Impact of hBN-encapsulation on light absorption in 2D-TMD-based photodetectors

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INTRODUCTION

Although the impact of encapsulation ([1]) on electronic properties of monolayer (ML) Transition Metal Dichalcogenides (TMDs) has been addressed in several theoretical and experimental studies ([2], [3]), the assessment of the impact of hBN encapsulation and its van der Waals (vdW) gaps on light propagation and absorption in stacked structures is still pending. To do so, we have adapted and compared several models for light propagation through stacked materials covering a variety of approximation levels, applying them to the light absorption of an hBN-encapsulated ML MoS_2.

DISCUSSION

The impact hBN encapsulation has on the light absorption of MoS_2 is analyzed considering several models for light propagation: from the most simplistic treatments based on the Beer-Lambert (BL) law, that only considers reflection due to the most superficial coating layer, up to the Transfer Matrix Method (TMM), accounting the propagation of normal EM fields, including both multiple reflections and spatial interferences. Moreover, intermediate approximations like Incoherent Path Sum (IPS), that takes into account multiple reflections in each layer but neglects upwards transmission, and Incoherent TMM (ITMM), which assumes spatial incoherence are also discussed. Fig. 1 provides a graphical illustration of each method. The layered nature of the 2D materials is taken into account in the light propagation by the inclusion of the vdW gaps and the reflections originated by them. First, we have compared the propagated energy flux along an hBN-encapsulated ML MoS_2 with two stacks of 20 hBN monolayers for a wavelength $\lambda_0 = 561$ nm. The multiple reflections and interference have a strong impact on the overall intensity inside the material layers, as depicted in Fig. 2.

We have next analyzed the normalized absorption, i.e. the number of absorbed photons in the ML MoS_2 (N_{abs}) with respect to the total number of incident photons (N_0) as a function of the top (n_t) and bottom (n_b) hBN layers for $\lambda_0 = 561$ nm (Figs. 3 and 4). For BL, N_{abs} only changes when a top dielectric layer of hBN is included, as it enhances the optical coupling between air and MoS_2. No reflections at inner interfaces are included, so vdW gaps are not relevant for this model. For IPS and ITMM, vdW gaps generate additional reflections that reduce the magnitude of propagated light intensity. IPS does not include upward transmissions between adjacent layers. However, these paths, included by ITMM, do not seem to contribute substantially to the net result. TMM, on the contrary, evidences the importance of spatial coherence in this multilayered structure but the effect of varying the thicknesses of the encapsulating layers is rather weak due to how thin these are (6-7 nm at most).

On the other hand, the absorption rate predicted by TMM is very sensitive to the substrate thickness t_s due to interferences. The role of this parameter has been studied in the visible range, in Fig. 5. Tuning t_{s} can increase N_{abs} in more than one order of magnitude thanks to constructive interferences at ML MoS_2. TMM predicted absorption as a function of t_s for two different wavelengths is presented in Fig. 6, evidencing the periodic nature determined by the ration λ/t_s.

CONCLUSION

We have evaluated the impact of hBN encapsulation on the absorption of ML MoS_2 demonstrating that while vdW gaps have a strong effect on light propagation for models assuming incoherence, they affect in less than 1% to the result predicted by TMM. Interference has a noticeable relevance when thin layers are considered, so TMM stands out as the most appropriate method for characterizing light absorption in optoelectronic devices.

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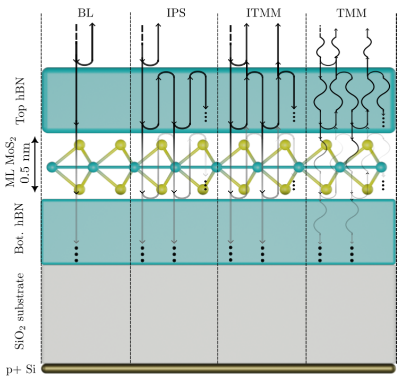

Fig. 1. Sketch of the stacked structure considered. The arrows represent the behavior of light beams according to each model.

