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Title	Investigating interface states and oxide traps in the MoS2/oxide/Si system
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Publication date	2021-06-09
Original Citation	Coleman, E., Mirabelli, G., Bolshakov, P., Zhao, P., Caruso, E., Gity, F., Monaghan, S., Cherkaoui, K., Balestra, V., Wallace, R. M., Young, C. D., Duffy, R. and Hurley, P. K.(2021) 'Investigating interface states and oxide traps in the MoS2/oxide/Si system', Solid-State Electronics, 186, 108123 (4pp). doi: 10.1016/j.sse.2021.108123
Type of publication	Article (peer-reviewed)
Link to publisher's version	10.1016/j.sse.2021.108123
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Download date	2026-11-02 01:19:41
Item downloaded from	https://hdl.handle.net/10468/13305



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Coláiste na hOllscoile Corcaigh

Solid-State Electronics 186 (2021) 108123

Contents lists available at ScienceDirect

Solid State Electronics

journal homepage: www.elsevier.com/locate/sse

Investigating interface states and oxide traps in the MoS_2/oxide/Si system

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ARTICLE INFO

The review of this paper was arranged by "Felice Crupi"

Keywords:
2D materials
Interface states
Oxide traps
MoS_2/oxide/Si system
MOSFET
Tunnel FET

ABSTRACT

This paper reports on the study of inverted metal-oxide semiconductor (MOS) structures formed through mechanical exfoliation of MoS_2 flakes onto Al_2O_3 or SiO_2 layers grown on degenerately doped *p* type silicon substrates. Using Au/Ni metal top contacts, multi-frequency capacitance and conductance characterisation were performed to investigate electrically active defects in the MoS_2/oxide structures. This data has been paired with physics-based ac simulations which indicate close to ideal interfacial properties.

1. Introduction

In recent years 2D materials have featured prominently in research, as they exhibit energy gaps which span from semi-metals through to wide band gap semiconductors with potential applications including sensors, electronics, and flexible display technologies [1,2]. In the area of insulating gate electron devices, the 2D structure of the semiconductor has the potential to result in near ideal semiconductor/oxide interface [3] properties, which is one of the main factors motivating research into MOSFET and tunnel FET devices based on 2D semiconductors. The application of multi-frequency capacitance and conductance measurements to investigate electrically active defects in MoS_2/oxide structures is a research area which has emerged in recent years [4–8], covering back-gated MoS_2 transistors [4] and top-gated [5–8] MoS_2 MOSFETs. The aim of this contribution is to extend the study of back gated metal/MoS_2/oxide/Si MOS structures, where the MoS_2 layer is thicker than the maximum depletion width. The results from three separate processes, combining experimental data and physics-based *ac* simulations, all indicate close to ideal interfacial properties.

2. Experimental methods and analysis

Fig. 1a shows an optical image of an inverted AuNi/MoS_2/Al_2O_3/p^+Si MOS capacitor, along a schematic of the structure (Fig. 1b) and cross sectional TEM images of the experimental devices (Fig. 1c). The structure was formed based on mechanical exfoliation of highly crystalline MoS_2 and subsequent transfer to the Al_2O_3 (23 nm)/p^+Si substrate. This process requires the flakes to have a large and flat surface area to allow for metal contact formation. In addition, the MoS_2 flake thickness should exceed the maximum depletion width. Hall measurements on the starting MoS_2 crystals provide an indication for the required flake thickness. [9] The Ni (5 nm)/Au (160 nm) metal contact was aligned with the 728 nm MoS_2 flake by optical inspection, with no subsequent processing prior to electrical measurements.

The multi-frequency (100 Hz to 1 MHz) CV response of the structure from approximately −9V to +5 V is shown in Fig. 2a. The CV response in the depletion region shows negligible/no dispersion suggesting a very low density of electrically active interface defects (D_{it}). The negative shift in the CV response yields a net fixed oxide charge density of 8.3×10^{12} cm^{-2} (+ve), assuming all the fixed oxide charge is located at the MoS_2/Al_2O_3 interface. The fixed oxide charge density is determined based on the shift of the flat band voltage from the ideal value. This positive charge is typically observed for ALD grown Al_2O_3 prior to H_2/

