A Theoretical Study on Spin-Filter Effect in Layered Materials

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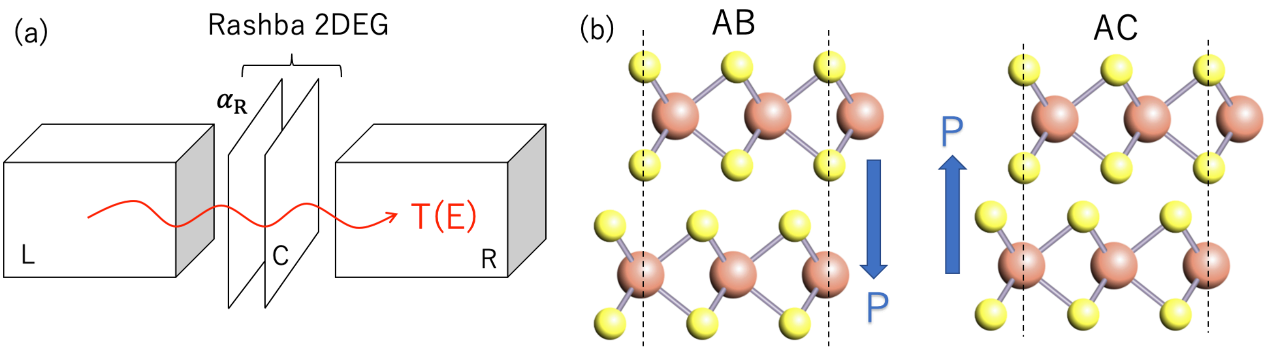
The symmetry of crystals has been deliberately controlled for optospintronic devices. The spin-orbit interaction, which couples the electron's spin and orbital motion, is attracting attention as a key effect in this process. For instance, MoS_2, one of the transition metal dichalcogenides (TMDs), is a direct bandgap semiconductor in a single layer and is characterised by a spin-dependent near-Fermi energy band dispersion. Such materials have quantum numbers that strongly reflect the symmetry of the system due to Rashba splitting caused by the breaking of inversion symmetry. Focusing on this property, we demonstrated the performance of a spin filter through model calculations of systems with Rashba-type band dispersion, as shown in Figure 1(a). The results revealed that the transmission function at the Fermi energy shows strong asymmetry between parallel and antiparallel configurations when the ratio of Rashba parameters in each layer is small.

It is known that polarisations occur in the direction perpendicular to the layers when TMDs are stacked alternately in layers [1]. We applied our previous research results to polarized layered materials and theoretically investigated the spin filter effect in systems with this stacking structure. In the presentation, we will discuss the relationship between the transmission function, band structure, and symmetry based on first-principles calculation results of an electronic device utilizing the polarization of bilayer 3R MoS_2.



(a) Two-dimensional Rashba model、α_R denotes the Rashba parameter. (b) Bilayer 3R Spontaneous polarisation of the AB/AC stacked structure of MoS_2, with opposite electrical polarisation depending on the structure.

Fig1 Model and spontaneous polarisation of the stacked structure of Bilayer 3R MoS_2.

[1] Fei, Z. Zhao, W.Palomaki, T.A. et al. Ferroelectric switching of a two-dimensional metal. Nature **560**, 336–339 (2018).