Optical properties of hafnium disulfide (HfS_2)

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Hafnium disulfide (HfS_2) belongs to layered materials. It comprises layers of hafnium and sulfur atoms which are bound by much weaker van der Waals interactions. An interest in HfS_2 is driven by its promising electrical properties as its expected room-temperature electron mobility is much higher than in other transition metal dichalcogenides. To unveil basic properties of HfS_2, optical studies were performed at low temperature.

HfS_2 is an indirect bandgap semiconductor. It was therefore rather unexpected to observe at liquid helium temperature a series of emission lines in the energy range of 1.4–1.5 eV [1]. The emission has been attributed to the recombination of neutral and charged excitons bound by the electron-attractive potential introduced by iodine molecules intercalated between layers of HfS_2. The I_2 molecules are introduced during the crystal growth as halogen transport agents in the chemical vapor transport (CVT) growth technique. Their presence in the crystal is confirmed by secondary ion mass spectroscopy. The ability of layered transition metal dichalchogenides to host intercalating molecules is well known. The TMDs comprise layers of tightly covalently bound layers of atoms separated by van der Waals gaps, in which the intercalants can be placed. In the case of halogen molecules, their large electron affinity results in a short range potential attracting electrons from the TMDs layers. The localized electrons interact with optically excited holes giving rise to bound excitons. The excitonic photoluminescence (PL) was observed in several molybdenum/tungsten sulfides/selenides: systems eg: $MoS_2:Cl_2$ [2] or $WS_2:Br_2$ [3].

Properties of the PL from bulk, CVT-grown HfS_2 will be reviewed. Classical statistical analysis of the PL intensity allows to distinguish two groups of transitions in the spectra: main X1 and X2 lines followed at lower energies by their replicas involving acoustic and optical phonons. The X1 and X2 emission lines are related to neutral and charged excitons. They combine conduction and valence band carriers in HfS_2, which are bound by the iodine molecule potential.

The effect of magnetic field on the investigated PL will also be reviewed.

[1] N. Zawadzka et al., Appl. Phys. Lett. **122**, 042102 (2023)

[2]. L. Kulyuk, et al., Phys. Rev. B **68** (2003) 075314.

[3]. L. Kulyuk, et al.,Phys. Rev. B **72**, (2005) 075336.