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https://doi.org/10.1016/j.sse.2021.108123
Received 18 May 2021; Received in revised form 30 May 2021; Accepted 2 June 2021
Available online 9 June 2021
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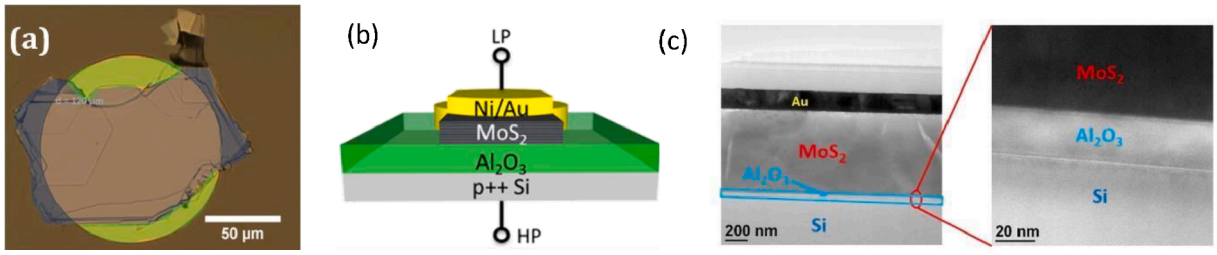


Fig. 1. Inverted MOS capacitor based on mechanically exfoliated MoS_2 (728 nm) transferred to 23 nm of ALD grown Al_2O_3 on degenerately doped p^+ type silicon (1×10^{-2} to 2×10^{-3} Ω.cm). The top metal is 5 nm Ni and 160 nm Au. a) Optical picture of the device showing the metal in contact with (green) the Si/Al_2O_3 substrate and (blue) the MoS_2. b) Schematic cross section of the device. c) Cross sectional TEM of the structure, with a zoomed in image of the $MoS_2/Al_2O_3/p^+$Si region. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

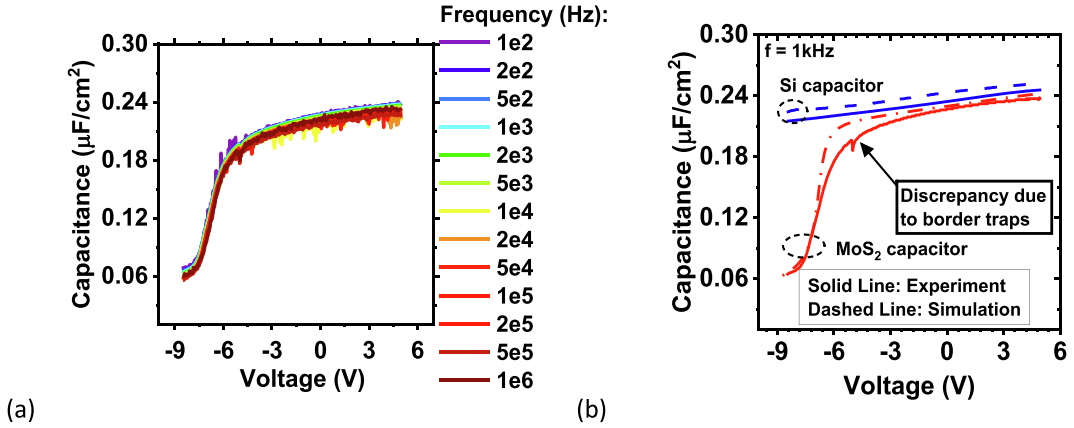


Fig. 2. (a) Experimental multi-frequency CV response of the NiAu/$MoS_2/Al_2O_3/p^+$Si described in Fig. 1. CV was recorded at room temperature. (b) 1 kHz CV responses of AuNi/$MoS_2/Al_2O_3/p^+$Si structure and the reference AuNi/$MoS_2/Al_2O_3/p^+$Si structure. The dashed lines are the physics based ac simulations of the structure.

N_2 annealing, and the density value obtained is consistent with other ALD grown films with a thickness around 24 nm [10].

In conjunction with the experimental data, physics-based ac simulations of the CV response based on TCAD software [11] are also presented. Fig. 2b shows the 1 kHz CV response for the case of the reference AuNi/Al_2O_3/p^+Si structure (blue) and the 1 kHz CV plot of the AuNi/$MoS_2/Al_2O_3/p^+$Si structure (red). The dashed lines are physics-based ac simulations of the CV response. The availability of the reference structure, with no MoS_2, allows a determination of the doping concentration in the p^+ silicon, which can subsequently be used in the simulation of the full AuNi/$MoS_2/Al_2O_3/p^+$Si structure. From the reference structure (AuNi/Al_2O_3/p^+Si), a boron doping concentration in the Si of 3×10^{19} cm^{-3} is obtained, consistent with the p^+ wafer resistivity range of 1×10^{-2} to 2×10^{-3} Ω.cm. For these simulations of the reference structure, the Al_2O_3 thickness is 23 nm (from TEM), with a dielectric constant of 6.5.

