A rigorous computational framework employing coupled-mode theory for assessing lasing with transition metal dichalcogenide bilayers in the nanoscale

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Abstract. A whispering-gallery mode nanophotonic laser cavity having as active medium a transition-metal-dichalcogenide (TMD) bilayer is examined. The proposed system is analysed and designed utilizing a strict and rigorous computational framework based on the coupled-mode theory. Our framework is capable of accurately and efficiently handling the gain properties of two-dimensional materials, such as contemporary TMD monolayers, multilayers, and heterostructures. The presented lasing cavity exhibits an adequately low pump threshold and light emission in the order of milliwatts is predicted. Exploiting the capabilities of the developed framework, we were in position to efficiently design the cavity as well as to estimate quantitative lasing parameters such as the pumping threshold and the lasing frequency.

1 Introduction

The study of micro- and nano-cavity lasers has attracted significant attention in the past decade due to their compact size, speed, and power efficiency [1]. The initial focus was on Fabry-Pérot and photonic crystal cavities and nano-cavity lasers exhibited notable performance metrics, which strengthened the research interest and led to other alternatives such as plasmonic or whispering-gallery mode cavities. More recently, two-dimensional (2D) materials were found to have interesting lasing capabilities and researchers started to experiment with their interaction with nanoscale systems. Transition metal dichalcogenides consist such a promising family of 2D materials, being capable of light emission in the deep near-infrared (NIR) and in the visible spectrum [2]. Importantly, each alternative TMD monolayer has a different bandgap giving in general flexibility to the design, which is further expanded when bilayers, multilayers, and TMD heterostructures come into consideration [2].

In this work, we present a rigorous computational framework that allows to systematically estimate the lasing characteristics *and* the output of a resonant system while also providing useful guidelines for designing efficient laser cavities. The framework is appropriatelly developed for considering sheet-type materials, respecting their 2D nature. We utilize this framework to analyse the lasing behaviour of an integrated whispering-gallery mode cavity, having as a gain medium a MoS_2/WSe_2 heterostructure (TMD heterobilayer) [3].

2 Coupled-mode theory framework

The proposed framework is based on the temporal coupled-mode theory (CMT) [4, 5], a powerful tool that allows for the accurate prediction of nonlinear systems response in the time domain without resorting to the solution of Maxwell's equations. Linear full-wave simulations are conducted to extract key parameters of the whispering-gallery cavity (resonance frequency, quality factor), which are then introduced in the simpler, time-dependent ordinary differential equations of CMT. The gain mechanism of the 2D bilayer is carefully treated by modeling both the carrier dynamics through an appropriate number of coupled rate equations, and by connecting them with the electromagnetic response of the system via an induced polarization field [4].

Following [4, 5], the cavity amplitude envelope $a(t)$ (assuming it oscillates at ω) is given by

$$\frac{\mathrm{d}a}{\mathrm{d}t} = -j(\omega - \omega_c)a - \frac{1}{\tau_\ell}a - \xi_1\left(\frac{\mathrm{d}p}{\mathrm{d}t} + j\omega_c p\right), \quad (1)$$

and the induced polarization envelope $p(t)$ by

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\omega_m^2 - \omega^2 + j\omega\Gamma_m}{\Gamma_m + j2\omega}p - \frac{\sigma_m}{\Gamma_m + j2\omega}\Delta N a. \quad (2)$$

The cavity (ω_c and $1/\tau_\ell$), gain material (ω_m and Γ_m), and coupling characteristics (ξ_1 and σ_m) are all meticulously included in the framework. The population inversion ΔN emerges generally from a multi-level carrier system, which is also coupled with Eqs. (1) and (2) to correctly encapsulate the various interactions that take place. Our MoS_2/WSe_2 heterobilayer can be modeled by a relatively simple three-level system [3], as schematically depicted in Fig. 1(b). Moreover, in the general case of mismatch between the cavity resonance and the gain peak frequency of the material (i.e., when $\omega_c \neq \omega_m$), the lasing frequency ω_L naturally emerges from the framework by a simple Fourier transformation of the envelope $a(t)$. Additionally, only by making a few simple but rational assump-

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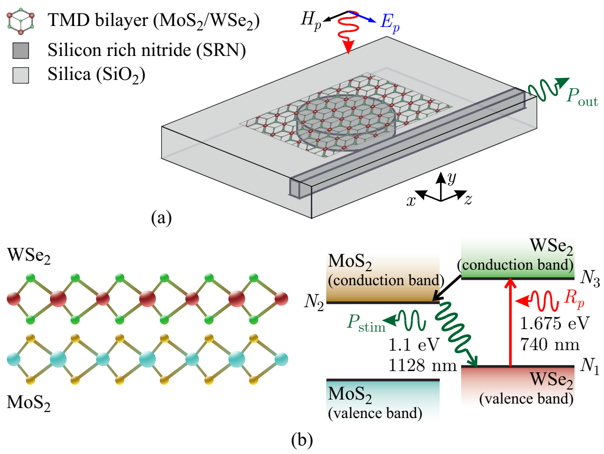

