Oral Presentation

THE EFFECTS OF SHORT-TERM AIR EXPOSURE OF MONOCRYSTAL $HFSE_2$ SURFACE

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One of the ways to improve silicon-based electronics is the integration of silicon with a material that possesses properties such as a sizable band gap (E_g) in the range of 1 - 2 eV and high room temperature carrier mobility (RTCM). $HfSe_2$, which belongs to transition metal dichalcogenides (TMDs) group, is a material that meets these requirements. Predicted RTCM of $HfSe_2$ is the highest among TMDs (3500 $cm^2\ V^{-1}\ s^{-1}$) [1]. Its bulk E_g is 1.1 eV and depends on the number of its layers and on the presence of HfO_2 in its subsurface, which widens the E_g up to 2 eV [2]. Due to the sensitivity of $HfSe_2$ to oxidation and its technological importance in possible future applications, we investigated this process for exfoliated bulk $HfSe_2$ crystal under ambient conditions. Our scanning electron microscopy studies show early oxidation with a rapid increase in the Se-rich blister coverage. X-ray photoemission data reveals diffusion of O atoms into the bulk and HfO_2 formation. Raman spectroscopy results confirm the coexistence of $HfSe_2$ and HfO_2 on the surface. Additionally, we confront the experimental findings with the density functional theory predictions.

[1] W. Zhang, et. al, Nano Res. 7 (2014) 1731–1737.

[2] Q. Yao, et. al, J. Phys. Chem. C, 122 (2018) 25498–25505.

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