Mapping domains and domain junctions in mono- and multi-layer TMDs using 4D-STEM: toward property controlled 2D device materials

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Despite the increasing interest in 2D material-based devices, synthesized 2D layers generally contain inevitable intrinsic growth-related atomic defects, which are the cause of a discrepancy between the properties measured in synthesized materials and those theoretically predicted from a perfect model system. Among many atomic defects, a grain boundary is one of the dominant structural defects determining the intrinsic properties of 2D materials [1]. Identification of domains and quantitative localization of domain junctions on a large scale have become critical requirements for the development of high quality 2D materials and theoretically modeling 2D material-based device performance.

In this work, we demonstrate multi-scale analytical process using four-dimensional scanning transmission electron microscopy (4D-STEM) that is a new acquisition technique allowing to record a diffraction pattern at each pixel of the electron beam scanning position [2]. The generated 4D-datacubes provide local structural information with high precision and enable numerically reconstructing selected structural information as real space images.

We present here the capability of 4D-STEM techniques for the quantitative investigations of; i) rotational and polar inverted domains in wafer-scale highly oriented epitaxial WS_2 monolayers grown by MOCVD and ii) lateral and vertical distribution of domains in multilayers (>10 MLs) $PtSe_2$ grown by MBE. The position and intensity ratio, arising from dynamic scattering, of diffraction spots are used to identify local orientation and polar direction in monolayer systems [3]. The lateral and vertical distribution of domains in multilayer 2D films is analyzed by combining 3-dimensionally resolved in-plane orientation map and a local stacking quality assessment using moiré signal arising from vertical misalignment in the film. The results are then associated with an in-depth atomic structure analysis which categorizes the type of domain junctions localized in the large scale maps.

Finally, this analytical process will allow to correlate structural configurations, quantitatively resolved from atomic to micron scales, with electric and optical properties, which provide great insights into structure-property relationships in synthesized 2D device materials.

References

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Figures

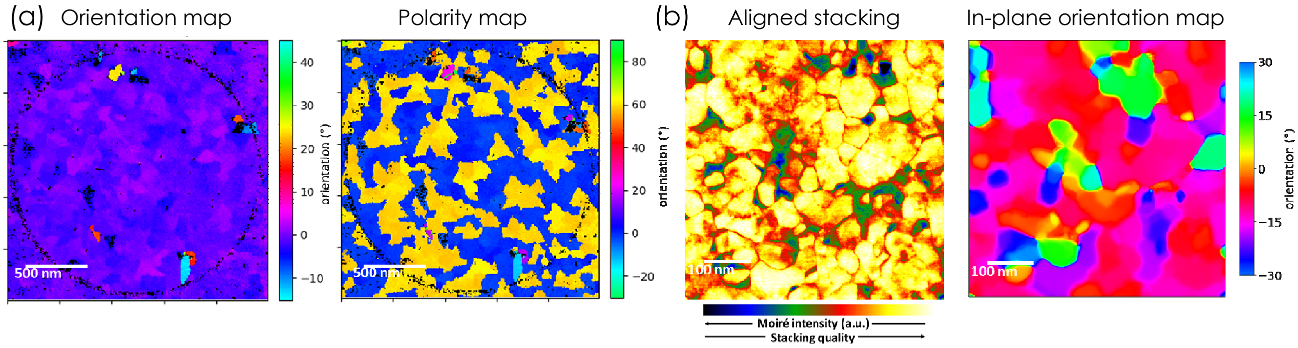

Figure 1: (a) Orientation and polar maps of wafer-scale highly oriented epitaxial monolayer WS_2 [3] and (b) Stacking quality and domain junction map, and 2D orientation map of $PtSe_2$ (>10MLs).