Defect-related emission spectra of HfS_2

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Transition metal dichalcogenides (TMDs) are two-dimensional layered van der Waals semiconductors have emerged as fascinating materials for exploring novel excitonic phenomena. The main focus of researchers has been focused until now on Mo- and W-based compounds. Recently, hafnium-based TMDs (i.e. HfS_2 and $HfSe_2$), have drawn more attention due to their very effective electrical response, which justifies a need to uncover the basic properties of the materials [1]. The optical emission of the HfS_2 bulk crystal grown by chemical vapor transport method is investigated using the photoluminescence (PL) technique in a broad range of temperature (5-300 K) and magnetic fields up to 30 T. The low-temperature (T=5 K) PL spectrum of HfS_2 comprises several emission lines apparent at around 1.50 eV, see Fig. (a). The overall line shape of the HfS_2 spectrum stays the same at several points of the crystal, on three samples of different origin. Some details of the spectrum vary from point to point with the appreciable energy shifts between thin layers and the bulk. In order to investigate the origin of the observed lines, the helicity-resolved PL spectra were measured in magnetic fields up to 30T (out-of-plane configuration), see Fig. (b). Most observed emission lines split with the effective g factor equal to 2.0±0.1 and are characterized by large quadratic diamagnetic shifts transforming into linear dependences at the highest fields. In contrast, different polarization schemes can be observed with both Zeeman-split and highly polarized lines of similar intensities (A), one polarized, dominant Zeeman-split line (B) or both Zeeman-split components partially polarized (Z). Both theoretical calculations and EELs experiments point to the HfS_2 indirect band gap at the energy of about 2 eV [2]. It is therefore reasonable to attribute the observed emission to yet unknown defect in HfS_2. The possible attribution of the defect is analyzed in the context of the observed PL properties and the features of the growth technology used to produce the crystals.

References

[1] S. Lukman, et al., Nature Nanotechnology, 15 (2020), 675
[2] C. Habenicht, et al., Physical Review B, 98 (2018), 155204

Figures

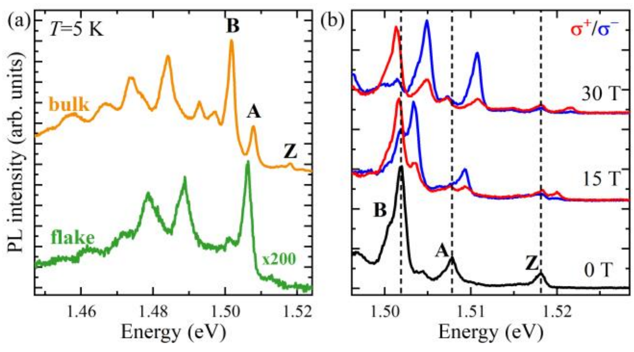

Figure 1: (a) The low-temperature PL spectrum of thin (several microns thick) layer and bulk HfS_2. (b) The helicity-resolved PL spectra of bulk HfS_2 at selected out-of-plane magnetic fields.