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NbO as gate electrode for *n*-channel metal-oxide-semiconductor field-effect-transistors

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Niobium mono-oxide (NbO) is investigated as a potential candidate for gate electrode to replace poly-silicon gate in metal-oxide-semiconductor field-effect transistors. NbO was found to have a work function of 4.18±0.05 eV on SiO_2 and to be stable up to 1000 °C with SiO_2 and HfO_2 gate dielectrics. The low work function and high stability make NbO suitable for *n*-channel metal-oxide-semiconductor field-effect transistors devices. The method of deposition is critical during the fabrication to minimize the incorporation of Nb, NbO_2, and Nb_2O_5 which are detrimental to the stability and conductivity of the gate electrode and extra care is needed to avoid further oxidation of NbO. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1759780]

The rapid shrinking of device feature sizes requires a high-κ gate dielectric and metal gate to replace thermal oxide and poly silicon in the near future. In order to satisfy the threshold voltage requirements, the work function of the gate material should be close to the conduction and valence band for *n*-channel metal-oxide-semiconductor field-effect transistor (NMOSFET) and p-channel metal-oxide-semiconductor field-effect transistor, respectively.[1] To qualify as a gate electrode, the material must be stable during the process at high temperatures. Only a limited number of materials satisfy the criteria for a gate electrode, and the low work function requirement for NMOSFET is one of the most difficult to meet.[2]

One approach to achieve a low work function metal gate is to vary the concentration of one component in a binary alloy, such as Ta in $RuTa_x$ and N in MoN_x.[3,4] However, when the work function of these alloys is targeted to below 4.3 eV, the thermal stability tends to deteriorate quickly. Currently, no viable candidate material with the targeted 4.2 eV work function for NMOSFETs has been demonstrated. In this work, we report our findings on NbO and how it satisfies many of the stringent requirements as a gate metal candidate for NMOSFET.

Fully oxidized niobium oxide (Nb_2O_5) has been extensively studied as an alternative candidate to replace SiO_2 as gate dielectric in complementary metal-oxide-semiconductor (CMOS) devices,[5] and as a cathodic electrochromic material for application in solar energy management, display devices, and sensors.[6] Partially oxidized niobium (NbO_x with x from 1 to 2) was studied as a variable resistor in superconducting circuits.[7] Due to the exothermic nature of reactions for NbO to be further oxidized to form NbO_2 and Nb_2O_5,[8] the methods for NbO deposition are severely limited and published reports on Nb mono-oxide are rare. Many methods have been used to deposit niobium oxides but reactive sputtering is so far the only method used to produce NbO films.[9,10] Pulsed laser deposition is another possible technique to deposit NbO, although it is not suitable for mass production.[6]

In this study, NbO films are sputter deposited in a dc magnetron sputtering system at room temperature using a Nb (purity 99.95%) target and a mixture of Ar and O_2 gases. Ar and O_2 gas are separately controlled by mass flow controllers and the total gas pressure during film deposition is maintained at around 6 mTorr. It is reported that for reactive sputter deposition of metal-oxide films at low temperature, the condition of the sputter chamber has a big influence on the film composition,[11] and it is definitely so for NbO deposition. The resulting composition of the NbO_x film is found very sensitive to chamber condition and it is an important step to condition the chamber before the film deposition. Fine control of the gas ratio as well as the sputtering power is also crucial to obtain the single phase film. Figure 1 shows the x-ray diffraction (XRD) phase scans of several films deposited under a variety of conditions. By reducing oxygen partial pressure $[P_{O_2}/(P_{O_2}+P_{Ar})]$, and by increasing sputtering power, the oxygen content in the film is reduced sufficiently to eliminate NbO_2 and form predominantly single phase NbO. As-deposited NbO film has small crystal size and higher resistivity; after annealing at 800 °C for 5 min in Ar, the crystal size increased from 2 to 40 nm and resistivity decreased from around 800 $\mu\Omega$ cm to a level of 80