In the case of the simulations for the AuNi/$MoS_2/Al_2O_3/p^+$Si structure, TCAD models for MoS_2 are not yet available. The MoS_2 parameters used in the simulations are: energy gap = 1.20 eV, electron affinity = 4.5 eV, electron effective mass = 0.57, hole effective mass = 0.8. The carrier density versus Fermi energy is taken from [12,13]. Fitting of the simulated CV response to the experimental response yields an *n*-type doping concentration in the MoS_2 of 1.75×10^{17} cm^{-3}. The effective fixed positive charge in the Al_2O_3, has an equivalent value of 8.3×10^{12}

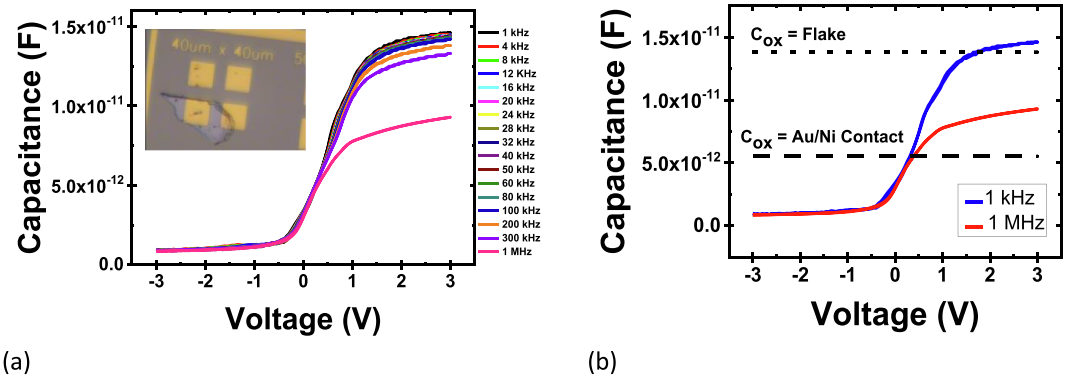


Fig. 3. (a) Experimental multi-frequency CV double sweep response at room temperature. The voltage range is between −3V and +3 V and the frequencies vary between 1 kHz and 1Mhz. The inset shows an optical image of the AuNi/$MoS_2/SiO_2/p^+$Si structure. (b) The CV response at 1 kHz and 1 MHz with the expected maximum capacitance shown as a dotted line for the cases where the area is defined by the Ni/Au contact and where the area is defined by the MoS_2 flake.

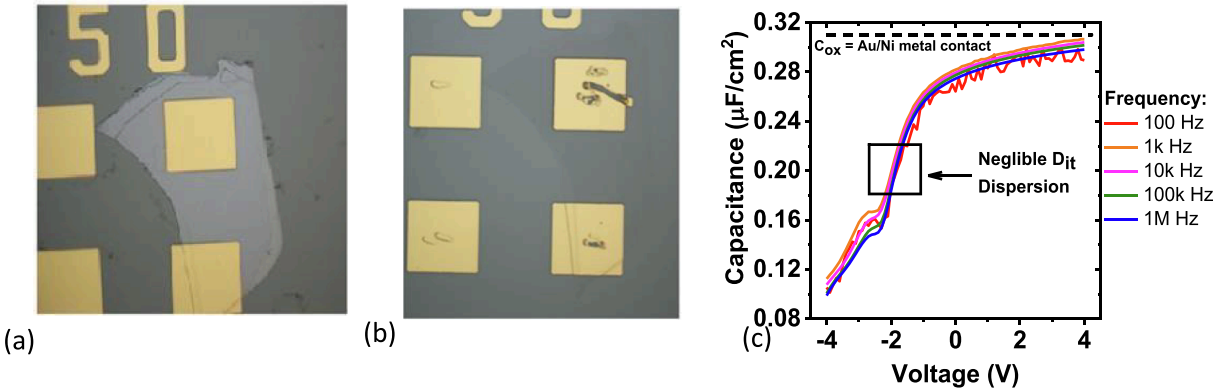


Fig. 4. a) Top view optical image of the AuNi/MoS_2/Al_2O_3/p^+Si structure where the Ni(5 nm)/Au(160 nm) contacts and the MoS_2 flake are both visible, (b) the same structure after reactive ion etching of the MoS_2 layer using the Ni/Au as a hard mask. Note that an impression remains of the original flake position due to the height differences during the reactive ion etching. The marks on the Ni/Au pads are probing marks. c) Corresponding experimental multi-frequency CV response of the AuNi/MoS_2/Al_2O_3/p^+ Si shown in Fig b) (top right square). CV was recorded at room temperature and the sweeps were performed from −4V to +4 V. The CV response demonstrates negligible CV dispersion in depletion.

cm^{-2} (+ve) located at the MoS_2/Al_2O_3 interface. It is noted that while the MoS_2 crystal used for the mechanical exfoliation was not intentionally doped, Hall analysis performed on the starting bulk crystal [9] yielded an *n* type semiconductor with a doping concentration of ~10^{17} cm^{-3} consistent with the value extracted from fitting the experimental CV response. The CV simulations, with no interface states included, fit the CV response in depletion. There is a small discrepancy at approximately −5V, when the Fermi level at the surface reaches the MoS_2 conduction band edge, which is likely due to oxide traps in the Al_2O_3 (also referred to as border traps) [14]. However, the overall results demonstrate a close link between the theoretical and experimental data, without the inclusion of electrically active interface defects.

