NANOGRAVIMETRIC AND PHOTOELECTROCHEMICAL STUDY OF SILICON PASSIVATED BY ULTRATHIN HAFNIUM OXIDE LAYER

E. Juzeliūnas*, P. Kalinauskas, L. Staišiūnas, A. Grigucevičienė, K. Leinartas, A. Selskis

Centre for Physical Sciences and Technology, Saulėtekio av. 3, LT-10257 Vilnius, Lithuania
**e-mail: eimutis.juzeliunas@ftmc.lt*

Hafnium oxide due to its good optical transparency, wide band gap, photoluminescence, high dielectric constant, considerable chemical stability is widely applied in various fields: capacitors, switching memories, field effect transistors, heat mirrors, biomedical sensors, corrosion protective systems for microelectronics and active metals [1-4]. Recently ultrathin HfO_2 layers were studied as promising material to enhance efficiency and stability of organic solar cells. However, a photoelectrochemical (PEC) properties of Si-HfO_2 system are known insufficiently. This study is focused on PEC behavior of p-Si with ultrathin ALD HfO_2 layers in acid perchlorate solution. The quartz crystal nanobalance (QCN) and PEC measurements (illumination: λ = 505 nm and N = 50 mW cm^{-2}) at open circuit were used to assess the dynamics of the electrode mass and photocharging in real time.

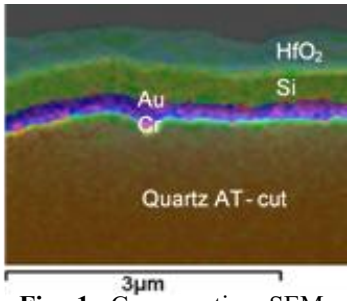

Fig. 1. Cross-section SEM image of the QCN sensor is composed of Cr/Au/Si/HfO_2 layers on quartz

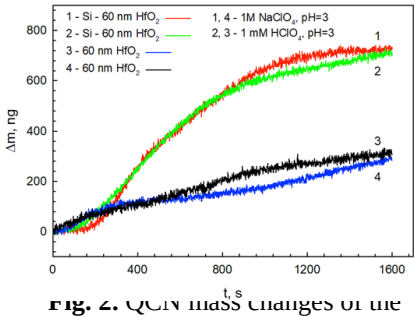

Fig. 2. QCN mass changes of the samples with 60 nm HfO_2 layer on Si (1,2) on Au (3,4) substrates in 1 mM $HClO_4$ and 1 M $NaClO_4$

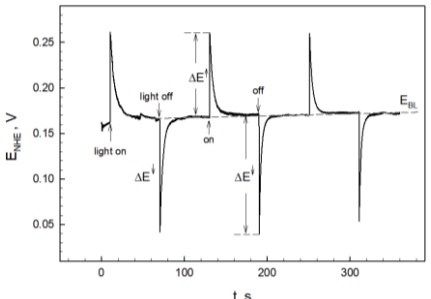

Fig. 3. Photopotential variation at open circuit of p-Si coated with 60 nm HfO_2 in 1 M $NaClO_4$ (pH 3) when illumination is chopped at 1 min intervals

The QCN measurements with HfO_2 film on Si and Au substrates indicated electrolyte intake rate into the oxide film. The differences in a mass variation of Au and Si based samples were attributed to different electrochemical potentials of the substrates. No indications of HfO_2 dissolution were observed. The mass gain effect did not depend on perchlorate concentration. The photo-potential variations of p-Si coated with 10 nm and 60 nm HfO_2 layers showed nearly ideal polarizability; no Faradaic process was induced during the illumination at open circuit. The HfO_2 films also exhibited a high passivation degree of electron transfer to the solution, which was evident from inhibition of the cathodic photocurrents of hydrogen reduction.

Acknowledgement. The research received funding from the Lithuanian Scientific Council under project agreement 1200-PL479

References

1. Hong Yu (Ed.), Hafnium: chemical characteristics, production and applications, South University of Science, Technology of China, Shenzhen, 2014.
2. Fohlerova Z, Mozalev A, Anodic formation and biomedical properties of hafnium-oxide nanofilms, J Mater Chem. B, 7 (2019) 2300-2310; doi.org/10.1039/C8TB03180K.
3. Li M, Jin Z, Zhang W, Bai Y, Cao Y, Li W, Wu D, Li A (2019) Comparison of chemical stability and corrosion resistance of group IV metal oxide films formed by thermal and plasma-enhanced atomic layer deposition. Sci. Rep., 9:10438 (2019); doi.org/10.1038/s41598-019-47049-z.
4. Staišiūnas L, Leinartas K, Juzeliūnas E, Bučinskienė D, Grigucevičienė A, Kalinauskas P, Selskis A, Stanionytė S, Anticorrosion performance of hafnium oxide ultrathin films on AZ31 magnesium alloy. Surf Coat Technol., 397 (2020) 126046; doi.org/10.1016/j.surfcoat.2020.126046.