

The optical properties and the interference effects of monolayer WSe₂ exfoliated on hBN/SiO₂/Si substrates

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Thin films of hexagonal boron nitride (hBN), due to its layered structure and insulating properties, are widely used as weakly interacting substrates for transition metal dichalcogenides (TMDCs). It has been shown that encapsulating monolayers (ML) of the TMDC in hBN can efficiently suppress inhomogeneous broadening of the exciton linewidth on account of reduction of influence of the environment on material properties. Beside those obvious advantages of using hBN in TMDCs heterostructures, there are other unexplored effects that influence their optical properties.

In this work, we present detailed experimental studies of the optical properties of monolayer WSe₂ exfoliated on hBN/SiO₂/Si substrates along with numerical simulations of the interference effects. We performed photoluminescence (PL) and Raman scattering measurements of monolayer WSe₂ exfoliated on hBN/SiO₂/Si heterostructures with more than 20 different thicknesses of hBN and SiO₂ thicknesses equal 200 nm and 300 nm. From the experimental results we found that hBN thickness has strong impact on intensity of the PL and the Raman signals. Enhancement factors of those signals, resulting from interference effects, have been modeled theoretically using transfer matrix method. Calculations of enhancement show that intensity of emitted signal strongly depends not only on hBN thickness, but also on the underlying SiO₂ thickness (d_{SiO_2}), as well as on excitation (λ_0) and emission wavelengths (Fig. 1). Calculated factors are in very good agreement with obtained experimental values. Enhancement factor maps show impact of hBN thicknesses and excitation wavelength on emission intensity. The highest emission intensity, in the wavelength region of interest, is obtained for specific excitation wavelength and hBN thickness.

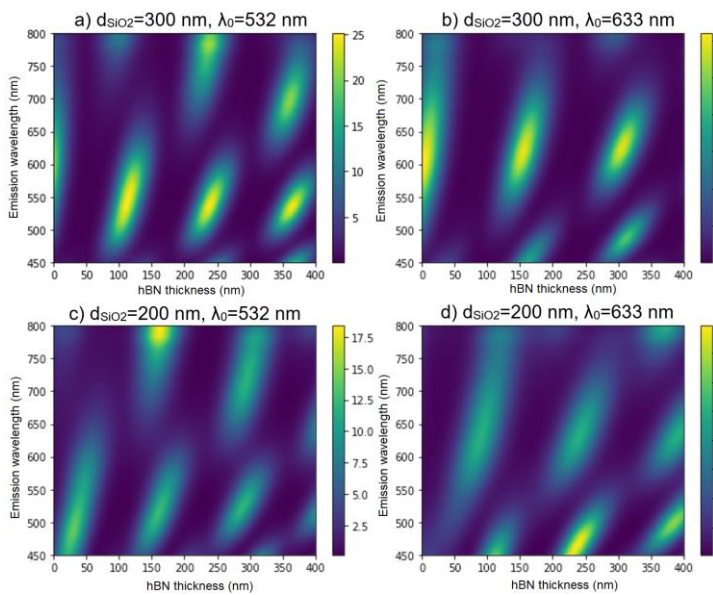


Fig. 1. Enhancement maps calculated for the stack of WSe₂/hBN/SiO₂/Si for the following parameters: a) $d_{\text{SiO}_2}=300$ nm, $\lambda_0=532$ nm, b) $d_{\text{SiO}_2}=300$ nm, $\lambda_0=633$ nm, c) $d_{\text{SiO}_2}=200$ nm, $\lambda_0=532$ nm, d) $d_{\text{SiO}_2}=200$ nm, $\lambda_0=633$ nm.

Additionally, we have found the impact of hBN thickness on the shape of the PL spectra of WSe₂ monolayers which cannot be explained by the interference effects. At room temperature we observe in PL spectra of WSe₂/hBN heterostructures lines below exciton and trion emission which we attribute to localized excitons. Our results show that different dielectric environments of the WSe₂ monolayers leads to the reduction of the both energy gap (E_g) and Coulomb binding energies (E_b).