

AN ANALYSIS OF OXIDATION DYNAMICS FOR GROUP IV TRANSITION METAL DICHALCOGENIDES

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The reactivity of group IV transition metal dichalcogenides (TMDs) in ambient air offers a unique way for the single–step formation of oxides with high dielectric constant (HfO₂, ZrO₂) directly on the native TMD conducting channel [1]. However, implementing this process in device fabrication requires a thorough understanding of the surface oxidation of those TMDs.

In this study, we determine the oxidation dynamics of bulk group IV TMDs (HfSe₂, HfS₂ and ZrS₂) across the timescale from minutes to weeks, using complementary surface characterization techniques. SEM and AFM reveal fundamentally different morphological features during native oxide growth. While HfSe₂ displays rapid surface modification evidenced by the nucleation of Se–rich blisters, the sulfides (HfS₂ and ZrS₂) develop nanoscale pits over prolonged ambient air exposure. Similarly, Raman spectroscopy reveals that the vibrational modes of HfSe₂ are affected within hours of exposure, while those of HfS₂ and ZrS₂ are not.

To evaluate changes in the chemical composition, we utilized XPS and EDX, which show the progress in formation of transition metal oxides. This study comprehensively describes the oxidation dynamics in the context of chemical composition, morphology and physical property changes in the TMD materials with different surface reactivity. 

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