# Defect Grating Simulations: Perturbations with AFM-like Tips

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*A defect grating in a silicon on insulator waveguide is simulated. We consider spectral changes in the optical transmission when a thin silicon nitride or silicon tip is scanned across the defect. The tip perturbs the resonance field, moving its peak wavelength and possibly changing its shape and quality factor. For the nitride tip, the influence is mostly a spectral shift; for silicon, the change of the resonance shape is pronounced. In particular for the nitride tip we observe a close correspondence between the wavelength shift as a function of tip position, and the local intensity in the unperturbed structure.*

## Introduction

Photonic crystals have the property that in a perfect crystal, a band of wavelengths is unable to propagate through the crystal. By introducing defects, extra states can be created which allow light to be transmitted; for example, a row of holes may be removed to create a photonic crystal waveguide. The crystal may be engineered to offer more functionality; for example, an extra defect may be created near or inside the waveguide, which can cause strongly wavelength-dependent behaviour and high local field intensities. These resonances can be very sensitive to perturbations. [1] shows that probing a photonic crystal microcavity by a silicon nitride or silicon AFM (Atomic Force Microscopy)-like tip can cause strong variations in the transmitted power.

In this paper, we perform simulations on a grating with a defect in a two-dimensional silicon on insulator waveguide structure. A very thin silicon nitride or silicon tip is scanned over the surface of the grating, and the transmitted, reflected and scattered powers are analyzed. We will show that there is both a wavelength shift of the resonance and a deformation of the spectrum, and that the wavelength shift can be correlated very well with the local intensity at the location of the end of the tip in the unperturbed structure.

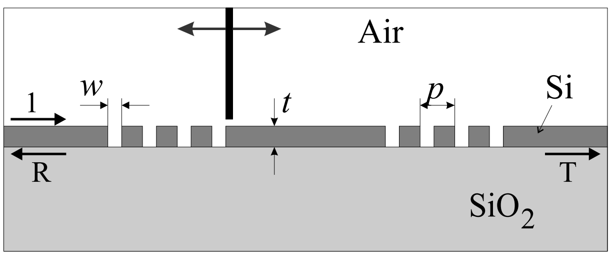


Figure 1: Silicon on Insulator waveguide structure. The refractive indices are: Si - 3.4, $Si_3N_4$ - 2.0, $SiO_2$ - 1.0, Air - 1.0. The waveguide thickness $t$ is 220 nm, the grating hole width $w$ 150 nm, and the grating period $p$ 380 nm. The width of the rectangular perturbing $Si_3N_4$ or Si tip is 40 nm. The defect is four filled holes long (so the length of the waveguide between the inner holes is $(4*0.38+0.23)\,\mu\text{m} = 1.75\,\mu\text{m}$).

Figure 1 shows the waveguide structure under consideration. Simulations are performed by means of a Quadridirectional Eigenmode Propagation (QUEP) method [2]. This method divides the structure into horizontal and vertical slices, and uses eigenmodes of these slices to describe the complete field. The horizontally and vertically propagating fields are coupled at the boundaries of the computational window, such that the boundaries are transparent for outgoing radiation and for influx of the the desired fields.

## Simulations

Into the structure of Figure 1 we insert the guided TE-polarized slab mode from the left, and analyze the transmitted and reflected modal powers $T$ and $R$. Since the waveguide is monomodal, the scattered power $S$ is equal to $1-R-T$. The spectrum of these quantities is shown in Figure 2.

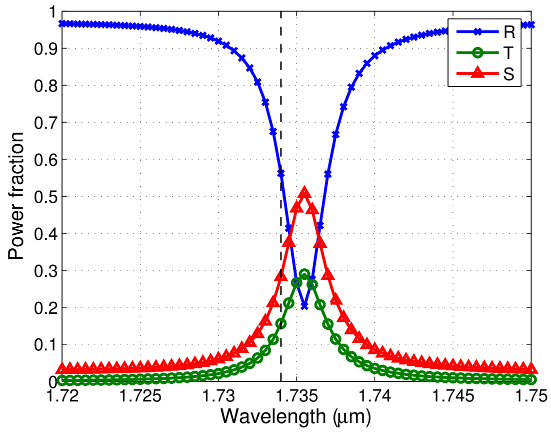


Figure 2: Spectrum of the structure of Figure 1 for unit input from the left; $R$ is the reflected modal power, $T$ is the transmitted modal power, and $S$ is the scattered (lost) power.