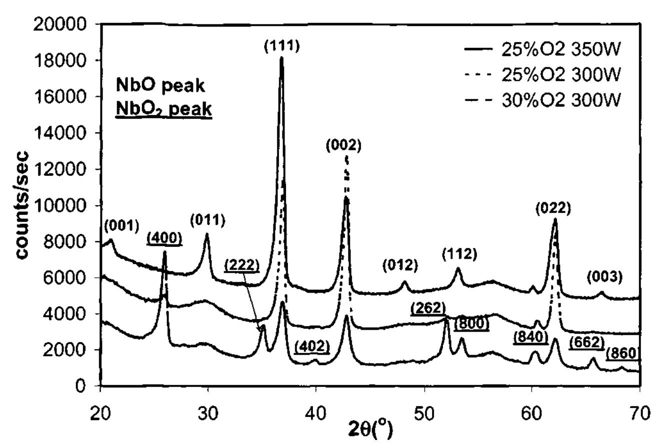

FIG. 1. XRD phase scans of niobium oxide films deposited under different oxygen concentration and sputtering powers. Samples were measured after 800 °C 5 min anneal in Ar.

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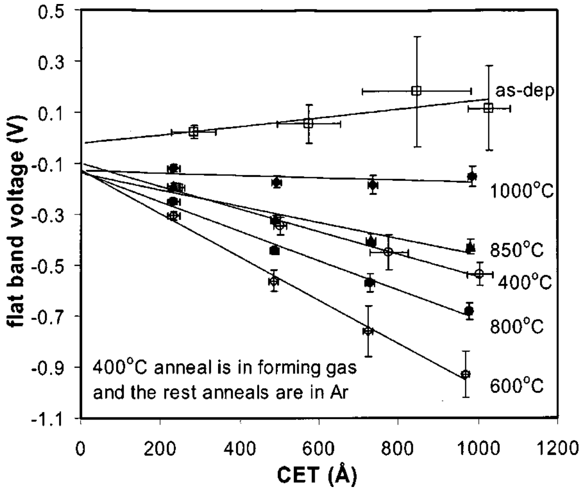

FIG. 2. V_{fb} vs CET for NbO measured over a series of anneals. Gate dielectric is SiO_2 with different thicknesses, error bar in the figure is the cross-wafer variation. Work function value could be extracted from y intercepts.

$\mu\Omega$ cm and is equivalent to those of typical metals.

In order to measure work function, a 160 nm NbO film is sputter deposited on a specially prepared wafer with various SiO_2 thicknesses,[12] photolithographically patterned, and dry etched. A SF_6 and N_2 gas mixture in a Lam 9600 etch tool was used to etch NbO. Good etch selectivity of around 13:1 was seen for NbO on HfO_2 but was poor for NbO on SiO_2 (around 1:2). An e-beam evaporated Nb sample is also made and measured in the same fashion for comparison. *CV* measurements on 100×100 μm^2 capacitors were performed as-fabricated and throughout a sequence of anneals. Figure 2 plots flatband voltage (V_{fb}) *versus* capacitive equivalent thickness (CET) for NbO. The big error bar on the as-deposited state is related to the composition inhomogeneity of the film. The y intercepts of the linear fits for data from various annealing steps are close to each other indicating a stable work function, however, the slope of the line changes throughout the annealing sequence implying changes in effective charge density during anneals.

