MS21 Aperiodic crystals in organic and inorganic compounds and soft condensed matter

MS21-1-5 The incommensurate composite structure of the misfit layer compound  $PbS_{1.12}VS_2$  #MS21-1-5

## C. Antunes Correa <sup>1</sup>, J. Volný <sup>2</sup>, K. Uhlířová <sup>2</sup>, T. Verhagen <sup>2</sup>

## <sup>1</sup>Institute of Physics of the Czech Academy of Sciences - Prague (Czech Republic), <sup>2</sup>Faculty of Mathematics and Physics, Charles University - Prague (Czech Republic)

## Abstract

Transition metal dichalcogenides (TMD) have been attracting attention due to their promising use in photonic [1,2], biological [3], and chemical applications [4]. As an alternative to the standard light-emitting devices (LEDs), which lacks the emission of chirally polarized light at room temperature, TMD semiconductors can be used to obtain intrinsically and controllable chiral LEDs. One of the configurations of chirally polarized LED configurations is the stacking of different types of semiconductors [5]. The whole spectral range from the far-infrared to the ultraviolet can be spanned by creating heterostructures formed by superlattices of two layers of semiconductors. Misfit layer compounds (MLC) [6] intrinsically form a superlattice consisting of stacking of a layer of a transition metal monochalcogenides (TMM) and one of a TMD, with a general composition of  $(MS)_{1+x}TX_2$ , where, M is Sn, Pb, Sb, Bi, or a rare earth element; T is Ti, V, Cr, Nb or Ta; X is S or Se; 0.08 < x < 0.28.

In this work, single-crystals of  $tPbS_{1.12}VS_2$  were prepared by chemical vapour transport, which were measured using single-crystal X-ray diffraction. The crystal structure is an incommensurate composite with alternated stacking of the subsystems PbS and VS<sub>2</sub>, with the stacking perpendicular to the ab plane. The interaction between the sublattices corresponds to a perturbating potential, which causes the modulation of each of the sublattices and, consequently, satellite reflections are present on the diffraction patterns. The crystal structure will be described using the superspace group formalism, where a wave vector **q** is the reciprocal lattice vector **b**\* from the subsystem VS<sub>2</sub> and is a modulation of the subsystem PbS.

## References

[1] Krasnok, A.; Lepeshov, S.; Alú, A. Nanophotonics with 2D Transition Metal Dichalcogenides [Invited]. Opt. Express 2018, 26 (12), 15972. https://doi.org/10.1364/OE.26.015972.

[2] Mak, K. F.; Shan, J. Photonics and Optoelectronics of 2D Semiconductor Transition Metal Dichalcogenides. Nature Photon 2016, 10 (4), 216–226. https://doi.org/10.1038/nphoton.2015.282.

[3] Hu, H.; Zavabeti, A.; Quan, H.; Zhu, W.; Wei, H.; Chen, D.; Ou, J. Z. Recent Advances in Two-Dimensional Transition Metal Dichalcogenides for Biological Sensing. Biosensors and Bioelectronics 2019, 142, 111573. https://doi.org/10.1016/j.bios.2019.111573.

[4] Lv, R.; Robinson, J. A.; Schaak, R. E.; Sun, D.; Sun, Y.; Mallouk, T. E.; Terrones, M. Transition Metal Dichalcogenides and Beyond: Synthesis, Properties, and Applications of Single- and Few-Layer Nanosheets. Acc. Chem. Res. 2015, 48 (1), 56–64. https://doi.org/10.1021/ar5002846.

[5] Withers, F.; Del Pozo-Zamudio, O.; Mishchenko, A.; Rooney, A. P.; Gholinia, A.; Watanabe, K.; Taniguchi, T.; Haigh, S. J.; Geim, A. K.; Tartakovskii, A. I.; Novoselov, K. S. Light-Emitting Diodes by Band-Structure Engineering in van Der Waals Heterostructures. Nature Mater 2015, 14 (3), 301–306. https://doi.org/10.1038/nmat4205.

[6] Wiegers, G. A. Misfit Layer Compounds: Structures and Physical Properties. Progress in Solid State Chemistry 1996, 24 (1–2), 1–139. https://doi.org/10.1016/0079-6786(95)00007-0.