Optical properties of $MoTe_2$ monolayers in various dielectric environments

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Molybdenum ditelluride ($MoTe_2$) belongs to a broad family of widely studied transition-metal dichalcogenides (TMDs) with several well recognizable members: MoS_2, $MoSe_2$, WS_2, and WSe_2. However, the properties of $MoTe_2$ are still not very well known, and ongoing research continuously uncovers the exciting physics of this material. The bulk $MoTe_2$ can be synthesized in semiconducting 2H as well as semimetallic 1T' phases and the transition from one to the other with application of a relatively small tensile strain has been observed. From the optical applications point of view 2H-$MoTe_2$, in its multi-layered form, is an indirect bandgap semiconductor with the gap energy of E_g ~0.93 eV (~1300 nm). Transition to the direct bandgap material with the E_g ~1.1 eV (~1130 nm) occurs when $MoTe_2$ is thinned down to a single monolayer (ML). These peculiar properties make the $MoTe_2$ ML and its derivatives interesting candidates for infrared light emitters that can compete with hardly controlled black phosphorus in this spectral region.

In this work, we present the result of first comparative studies on optical properties of mechanically exfoliated uncapped and hexagonal boron nitride (h-BN)-encapsulated MLs of $MoTe_2$ deposited on the Si/SiO2 substrates. The Raman spectroscopy confirms the presence of a single layer of $MoTe_2$ in the investigated structures by revealing the lack of the B^1_{2G} mode that exists in a few-layer-thick material. High spatially-resolved photoluminescence (PL) experiments at T=4.4 K show two inhomogeneously broadened emission bands near 1.1 eV attributed to recombination of neutral (X) and charged (T) exciton states. The reflectivity contrast (RC) experiment is consistent with the suggested assignment of those optical transitions. Interestingly, h-BN encapsulation of $MoTe_2$ strongly affects considered transition energies, as well as the trion binding energy - the redshift of the exciton transition band of h-BN/$MoTe_2$/h-BN is observed in respect to the non-encapsulated ML and the trion binding energy is reduced by ~5 meV. These differences in optical properties between uncapped and h-BN-encapsulated $MoTe_2$ MLs are most likely related to the modification of the dielectric environment – which affects free-particle bandgap and exciton binding energy – as well as to the apparent changes in the Fermi energy that influences the many-body interactions.

The temperature-dependent PL experiment let to examine the stability of X and T complexes in both structures and revealed similarities between them. While exciton emission is observed between T=4.4 K and 300 K, the T emission tends to vanish above 80 K. Careful analysis of temperature evolution of the exciton energy and its spectral broadening allowed to extract a set of relevant parameters, giving an insight into exciton-phonon coupling strength in both structures. Finally, the time-resolved photoluminescence experiment confirmed that exciton and trion decay is very short and its dynamics can be faster than the resolution of the setup (less than 2-3 ps).

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