Further studies were performed using different deposition and fabrication facilities, where MoS_2 was exfoliated on heavily doped SiO_2 (10 nm)/p^+Si and capacitor structures were formed using Ni(5 nm)/Au (160 nm) metallisation. In this case, the MoS_2 flake was not etched, and the resulting multi frequency CV responses of the structure highlight an effect which is evident when the dimensions of the flake exceed the dimensions of the metal contact. The multi-frequency (1 kHz to 1 MHz) CV sweeps performed between −3V and +3 V are shown in Fig. 3a. In this case, the CV responses are double sweep hysteresis curves with no hold time in the accumulation region (+3V) of the SiO_2/Si and the MoS_2/SiO_2 interfaces. In Fig, 3a the capacitance is plotted as the measured value, and not normalised to μF/cm^2, as the effective area of the sample is not a unique value for all *ac* signal frequencies. The expected maximum capacitance, based on the metal contact area of the 40 μm × 40 μm square, is 5.52 × 10^{-12}F and is shown as a dashed line in Fig. 3b. At *ac* signal frequencies from 1 kHz to approximately 100 kHz, electrons can follow the ac signal throughout the MoS_2 layer, beyond the metal contact, and therefore the area of the sample for the conditions of maximum capacitance is defined by the flake area as opposed of the metal contact area. Based on an estimated flake area of 4 × 10^{-9} m^2, the expected maximum capacitance value is 1.38 × 10^{-11}F and the experimental data showed the maximum capacitance to be 1.46 × 10^{-11}F. A significant observation from the CV response is that negligible hysteresis in the CV is present.

A repeat of the process is shown in Fig. 4. In this case the Ni(5 nm)/Au(160 nm) metal was used as a hard mask during reactive ion etching of the MoS_2 (the MoS_2 flake averaging ~350 nm in height) on doped Al_2O_3 (20 nm)/p^+Si. This approach allows a well-defined area of MoS_2 in the capacitor structure. The gas used during etching was SF_6 (5sccm)/Ar (45sccm) for 30 s at 100 W and 6mT. An image of the initial flake outline is still visible in Fig. 4. b due to the height difference (MoS_2 and Al_2O_3) during the etch process. Following the etching process, Fig. 4c demonstrates a good agreement between the theoretical maximum oxide capacitance of 0.31 μF/cm^2 (dashed line) and the experimental values. This sample also shows negligible frequency dispersion in depletion from 0 to −2 V. The origin of the ledge in the CV response at ~2.5 V could be a consequence of deep depletion in the MoS_2 substrate or an interface defects response, and requires further study.

The observation of a negligible interface state density and negligible hysteresis from the multi-frequency CV response is technologically advantageous, but also somewhat unexpected, as the surface of exfoliated MoS_2 is known to contain a high density of structural defects on the surface when imaged by STM [15], where density values can exceed 10^{12} cm^{-2}. In addition, it is reasonable to expect single or multiple atomic steps in the MoS_2 surface which is placed in contact with the Al_2O_3 or SiO_2 surface. Our results indicate that these defects are either: not electrically active or are passivated between exfoliation and subsequent transfer to the SiO_2/Si substrate.

3. Conclusion

In conclusion, these results demonstrate that interface state density values below the detection limit can be achieved between crystalline MoS_2 and amorphous Al_2O_3 or SiO_2, supporting one of the main motivations for using 2D semiconductors in MOSFETs and Tunnel FETs. More studies are currently underway to investigate the structural, chemical, and electronic properties of this interface and to understand why we observed negligible densities of electrical active interface defects as well as negligible CV hysteresis.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors from the Tyndall National Institute acknowledge the financial support of Science Foundation Ireland through the AMBER 2 (12/RC/2278_P2), UNITE (13/US/I2862) and INVEST (15/IA/3131) projects and the European Union through the ASCENT + project (Grant Agreement No. 654384). The authors from the University of Texas at Dallas acknowledge the financial support of The National Science Foundation CAREER Award (ECCS-11139986).

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Emma Coleman: Position: PhD student. Supervisors: Prof. Paul Hurley, Dr. Karim Cherkaoui & Prof. Colm O' Dwyer. Bachelor's Degree: Chemistry, University College Cork. Area of research: 2D Materials & Devices. More specifically, 2D transition metal dichalcogenides which exhibit a range of electronic properties spanning from semi-metals through to wide bandgap semiconductors. .