Growth, structure and sulfurization of epitaxial $PtSe_2$: towards a Janus transition metal dichalcogenide

Roberto Sant[1]
Maxime Gay[2], Alain Marty[3], Rania Harrabi[4], Simone Lisi[1], Celine Vergnaud[3], Minh Tuan Dau[3], Olivier Renault[2], Johann Coraux[1], Matthieu Jamet[3], Gilles Renaud[4].
[1]*Univ. Grenoble Alpes, CNRS, Institut Néel, 38000 Grenoble, France*
[2]*Univ. Grenoble Alpes, CEA, LETI, 38000 Grenoble, France*
[3]*Univ. Grenoble Alpes, CEA, IRIG/DEPHY/SpinTec, 38000 Grenoble, France*
[4]*Univ. Grenoble Alpes, CEA, IRIG/MEM/NRS, 38000 Grenoble, France*

Abstract

Annealing transition metal dichalcogenides (TMDCs) with MX_2 stoichiometry - M is a metal and X a chalcogen atom - in the gaseous atmosphere of a different chalcogen (Y) precursor is a viable route to form ternary $MX_{(1-x)}Y_x$ alloy compounds [1]. In epitaxial single layer (SL) TMDCs, a careful choice of the process parameters can lead to the substitution of the chalcogen atoms in the top layer but not in the bottom one. These ordered XMY-type alloys are called "*Janus*" after the bi-face Roman god. This configuration breaks the vertical mirror symmetry and introduces an intrinsic built-in electric dipole [2]. We grew SL $PtSe_2$ by direct selenization of a Pt(111) surface in ultra-high vacuum (UHV) and we attempted its conversion into the corresponding Janus SePtS SL TMDC by sulfurization in H_2S gas. We monitored the growth and the sulfurization by combining *in situ* and *operando* synchrotron X-ray surface diffraction (SXRD) and *ex situ* X-ray photoemission spectroscopy (XPS). Depending on the annealing conditions, i.e. temperature and exposition time, the Se-by-S substitution in $PtSe_2$ can lead either to a Janus alloy or to a complete transformation into a sulfide. Most interestingly, the process does not alter the structure of the as-grown $PtSe_2$, which is strongly distorted and pinned to the Pt substrate by a coincidence site lattice – as demonstrated by the quantitative analysis of the diffraction data. Our work suggests a new way of preparation of 2D Janus materials and provides interesting insights about the atomic structure of epitaxially grown 2D TMDCs. By virtue of the chemical asymmetry, Janus SePtS is predicted to exhibit properties such as Rashba effect and/or out-of-plane piezoelectricity, which are forbidden by symmetry in its binary analogues [3].

References

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Figures

Figure: Schematic of the sulfurization process (annealing in H_2S gas pressure) by which SL $PtSe_2$ is transformed into a Janus SePtS compound.