Advanced X-ray diffraction methods for van der Waals epitaxic films

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Potential applications in spintronica and quantum computing are among the reasons that have motivated recent researches in epitaxial films of layered materials with van der Waals (vdW) gap. Bismuth chalcogenide compounds are typical examples of this class of materials with interesting properties as three-dimensional topological insulators (TI). The vdW gaps allow TI films to be growth on a variety of substrates with lattice mismatch ranging from 0.04% to about 20%. The weak nature of the vdW bonds prevent formation of electrically active interface defects such as misfit dislocations, i.e. unpaired covalent bonds at film/substrate interfaces often observed in epitaxy of semiconductors. However, weak vdW bonds between adjacent layers make almost impossible to obtain films that are perfectly coherent to the substrate, even in the case films with very small lattice mismatch. The impact of this absence of coherence on film crystalline quality and electrical properties are subjects of current investigations. In this presentation, we will describe two x-ray diffraction methods developed to address films based on vdW epitaxy. The first method exploits hybrid reflections [1,2] to probe lattice mismatches with astonishing accuracy of 0.002%, which is at least 20 times better than other methods currently available. With this method we can see that even in films where the nominal mismatch is very small, interface coherence depends on the growth parameters. In the other method, experimental and theoretical integrated intensities of asymmetric reflections with different in-plane components are compared to extract values of lateral atomic disorder in the films. Both methods are applied in a series of bismuth telluride films grown as a function of temperature and

additional flux of tellurium by MBE on BaF_2 (111) substrates.

[1] E. H. Smith et al. Appl. Phys. Lett. 111, 131903 (2017).
[2] S. L. Morelhao et al. Appl. Phys. Lett. 112, 101903 (2018).