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The Effects of AlN Passivation Layer to Metal Work-Function and Band Alignment of Metal Oxide Semiconductor Devices

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Abstract

The effects of AlN passivation layer have been studied on Ni/HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ for metal oxide semiconductor devices application. It is found that the AlN layer induces a dipole $\delta = 0.18$ eV between HfO_2 and substrate. The dipole value extracted from capacitance-voltage ($C - V$) characteristics performs an excellent agreement with X-ray photoelectron spectroscopic (XPS) measurement. The effective work function (EWF) $\phi_{m,eff}$ of Ni, valance band offset ΔE_V, electron affinity χ, and conduction band offset ΔE_C of HfO_2 are obtained by 5.39, 2.84, 2.61, and 1.89 eV, respectively. Its energy band gap is found in 5.45 eV which is consistent with that of earlier report.

1. Introduction

Among many high-k materials will be applied in the future CMOS devices, HfO_2 has now emerged as the choice for oxide layers due to large permittivity. But HfO_2 layer suffers from process dependent threshold voltage variation, the difficulty in achieving band edge work function value, and trap creation. In recently, it is believed that AlN interface layer (AlN-IL) can be used to passivate $In_{0.53}Ga_{0.47}As$ interface and reduce density of interface trap (Dit) to ~10^{11} cm^{-2} for metal oxide semiconductor capacitors devices (MOSCaps) [1]. However, the addition of this layer maybe affects to band alignment of these devices and effective work function (EWF) of metal. It was also found that the EWF of metal in contact with high-k dielectric differed from its work function (WF) in vacuum and strongly depended on its chemistry and its interface [2]. So in this study, we focus on discussion about the effect of AlN-IL to EWF of Ni and the band alignment of Ni/HfO_2/AlN/$In_{0.43}Ga_{0.47}As$ MOSCaps.

2. Experimental

Wafer used in this paper is $5\times10^{17}/cm^3$ Si-doped n-type with 100 nm $In_{0.53}Ga_{0.47}As$ layer grown by solid source molecular beam epitaxial on n^+-InP substrate. The process to fabricated AlN-IL could be found elsewhere [1]. For EWF extraction, 5 cycles of AlN-IL were deposited followed by the growth of 80 cycles, 120 cycles, and 160 cycles' thermal-ALD-HfO2 films. After that all samples were annealing in forming gas (FG) at 450°C for 5 minutes by rapid thermal annealing (RTA) before Ni/Au gate contacts and Au/Ge/Ni/Au backside ohmic contacts deposition. Finally, all samples were annealed at 350°C for 30s in FG.

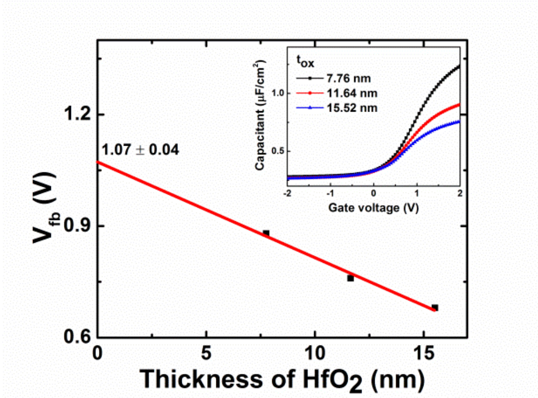

Fig. 1 The V_{FB} versus. HfO_2 thickness plot for Ni gates. Using Eq. (1), the inset shows C-V characteristics of three samples with different thickness

3. Result and discussion

The EWF was calculated by using the following equation:

$$V_{FB} = \phi_{m,eff} - \phi_S - \left(Q_f \frac{\varepsilon_{SiO_2}}{\varepsilon_{ox}^2} t_{ox} + \frac{1}{2} \rho_{ox} \frac{\varepsilon_{SiO_2}}{\varepsilon_{ox}^2} t_{ox}^2\right) + \delta, \quad (1)$$

where V_{FB} is the flat band voltage extracted by the second derivative method, $\phi_{m,eff}$ is the EWF of metal, ϕ_S is the semiconductor WF, Q_f is the interface fixed charges, ε_{SiO2} is the permittivity of SiO_2, ε_{ox} is the permittivity of HfO_2, t_{ox} is its thickness, ρ_{ox} is bulk HfO_2 charge density, and δ is the dipole caused by AlN-IL.

