An experimental study of bulk HfS_2, ZrS_2 and $HfSe_2$ monocrystal surfaces exposed to ambient air

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HfS_2, ZrS_2, and $HfSe_2$ belong to the group IV transition metal dichalcogenides (TMDs). These materials are promising for next-generation electronics due to their tunable band gaps (1–2 eV) and high predicted carrier mobilities at room temperature [1]. While many TMDs are chemically inert, group IV TMDs oxidize when exposed to air. Understanding how this oxidation affects their physical properties and surface morphology is critical for their use in electronic devices.

In this study, we investigate bulk HfS_2 and ZrS_2 monocrystals exposed to ambient air and compare our findings to the observations we made for the oxidized $HfSe_2$ [2]. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) images reveal clear differences in surface morphology: $HfSe_2$ develops characteristic selenium-rich blisters, while the sulfur-based TMDs (HfS_2 and ZrS_2) show the formation of pits with electronic and mechanical properties that differ from those of the surrounding area. Further Raman spectroscopy data reveals that $HfSe_2$ vibrational modes change rapidly due to the ambient air exposure of the material, whereas the vibrational properties of HfS_2 and ZrS_2 remain stable. Finally, X-ray photoemission spectroscopy (XPS) and energy-dispersive X-ray spectroscopy (EDX) show that the sulfur-based TMDs are significantly more chemically stable in ambient air than $HfSe_2$.

These results offer a comprehensive description of the surface oxidation of chosen TMDs, which is crucial in the context of the material selection and technological processing requirements for future group IV TMD-based devices.

Acknowledgements:
The authors acknowledge the financial support of Ministry of Science and Higher Education under project no. 0512/SBAD/6220 and project no. 0512/SBAD/2620.

References

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