In order to make sure the changes due to perturbations are as large as possible, we tune the wavelength to the left flank of the resonance, at 1.734 $\mu$m (the dashed vertical line). At this wavelength, Figure 3 shows the absolute value of the field.

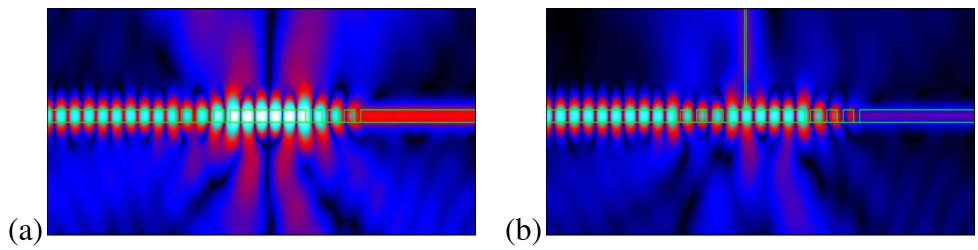


Figure 3: Logarithm of absolute value of the principle dielectric component of the field in the defect grating at a wavelength of 1.734 $\mu$m. a: without tip; b: with silicon tip

A 40 nm wide rectangular silicon nitride or silicon tip is scanned horizontally across the surface of the structure, at a height of 10 nm above the waveguide. The most pronounced perturbation of the resonance occurs when the tip is placed close to the field maxima visible in Figure 3a; Figure 3b shows an example. By evaluating $R$, $T$ and $S$ at each location of the tip, Figure 4 is obtained. The tip switches, or at least modulates, the transmission through the structure. Obviously, the tip moves the transmission further out of resonance (increase of $R$, decrease of $T$ and $S$), with a pattern that relates (nonlinearly) to the local intensity in Figure 3a [1].

[1] At a wavelength of e.g. 1.737 $\mu$m, the opposite effect can be observed; the tip moves the transmission into resonance, and $R$ is decreased while $T$ and $S$ increase.

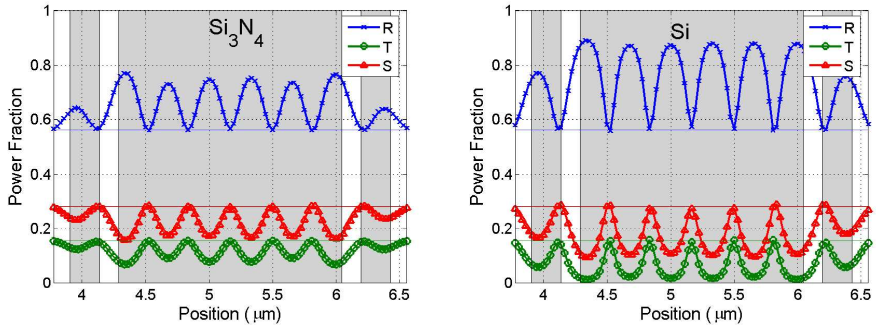


Figure 4: Reflected, transmitted and scattered power as a silicon nitride (left) or silicon (right) tip is scanned over the surface around the central defect (gray patches: high index regions). The horizontal lines denote the values without the tip.

We now look at the spectral properties of the perturbation. In first approximation, we assume that the only effect of the perturbation is a wavelength shift of the resonance. Under that assumption, each of the curves of Figure 4 can be directly related to a wavelength shift by finding the wavelength difference needed in Figure 2 to obtain the altered values of the three powers. These estimations are shown in Figure 5.

