

The misfit layer compound PbSVS₂: a composite structure with twins

Transition metal dichalcogenides (TMD) have been attracting attention due to their promising use in photonic, biological, and chemical applications. 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 controllable chiral LEDs. One of the configurations of chirally polarized LED configurations is the stacking of different types of semiconductors. 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) 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 $(MS)_{1+x}TX_2$. Here, M is Sn, Pb, Sb, Bi, or a rare earth element; T is Ti, V, Cr, Nb, or Ta; X is S or Se; $0.08 \leq x \leq 0.28$.

In this work, single crystals of PbSVS₂ were prepared by chemical vapor transport and were measured using single-crystal x-ray diffraction. The crystal structure is an incommensurate composite with alternated stacking of the subsystems PbS and VS₂, with the stacking perpendicular to the ab plane. The interaction between the sublattices corresponds to a perturbing 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, and I will present the trick behind scenes to elucidate the crystal structure of a composite with twins.

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