly due to the tendency of the gate material to restructure during the high temperature operation. This depends on several parameters like grain size and substrate but also on the melting point of the metal, which for Ir is considerably higher (2410°C) as compared to Pt (1772°C) [25]. The better stability of Ir is reflected in the stability tests in Fig. 5. This makes it even more interesting to investigate Ir also at higher operation temperature in future work.

More work should be performed e.g by DRIFT (Diffuse Reflectance IR Fourier Transform) spectroscopy [23] to reveal the details in the detection mechanism in these measurements. For example, the extremely high response to high concentrations of

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methanol for the Pt gate SiC-FET sensor will be interesting to study. More quantumchemical calculations on the reaction mechanisms will also be carried out. In particular more detailed studies are necessary to better understand the difference in response behavior between Pt and Ir as a consequence of their different electronic structure (both Pt and Ir are cubic close packed metals). The interplay between methanol, hydrogen and oxygen on Pt and Ir surfaces is especially interesting to study in relation to the results in Table 2. Further studies are planned to investigate the methanol response over a larger concentration range starting at around 10 ppm. The response to Ir at temperatures above 300°C may give interesting results and will be investigated. There are other sensing materials with potential for selective methanol sensing and interesting to include in a sensor array, which might be needed in order to reach a viable methanol sensor system.

5. Conclusions

Methanol is an interesting alternative vehicle fuel, either in itself in an internal combustion engine or as a hydrogen source for fuel cells The possibility to synthesize methanol from carbon dioxide has increased the interest even more, and justifies sensor development. Silicon carbide based FET sensors were tested regarding their response to methanol at elevated temperature. Two catalytic gate metals, Ir and Pt, were tested so far. The Pt gate FET sensor (operation temperature 200°C) showed higher sensitivity to methanol compared to the Ir gate sensor (operation temperature chosen to 250°C) but the stability of the sensor was found to be better for the latter one. The response curves were non-Langmuir in nature, which could be due to the adsorption energies being dependent upon the degree of coverage as supported by quantum-chemical calculations. Both

sensors showed a low response to propene, while the response to hydrogen is even higher as compared to methanol and also with clear cross sensitivity at the chosen operation temperatures for methanol detection. More sensing materials are interesting for future studies and the detection mechanism needs further clarification. For example, a very high response of the Pt gate sensor implies that not only dissociated hydrogen atoms are involved in the detection of methanol.

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Table captions:

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Table 2. Selectivity and cross sensitivity studies. Response of Ir gate and Pt gate SiC-FET sensors at different concentrations of hydrogen, propene and mixtures of these gases with methanol in 10% O_2 / N_2 as carrier gas at the chosen operation temperature for methanol detection.

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Author Biographies

Jayita Kanungo received her Ph.D degree in Engineering from Jadavpur University, India, 2010. Now she is working as a research associate at IC Design and Fabrication Centre, Department of Electronics and Telecommunication Engineering, Jadavpur University, Kolkata, India. Her main research interest is development and applications of gas sensor materials and devices.

Mike Andersson received his Ph.D. in applied physics at Linköping University 2007 and completed a Post Doc in sensor science in 2009. He is currently working as a research scientist within the sensor science group at Linköping University as well as within SenSiC AB. His main research interests concern chemical sensors for high temperature and environmental applications.

Zhafira Darmastuti, PhD student at Applied Physics, Linköping University. She has academic and industrial background in Energy and Environment Engineering. Her main interest is chemical gas sensors for flue gas cleaning in power generation application.

Dr. Sukumar Basu is a retired professor of IIT Kharagpur, India and now he is associated with Jadavpur University, Kolkata, India as Research Advisor. His main topics of research are electronic materials and solid-state gas sensors. At present he is working on synthesis and characterizations of graphene and its oxide derivative for applications as hydrogen & hydrocarbon sensors. Prof. Basu has published about 200 papers in the peer reviewed national & international journals and proceedings of the international conferences. He has four book chapters and three Indian patents to his credit.

Per-Olov Käll, Professor in inorganic chemistry at Linköping University, Sweden. Käll, who received his PhD in inorganic chemistry at Stockholm University in 1991, has a main interest in materials chemistry. While in the beginning of his academic career Käll studied the synthesis and phase composition of structural ceramics, e.g. silicon nitride based ceramics, in recent years he has been working with synthesis and characterization of nano-sized metal oxide particles and thin films for applications in, e.g., sensors, magnetic resonance imaging, and optical devices. Käll is also interested in the energy issue and believes it is important to develop effective catalysts for the hydrogenation of CO₂ to MeOH and other energy rich hydrocarbons. He has published more than 40 articles in international peer-reviewed scientific journals and about 20 peer-reviewed conference proceedings. He is a member of the board of The Centre in Nano science and technology (CeNano) at Linköping University and of the editorial board of the newly launched journals *Open Journal of Inorganic Chemistry* and *ISRN Nanotechnology*.

Lars Ojamäe, Professor in Physical Chemistry at Linköping University since 2008. He received his PhD in inorganic chemistry at Uppsala University in 1993, worked as postdoc at the Ohio State University and at the University of Turin, as assistant professor at Stockholm University and associate professor and then full professor at Linköping University. He heads the physical chemistry subdivision. His research activities focus on computational-chemistry modeling of chemical reactions at surfaces, solar cells, hydrogen bonding and nanoparticles.

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Anita Lloyd Spetz, Professor in Sensor Science, Chemical Sensors at Linköping University, 2011–2014 50% FiDiPro professor, Oulu University, Finland. 1995–2006 she was at S-SENCE, Swedish Sensor Centre (centre of excellence). From 2007 she is the Vice Director of the VINN Excellence centre, FunMat, Functional nanostructured Materials. Her research involves SiC-FET high temperature gas sensors with MAX material ohmic contacts, wide band gap material transducers for biosensors, resonator sensors, soot sensors and graphene sensors. She runs application projects with industry, and she is member of the board of SenSiC AB for commercialization of SiC-FET sensors. She has published 160 papers in scientific journals and referenced conference proceedings, 10 book chapters, and has 4 patents.