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Calculating area density of Hf atoms by transmit absorption spectra

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Introduction

In this report, X-ray absorption is used to estimate the aera density of Hf atoms in the HfO_2 thin film (<10nm) grown on the fused SiO_2 substrate. To reach this purpose, a commecial Hf solution is employed to be the reference.

Experiment

Film deposition was carried out in an ultrahigh vacuum (7×10^{-8} Pa) radio-frequency (r.f) magnetron sputtering system[2]. A 3 in. metallic Hf (99.9% purity) disc was used as the sputtering target with argon as the plasma-generating gas. Oxygen flow in to be the reacting gas to form HfO_2. Fused SiO_2 substrate is heated to 400°C during the whole deposition process.

Four samples have been measured on the beamline by transmission mode under the exactly same condition: HfO_2/fused SiO_2, blank fused SiO_2 wafer, commercial Hf solution (1mg Hf atoms in 1ml 5%HF solution) in a polymer case which makes the thickness of the solution be 1cm along the X-ray path and, the last one, pure water in the same case to be the blank background of the solution. Special care has been taken to make sure that the X-ray is normally incident to the samples.

Theory and calculation

In transmission XAFS measurement, the experimental spectra is given by

$$\mu_{exp}t=\ln(I_0/I_t) \qquad (1)$$

Where I_0 and I_t are the value read from incident ion chamber and transmit ion chamber, respectively. They could be evaluated by the following equation [1]:

$$I=N_0(1-\exp(-\mu_{gas}(E)x))(E/32eV) \qquad (2)$$

Where N_0 is the total amount of photons per second incident on the ion chamber, E is the energy of photons. $\mu_{gas}(E)$ is the absorption coefficient of the gas in the chamber; x is the length of the chamber, so $1-\exp(-\mu_{gas}(E)x)$ is the photon percentage that the chamber absorbed.

Figure 1 shows the scheme of the transmission XAFS measurement. according to Lambert-beer law, the experimental spectra could be written as:

$$(\mu t)_{exp\_1}=\mu_{HfO2}t_{HfO2}+\mu_{air}t_{air}+\mu_{SiO2}t_{SiO2}-P \qquad (3)$$

Where $P=\ln((1-\exp(-\mu_{tgas}t_{tm}))/(1-\exp(-\mu_{igas}t_{im})))-\mu_{igas}t_{im}$, which keep constant once the measuring condition is determined. Similarly, when the sample is changed to blank fused SiO_2 wafer :

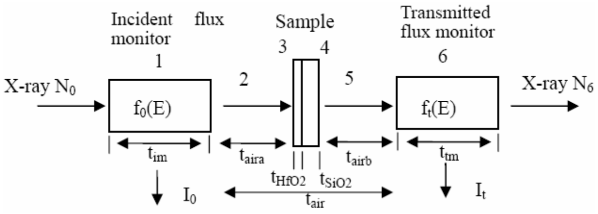

Fig. 1 Scheme for transmission XAFS measurement

$$(\mu t)_{exp\_2}=\mu_{air}t_{air}+\mu_{SiO2}t_{SiO2}-P \qquad (4)$$

So:

$$\mu_{HfO2}t_{HfO2}=(\mu t)_{exp\_1}-(\mu t)_{exp\_2} \qquad (5)$$

Therefore, the absorption of HfO_2 thin film is obtained by the subtracting the blank SiO_2 background. And the height of the K-edge jump represents the area density of the Hf atom in the film. The similar treatment is performed on the reference solution.

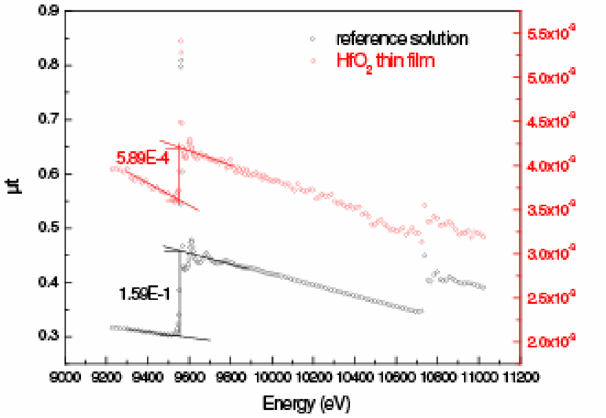

Fig. 2 Absorption of HfO_2 thin film and reference solution The area density of Hf atom in the film is calculated as: 5.89E-4/1.59E-1=3.704E-3mg/cm^2

References

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