

# Design and Analysis of Nano-Scale Resonators to be Integrated with Monolayer Heterostructures

**Brian Bemis**

**Electrical and Computer Engineering, Oregon State University**

**NNIN REU Site: Washington Nanofabrication Facility and Molecular Analysis Facility, University of Washington, Seattle, WA**

NNIN REU Principal Investigator: Dr. Arka Majumdar, Electrical Engineering and Physics, University of Washington

NNIN REU Mentors: Taylor Fryett, Electrical Engineering, University of Washington, and Alan Zhan, Physics, University of Washington

Contact: bemisb@onid.oregonstate.edu, arka@uw.edu, tfryett@uw.edu, azhan137@gmail.com

## Abstract:

Unprecedented material compatibility and unusual optoelectronic properties of single-atom thick monolayer materials have generated strong interest in building devices with them in the recent years. The full potential of such materials can, however, be realized if one stacks such materials, and integrates them with nano-scale resonators to increase the light-matter interaction. However, for this process to be effective with such monolayer heterostructures, specifically the interlayer excitons observed in previous results, the resonator must be able to support a transverse magnetic (TM) mode in order to possess a strong electric field in the direction perpendicular to the monolayer material stack, or the surface of the cavity. This requirement is fundamentally different from resonators designed for single monolayers, where light only with polarization parallel to the surface is effective. In this report, we present a design methodology to build photonic crystal resonators to support TM modes. Previous results used a much thicker geometry for the resonator, which poses a problem for fabrication due to long etching time. Using those as starting designs, using finite-difference-time-domain simulation, we design a cavity with only 250 nm thickness exhibiting TM resonances at 900-950 nm range, the typical wavelength range for the tungsten diselenide ( $WSe_2$ )-molybdenum diselenide ( $MoSe_2$ ) interlayer excitons. Additionally, we present a doubly resonant ring resonator that will be used to enhance the nonlinear properties of monolayer heterostructures.

## Introduction:

Current research involves optical resonators integrated with single two-dimensional (2D) material monolayers [1]. These resonators are stimulated using a transverse electric (TE) mode with light polarization parallel to the cavity surface and in-plane with the single-atom thick monolayer. However, when these monolayers are stacked together into 2D material heterostructures, interesting properties arise [2]. Of these properties, the presence of interlayer excitons [3] and applications to nonlinear optics are particularly noteworthy. In order to interact

with interlayer excitons, it is necessary to use light with a polarization perpendicular to the cavity surface and therefore in the direction of the interlayer excitons, or a TM mode. For our purposes, we are interested in  $WSe_2$ - $MoSe_2$  heterostructures that require a TM resonance at 900-950 nm wavelength range. We report on two designs for optical resonators, scaled to have a TM resonance in this wavelength range. To explore the use of heterostructures in nonlinear optics a doubly resonant ring resonator was designed for future experiments.

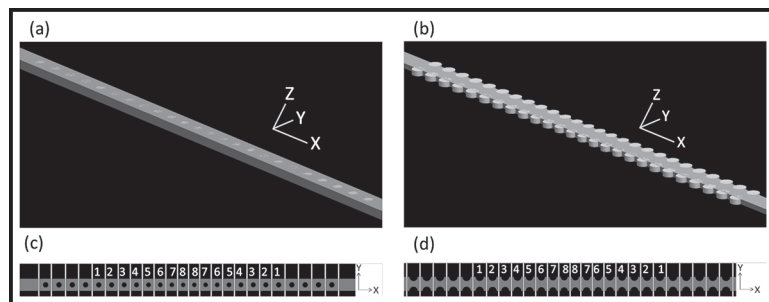


Figure 1: (a) Nanobeam schematic. (b) Fishbone schematic. (c) Nanobeam taper. (d) Fishbone taper.

## Simulation Procedure:

The first design was based on the photonic crystal nanobeam by Zhang, et al. [4]. However, when this design was scaled to have a resonance within 900-950 nm, it was 595.5 nm thick. Such a thick structure is difficult to etch, and in our design, the thickness was reduced to 250 nm and the periodicity was increased by 101.5 nm to be 300 nm, while the width was increased

by 75 nm to become 273.5 nm. The cavity periodicity and radii tapers, respectively, are described by the formulas:  $P(k) = 42(a+101.5 \text{ nm})/(42+k)$  and  $R(k) = 0.34(42a/(42+k))$  where “a” is the original periodicity and  $\{k: 1 \leq k \leq 8\}$  (see Figure 1). Note that the original periodicity was not increased for the radii formula as the radius parameter remained unchanged.