Figure 3 shows the extracted data from Fig. 2 for NbO and similar data for Nb. Work function of NbO reaches a stable value below 4.2 eV after a 400 °C anneal, while the work function of Nb changes in a bigger range during the

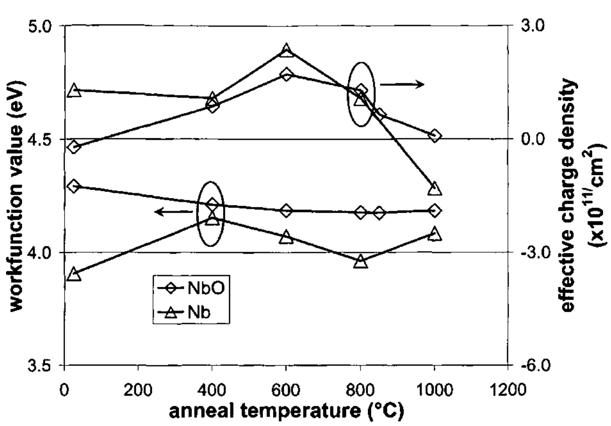

FIG. 3. Work functions and effective charge density change for NbO and Nb over a series of anneals.

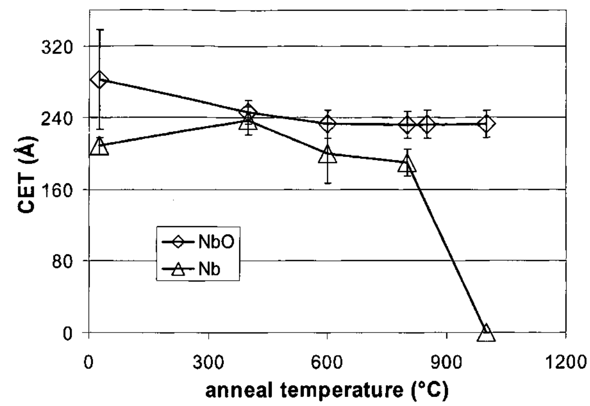

FIG. 4. CET stability of Nb and NbO on SiO_2.

course of anneals. As to the effective charge density, $NbO/SiO_2/Si$ gate stack also shows much more stable property than $Nb/SiO_2/Si$ gate stack during anneals. To further study the interaction when NbO and Nb are in contact with SiO_2, Fig. 4 plotted the CET changes for NbO and Nb on around 24 nm SiO_2 gate dielectrics as part of the work function measurement. It shows that CET values for as-deposited Nb and NbO are different due to the different nature of deposition methods but get very close after 400 °C anneal. After 600 °C anneal, CET for NbO is very stable while CET for Nb continues to decrease, indicating a continuous reaction between Nb and SiO_2. After 1000 °C anneal, the Nb capacitor is shorted.

To test the feasibility of integrating NbO into CMOS fabrication, NbO capacitors on high-*k* gate dielectric were fabricated on 7 nm of atomic-layer-deposition (ALD) HfO_2[13] and CET change is monitored during anneals. It was found from 400 to 1000 °C, CET changed from 3.3 to 3.0 nm with 0.3 nm change happening at 800 °C anneal. We attribute this change to the densification of ALD HfO_2. NbO demonstrates a good stability with HfO_2, and is a potential candidate for future gate electrode application in NMOSFETs.

Traditional self-aligned NMOS transistors were also fabricated. NbO on ALD HfO_2 gate stack experienced 850 °C 5 min anneal for the source/drain implant activation. Anneals were carried out in a rapid thermal processing system with an oxygen free ambient to avoid further oxidation of NbO. Finished device shows a threshold voltage (V_{th}) of 0.75 V, 0.3–0.5 V higher than the expected value. This could be attributed to the charge effect in HfO_2 layer and requires further study.[14,15] Besides the V_{th}, devices show good transport characteristics as well as good uniformity and repeatability across the wafer.

In conclusion, a sputter deposited film of NbO is proposed as a low work function gate electrode for NMOSFETs with a measured value of 4.18 ± 0.05 eV. The sputter conditions are tuned to prevent significant Nb, NbO_2, and Nb_2O_5 content in the film. The NbO gate electrode is stable with gate dielectrics up to 1000 °C anneal and can be etched in conventional etch tools with fluorine based etchants. With HfO_2 gate dielectrics, high etch selectivity is achieved and etch can be stopped at the HfO_2 layer. Our experiment shows that NbO is highly compatible with high-κ HfO_2 gate dielectric and traditional self-aligned device flow.

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