Strain and defect modulations of electronic structure in transition-metal dichalcogenides

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In 2011, transition-metal dichalcogenides (TMCs) have started their renaissance as potential materials for nano- and opto-electronics due to their extraordinary electronic properties arising from quantum confinement (exfoliation). Though known for over 40 years, bulk 3D TMCs are no threat to traditional silicon-based electronics. The situation has changed in 2011, when Nicolosi and co-workers have shown that 3D TMCs are easy to process using liquid exfoliation and large-area single layers can be produced at low costs. Exfoliation to monolayers changes significantly electronic properties of TMCs. Kis and co-workers utilized this phenomenon and in the beginning of 2011 they produced the first field-effect transistor (FET) based on MoS_2 monolayer. Shortly after, a logical circuits and amplifiers were produced. Silicon-based FETs often suffer from heat dissipation. Therefore, to improve nanoelectronic devices one could replace silicon with materials that perform better at smaller scale, such as layered TMCs.

In this work, we show that electronic properties of TMC layered and tubular materials can be tuned by mechanical deformations (so-called straintronics). Tensile strain applied to the material affects strongly electronic structure and transport properties, resulting in the semiconductor-metal transition for elongations as large as 10%. It also does have a strong effect on the phonon dispersion, causing softening of the in-plane E modes by ~3 cm^{-1} per percent of strain, and of the out-of-plane A modes by ~1 cm^{-1} per percent of strain (see Figure top panel). Hence, Raman spectroscopy qualifies as an excellent tool to monitor tensile tests of TMDs, both in 2D and in tubular forms.[1]

Electronic properties are also strongly changed in the presence of defects, such as point vacancies or grain boundaries (see Figure bottom panel). As in the pristine TMC monolayer transport is almost direction-independent, local defects change the situation completely, reducing conductance in some cases by more than 50%.[2]

References

[1] Ghorbani-Asl, Zibouche, Wahiduzzaman, Oliveira, Kuc, Heine, Sci. Rep., **3**, (2013) doi:10.1038/srep02961

[2] Ghorbani-Asl, Enyashin, Kuc, Seifert, Heine, PRB, **88**, (2013), 245440