The second design was based on the “Fishbone” version of the photonic crystal nanobeam by Lu, et al. [5]. However, this design also faced similar challenges and was adjusted from a thickness of 370 nm to 250 nm; while the periodicity was increased by 30 nm to become 400 nm and width was increased by 50 nm to become 420 nm. The cavity periodicity and radii tapers, respectively, are described by the formulas:  $P(k) = (1-0.02k)(a+30 \text{ nm})$  and  $R(k) = 0.34((1-0.02k)a)$  where, again, “a” is the original periodicity and  $\{k: 1 \leq k \leq 8\}$ .

The doubly resonant ring resonator was designed for two modes, one at twice the frequency of the other to enhance both the fundamental and the second harmonic frequency. This resonator will be used to explore the application of heterostructures to nonlinear optics. The 330 nm thick silicon nitride (SiN) ring resonator on a silicon dioxide (SiO<sub>2</sub>) base consists of a waveguide with a width set to 1193 nm such that the 1550 nm and 775 nm

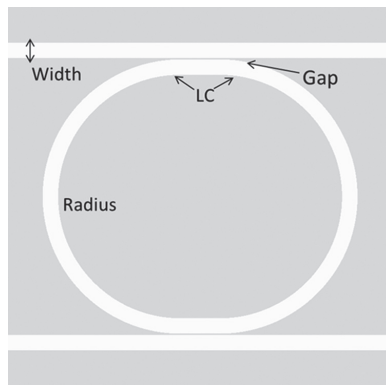


Figure 2: Ring resonator schematic.

modes have the same effective index, giving the modes significant overlap which allows the creation of higher frequency photons. The waveguide was separated by a gap of 100 nm from a 10 μm radius ring with a coupling section length of 3 μm.

## Results and Conclusions:

In summary, three optical resonators were designed to be integrated with 2D material heterostructures.

As evident from the  $E_z$  fields of the nanobeam and fishbone designs in Figure 3, both resonators support a TM mode that will interact with the interlayer excitons in WSe<sub>2</sub>-MoSe<sub>2</sub> heterostructures. The ring resonator's electric field profile exhibits coupling for both modes (see Figure 4).

## Future Work:

Once these optical resonators are fabricated they will be integrated with 2D material heterostructures. Then these devices will be characterized in a confocal microscopy setup to be used in future experimentation.

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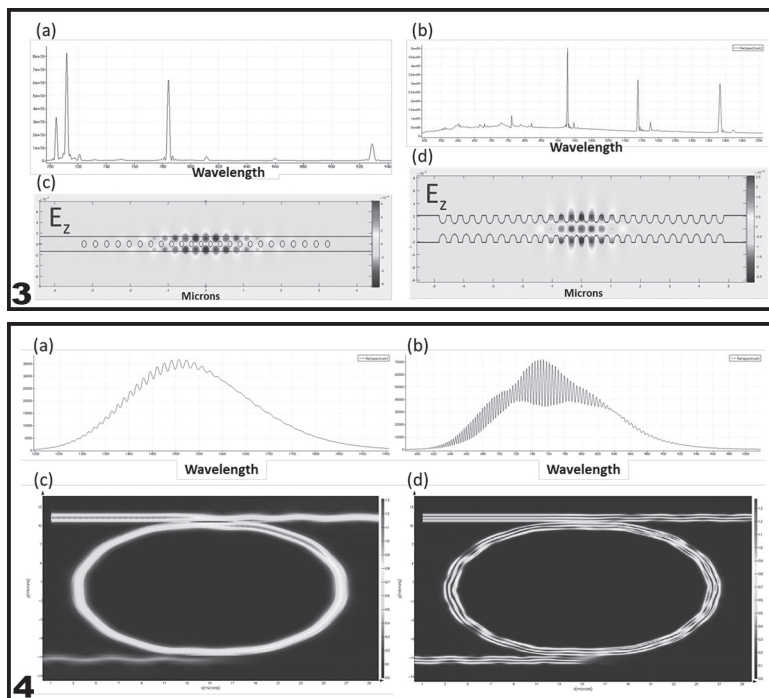


Figure 3, top: (a), (c) Nanobeam spectrum and  $E_z$  field profile. (b), (d) Fishbone spectrum and  $E_z$  field profile. Figure 4, bottom: (a), (c) 1550 nm mode spectrum and electric field profile. (b), (d) 775 nm mode spectrum and electric field profile.