Figure 1. (a) Schematic of the proposed whispering-gallery mode cavity (disk resonator) with the TMD heterobilayer on-top. The vertical pump illumination and the output channel are both clearly marked. (b) Atomic structure of the WSe_2, MoS_2 monolayers and the three-level energy diagram of the heterostructure, which allows for stimulated emission around 1128 nm due to the interlayer excitons formed between MoS_2 conduction and WSe_2 valence bands.

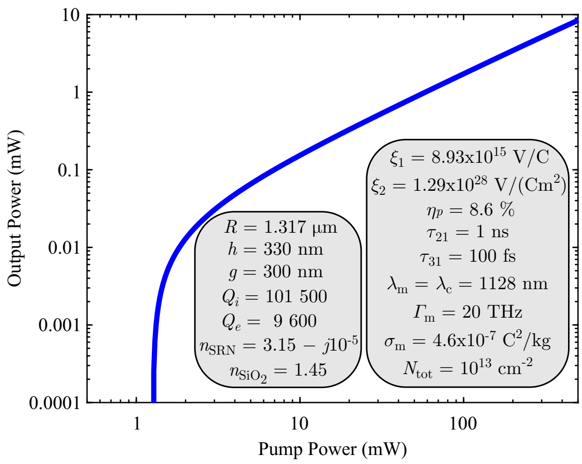

Figure 2. CW lasing output power of the proposed whispering-gallery cavity versus pump power. A low pump threshold of 1.3 mW is achieved and a clear, linear output is observed. The output power saturates for $P_p \sim 10$ W (not shown). Insets: Complete list of the parameters used for the simulation.

tions/simplifications, we are able to get a good estimation of the lasing frequency in a closed-form equation.

3 System design

The practical realization of the envisioned whispering-gallery mode cavity is a silica-cladded, silicon rich nitride (SRN) disk of radius R [Fig. 1(a)]. SRN is chosen for being transparent deep in the NIR where TMDs are able to emit light, in contrast to silicon which starts to exhibit important absorption below 1150 nm. By utilizing the developed framework in the proposed structure, we are able to evaluate that higher order modes with higher quality factors are more beneficial for lasing, despite their weaker interaction with the TMD bilayer. Thus, we opt for a disk with radious $R = 1.317$ μm and a high intrinsic quality factor of $Q_i \sim 101\,500$ (comprising radiation and bulk material ohmic losses). The TMD bilayer is vertically pumped by illuminating with a plane wave at 740 nm, with energy equal to the WSe_2 bandgap. This results in the formation of a vertical Fabry-Pérot cavity and the absorption efficiency is optimized when the height of the resonator is $h = 330$ nm. The structure emits light at 1128 nm due to an interlayer exciton formed between the MoS_2 conduction band and the WSe_2 valence band [Fig. 1(b)]. The emitted light is initially trapped inside the whispering-gallery cavity and then couples to the outside world through a bus waveguide placed near the cavity (300 nm edge-to-edge distance). The respective external quality factor is calculated around $Q_e \sim 9\,600$ since strong coupling between the cavity and the waveguide is desirable.

By solving the system of the ordinary differential equations that consist the developed framework, we are able to calculate efficiently the output power of the laser with respect to the pump excitation. The resulting continuous-wave (CW) output is depicted in Fig. 2. We can readily realize the lasing threshold which is around 1.3 mW. The output power is relatively high, reaching 10 mW for a pumping power of 592 mW. The emission remains linear for a wide pumping range, until starting to saturate for $P_p \sim 10$ W (not shown). The saturated output power is calculated in the vicinity of 120 mW.

4 Conclusion

To conclude, we have developed a rigorous computational framework that is capable of appropriately describing light emission in micro- and nano-cavity lasers with 2D gain materials. Since the framework is well-suited to model the emission from contemporary, sheet-type materials, we have used it to evaluate the performance of a whispering-gallery mode disk-type cavity, combined with a TMD heterobilayer. The proposed system exhibits a lasing threshold of 1.3 mW and emits with a 1.7% efficiency for a wide range of pumping before saturation.

This research work was supported by the Hellenic Foundation for Research and Innovation (HFRI) under the “First Call for HFRI Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment grant” (Project No. HFRI-FM17-2086).

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