Fig. 1 shows the extracted V_{FB} as a function of HfO_2 thickness. The good linear fit indicates that $Q_f \gg 1/2 . \rho_{ox} . t_{ox}$, namely the parabolic term of Eq. (1), is negligible. The inset is the $C - V$ curves at 1 MHz of three samples with different HfO_2 thicknesses. The flat in depletion region and the same in minimum capacitance of three samples indicate the stability of oxide quality.

Fig. 2(a) shows a schematic Band alignment of Ni/HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ MOSCaps, the fixed charge of AlN-IL induces a dipole between HfO_2 and substrate so there is a discontinuity for the vacuum level at

AlN/$In_{0.53}Ga_{0.47}As$ interface called δ. This discontinuity was observed in Fig. 2(b) when the V_{FB} shifts of 0.18 V in case there is an AlN-IL between HfO_2 and substrate.

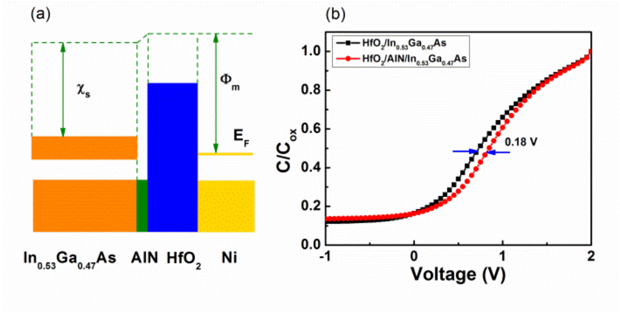

Fig. 2 (a) A schematic band alignment of Ni/HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ MOSCaps; (b) C-V characteristics at 1 MHz of the MOSCaps with and without AlN-IL

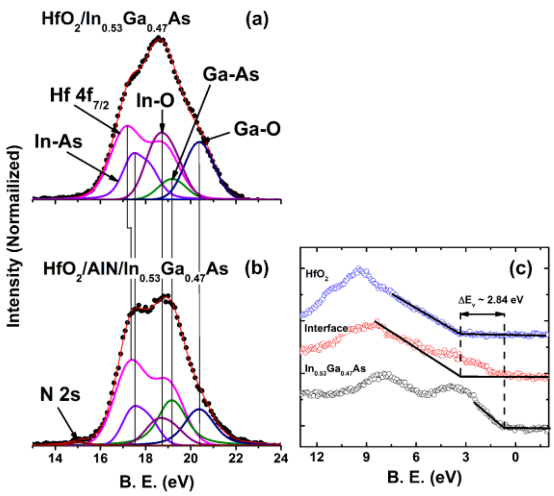

Fig. 3 XPS spectra of $Hf4f_{7/2}$, $In4d_{5/2}$, $Ga3d_{5/2}$, and N2s taken from (a) HfO_2/$In_{0.53}Gas_{0.47}As$ and (b) HfO_2/AlN/ $In_{0.53}Gas_{0.47}As$ interfaces; (c) Valance band maximum (VBM) of $In_{0.53}Ga_{0.47}As$ and ALD-HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ used to extract the valance band offset

