Structure, chemistry and electric field in epitaxially grown 2D layers investigated by 4D-STEM

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Epitaxial growth is a route to achieve highly crystalline continuous 2D layers. Molecular beam epitaxy (MBE) might lead to the formation of well-oriented large crystal with a great flexibility in the choice of the metals, allowing to realize van der Waals (vdW) heterostructures based on transition metal dichalcogenides (TMDs) with the desired configuration. In order to develop and control the synthesis of well-designed complex structures, multidimensional and multiscale structural analysis should be accessible in routine way. X-ray diffraction (XRD) gives a precise information on material quality regarding the crystallinity and the orientation distribution at mm scale, while scanning transmission electron microscopy (STEM) offers today the capability to study the detailled local atomic structures such as vacancies, grain boundaries as well as the associated chemical composition at atomic scale. However these techniques do not reveal complete material characteristiques because of the gap in scale between the information obtained by different techniques. Four dimensional (4D)-STEM is a new acquisition technique allowing to simultaneously record 2D images in real and recoprocal spaces [1]. Multiple information, from structure to electric field [2], at different scales can be reconstructed from signals appearing in diffraction pattern acquired at each pixel of the beam scan.

In this work, we demonstrate the use of 4D-STEM to study epitaxially grown 2D materials. Orientation and 1H-1T' phase maps in WSe_2 monolayers grown on vdW substrates are reconstructed at micron scale and directly correlated with both large scale XRD analysis and related atomic structures. In addition, the distribution of the charge density and the local electrostatic potential were also investigated at atomic scale by measuring the displacement of the centre of mass (CoM) of the transmitted beam. The results show the capacity to construct an overview of synthesized materials from mm scale down to atomic scale with information on structure, chemistry and electrostatic potential to study the growth mechanism and to explore the resulting physical properties.

References

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Figures

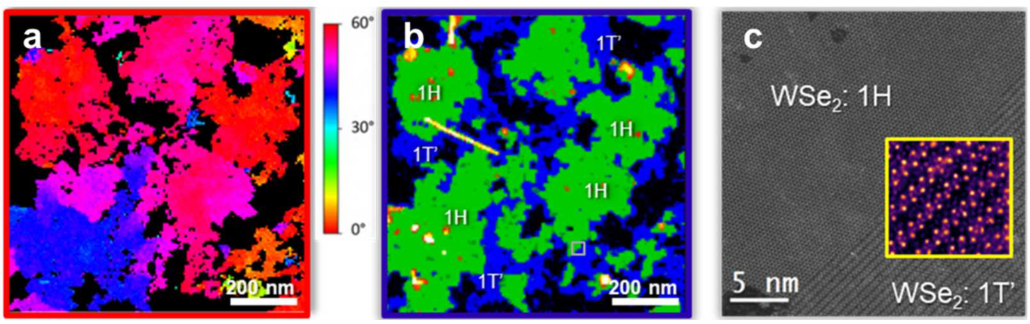

Figure 1: WSe_2 monolayer grown on mica substrate by MBE; (a) orientation and (b) phase maps reconstructed by 4D-STEM and (c) detailed atomic structure at interface between 1H and 1T' phases.