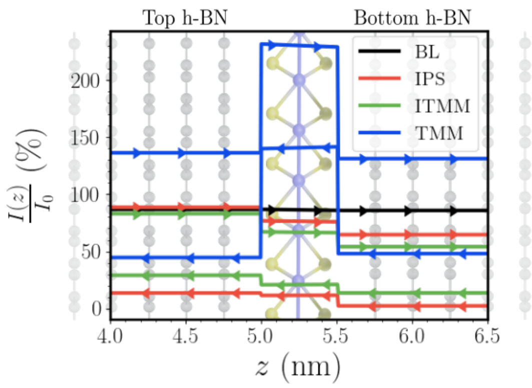

Fig. 2. Net forward and backward propagated energy flux vs. depth in the active region for $\lambda_0 = 561$ nm. Multiple reflections and interference have strong impact on the overall intensity inside material layers. vdW gaps were not included for the sake of clarity, and $n_b = n_t = 20$ and $t_s = 270$ nm were used.

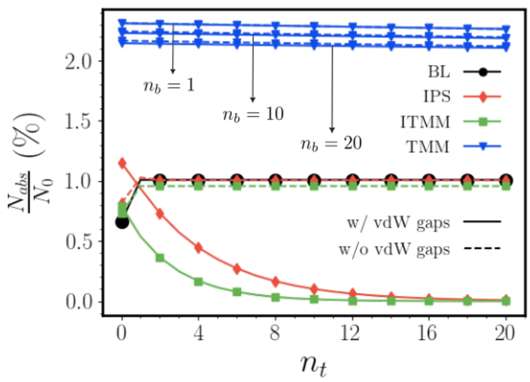

Fig. 3. Photon absorption rate vs. number of top hBN monolayers calculated with each model. For BL, IPS and ITMM, these curves correspond to $n_b \geq 1$. A substrate thickness of 270 nm was used.

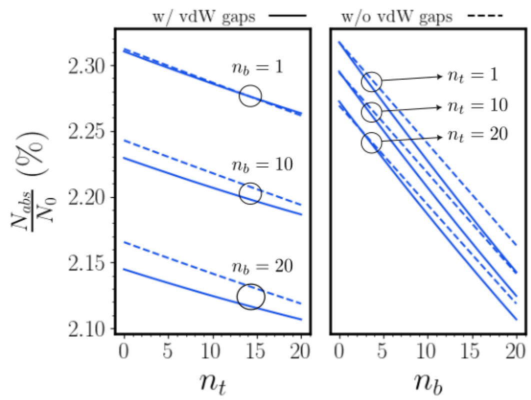

Fig. 4. Absorption rate predicted by TMM for different numbers of top and/or bottom h-BN monolayers, with $\lambda_0 = 561$ nm and $t_s = 270$ nm.

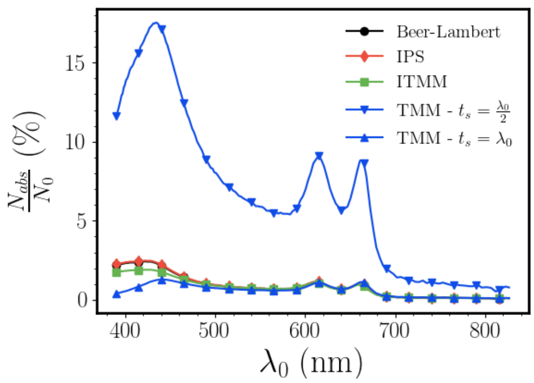

Fig. 5. Comparison of the four models in the visible range. While TMM overlaps with the rest of models for $t_{\text{subs}} = \lambda_0$, it approaches a resonance when $t_s \approx \lambda_0/2$, for which N_{abs} increases in a factor of about 10.

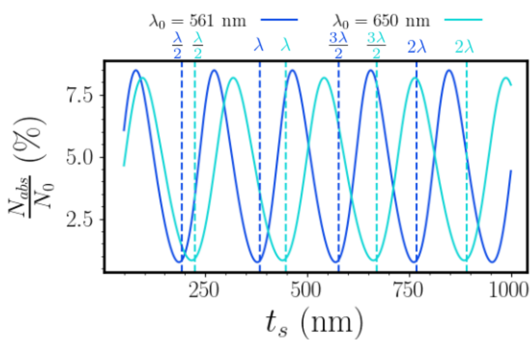

Fig. 6. Normalized N_{abs} vs. t_s for two different wavelengths 561 and 650 nm, according to TMM. The period is $\lambda/2$ in both cases, but resonances do not coincide with multiples of $\lambda/4$ nor $\lambda_0/4$ due to additional phase difference introduced by interfaces.