Comparative optical studies of ReS_xSe_{2-x} alloys

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Bulk ReS_2 and $ReSe_2$ are both direct band gap semiconductors belonging to the family of transition-metal dichalcogenides (TMDs). Unlike other TMDs such as MoS_2 or $MoSe_2$ they crystallize in a distorted structure of triclinic symmetry. The rhenium atoms in each layer are displaced from the centres of octahedral coordination units, forming a zigzag chain along the *b*-axis. The resulting lattice distortion leads to anisotropy of optical and electrical properties in the van der Waals plane. Furthermore, ReS_2 lacks band renormalization and the bulk behaves as decoupled monolayers, making bulk ReS_2 crystals an ideal platform to investigate exciton and phonon physics in two dimensions.

The ability to tune physical properties of ReS_2 is of great importance from both scientific and technological points of view. In particular, lattice defects and impurities may be exploited to change its electronic and optical properties. In this work, we focus on the optical properties of mixed crystals ReS_xSe_{2-x} ($0 \leq x \leq 2$). Additionally, we explore the effects of doping of pure members of this series with Nb. The samples were grown directly from the constituent elements (with respective purities: Re – 99.99%, S – 99.999%, Se – 99.999%) using the vapor transport method (CVT). To obtain nominal Nb concentration of 1-5%, the weight of doping material was determined stoichiometrically.

We conducted polarization-resolved photoluminescence measurements of the ReS_xSe_{2-x} series for varied excitation powers, in the range of temperatures from 16 to 100 K . The band gap energy varies smoothly with the composition *x*, indicating that the nature of the excitons is similar for all pure members of the ReS_xSe_{2-x} series. At 16 K the photoluminescence spectra of ReS_2 and $ReSe_2$ reveal two, well resolved excitonic transitions (X_1 and X_2) with opposite linear polarization dependence. The peak X_1 at lower energy is not allowed for light polarized perpendicular to the *b*-axis, whereas the X_2 is not allowed for light polarized along the *b*-axis.

We have also performed systematic Raman scattering measurements over the entire range of composition *x*. In Raman spectra of the pure members of the series we observe at least 12 active modes. Such high number of Raman peaks is caused by the low symmetry of the crystals and they involve mixing of in-plane and out-of-plane motion of the Re and S (Se) atoms.