Optical properties of ReS₂ single crystals doped with Nb

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Bulk rhenium disulphide is direct band gap semiconductor belonging to the family of transition-metal dichalcogenides (TMDs). Unlike other TMDs such a MoS_2 , $MoSe_2$ and WSe_2 , it crystallizes in distorted structure of triclinic symmetry [1]. Re atoms in each monolayer are displaced from the centre of octahedral coordination units forming zigzag chain along the b-axis. Lattice distortion leads to the anisotropy of optical and electrical properties in van der Waals plane. Furthermore, in ReS₂ the band renormalization is absent and bulk behaves as decoupled monolayers.

In this work, we focus on the optical properties of pure and Nb-doped ReS_2 single crystals. They were grown directly from the composite elements (Re: 99.99% pure; S: 99.999%) by the vapor transport method using I₂ as transport agent. To obtain nominal concentration 1-5% of Nb, the weight of doping material was determined stoichiometrically.

We performed systematic Raman scattering investigation on a series ReS_2 single crystals. In Raman spectra we observe 11 active modes in the range 100-400 cm⁻¹ for all contents of Nb. These Raman peaks are caused by low symmetry of the crystal and they are mixing of in-plane and outof-plane motion of Re and S atoms (Eg, Ag). However, certain modes have characteristic behavior. The Raman peaks at 149.4, 159.5 and



Fig.1 (a) Raman spectra measured under different configuration, (b) unpolarized Raman spectra (c) Raman spectra measured as a function of angle in relation to b-axis in $Z(XX)\overline{Z}$ configuration.

211.2 cm⁻¹ have different polarization tendencies and become prominent under certain configurations: $Z(XX)\overline{Z}$ or $Z(XY)\overline{Z}$ (Fig. 1a). Furthermore, they are strongly polarized both along and perpendicular to b-axis of the crystal (Fig.1c). Additionally, we conducted polarizationresolved photoluminescence measurements for varied power excitations in the range temperatures from 10 to 160 K. At 10 K the PL spectra reveal two, well resolved peaks X₁ and X₂ at 1.556 eV and 1.585 eV as well as two additional prominent features at higher energy side X₃ and X₄, at 1.636 eV and 1.647 eV, respectively. Our results confirmed a strong, opposite polarization dependence of low energy excitons: the X₁ is not allowed for light polarized perpendicular to b axis, whereas the X₂ is not allowed for light polarized along the b-axis. In contrast, higher excitonic transition detected at 1.556 eV is only weakly polarized. [1] Tongay S. et al, *Nature Comm.* **5**, 3252 (2014).