To better understand the δ value, the interfaces of both HfO_2/$In_{0.53}Ga_{0.47}As$ and HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ thin films were investigated by using X-ray photoelectron spectroscopic (XPS) in Fig. 3. From the measurement values, the positions of Hf $4f_{7/2}$, In $4d_{5/2}$, In-O, Ga $3d_{5/2}$, Ga-O peaks in Fig. 3(a) are 17.12, 17.40, 18.47, 19.00, 20.2 eV, respectively for HfO_2/$In_{0.53}Gas_{0.47}As$ interface. With AlN-IL in Fig. 3(b), all peaks positions had no change except the increase of 0.20 eV of Hf $4f_{7/2}$ peak to 17.32 eV and the appearance of N 2s peak at ~15 eV. This shift is also in agreement with the shift in V_{FB} due to the dipole $\delta = 0.18$ eV. The relative intensity of In-O and Ga-O peaks significantly decreases in Fig. 3(b) indicate the effects of AlN passivation layer reported in elsewhere [1]. AlN-IL reduced the reactions of In and Ga in substrate to oxygen in HfO_2 leading to the increase of oxygen vacancy in interface, one of the reasons rose Dit. By substituting the value of $\delta = 0.18$ eV into Eq. 1, the EWFs of Ni were obtained $\phi_m = 5.39 \pm 0.04$ eV. These values are higher than that in vacuum and that of earlier report. The reason is the difference between interfaces of HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ with that of HfO_2/SiO_2/Si. This higher of EWF was recently discussed by R. Winter et al when Al was used as gate metal for Al_2O_3/ $In_{0.53}Ga_{0.47}As$ substrate [2]. Fig. 3(c) shows the valance band maximum (VBM) of $In_{0.53}Ga_{0.47}As$ and ALD-HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ used to find valance band offset. Its value was deduced $\Delta E_V = 2.84 \pm 0.1$ eV.

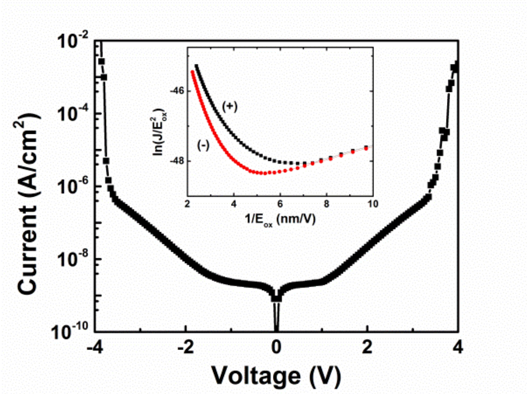

Fig. 4 Current density (J) as a function of gate voltage for Ni/HfO_2/AlN/$In_{0.53}Ga_{0.47}As$ MOSCaps of $t_{ox} = 7.76$ nm, the inset shows the electrical data in term of $\ln(J/E_{ox}^2)$ vs. $1/E_{ox}$

To derive the conduction band offset and electron affinity of HfO_2, the Fowler-Nordheim regime was used [3]. By extrapolating the slop of $\ln(J/E_{ox}^2)$ versus $1/E_{ox}$ shown in the inset of Fig. 4, the conduction band offset and electron affinity of HfO_2 are extracted by $\Delta E_C = 1.89 \pm 0.1$ eV, and $\chi = 2.61 \pm 0.1$ eV, respectively. The extracted values are slightly difference from that of earlier report [4] shows the effects of AlN-IL dipole to band alignment of device. However, by combining with ΔE_V value, the energy band gap of HfO_2 was found in 5.45 eV. This value is in excellent agreement with Chang et al group report [4].

3. Conclusion

In conclusion, the dipole of AlN-IL was derived $\delta = 0.18$ eV. The EWF of Ni was $\phi_{m,eff} = 5.39 \pm 0.04$ eV, while the values of conduction band offset, valance band offset, and electron affinity of HfO_2 were $\Delta E_C = 1.89 \pm 0.1$ eV, $\Delta E_V = 2.84 \pm 0.1$ eV, and $\chi = 2.61 \pm 0.1$ eV, respectively. These results could be used in controlling the threshold voltage of MOS devices.

Acknowledgements

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References

[1] *Quang Ho, L., et al., Electron Devices, IEEE Transactions on, 2014.* ***61****(8): p. 2774-2778.*

[2] *Winter, R., et al., Applied Physics Letters, 2014.* ***104****(20): p. 202103.*

[3] *Olivo, P., J. Sune, and B. Ricco, Electron Device Letters, IEEE, 1991.* ***12****(11): p. 620-622.*

[4] *Chang, Y., et al., Applied Physics Letters, 2008.* ***92****(7): p. 072901-072901-3.*