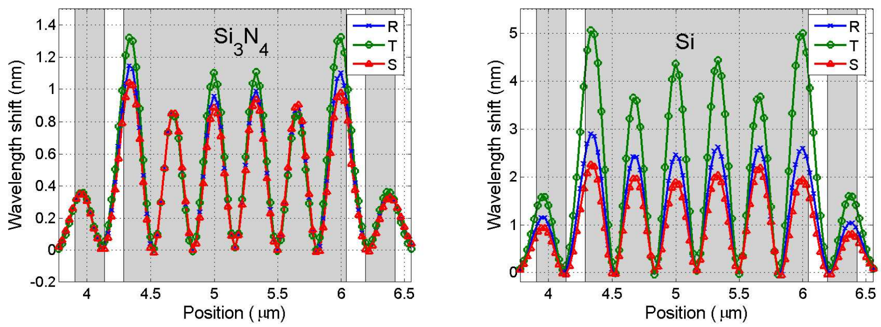


Figure 5: Estimated wavelength shift of the resonance for the silicon nitride (left) and silicon (right) tips; each line is the wavelength shift estimated by only considering the $R$, $T$ or $S$ curve in Figure 4. Note the different scales of the shifts in the two graphs.

If the assumption of a pure wavelength shift would hold, all three curves predicted by the three powers would yield the same resonance shift. For the silicon nitride tip, this is well satisfied at some tip positions; for the silicon tip, the three curves do not agree well anywhere.

As an example, the full spectrum of the structures with the tip at location 4.6664 $\mu$m, which is at the top of the third peak in Figure 5, is shown in Figure 6, and it is indeed clear that the spectrum at this location only shifts for the nitride tip, while it is significantly distorted for the silicon tip; the resonance is broadened and less pronounced.

Clearly, positioning the tip where the field intensity is negligible should not change the transmission. Conversely, at a position with a strong local intensity, a pronounced effect on the transmission and on the spectral properties can be expected. This is investigated in Figure 7, where we - admittedly rather arbitrarily- plot the average value of the estimated wavelength shift from the three curves in Figure 5, as well as the absolute value squared of the local electric field that would be at the end of the tip if there were no tip present.

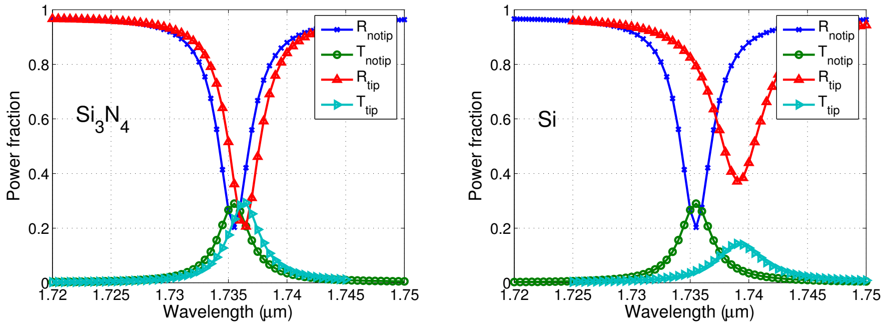


Figure 6: Spectra of the structure without and with a silicon nitride (left) or silicon (right) tip at location $4.6664\,\mu$m.

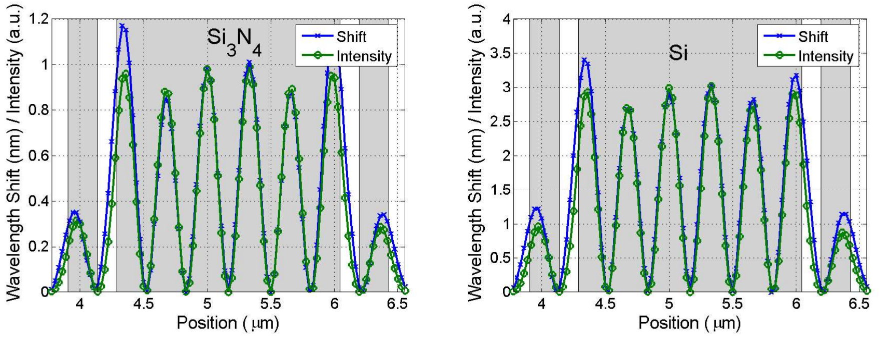


Figure 7: Comparison of the average wavelength shifts of Figure 5 to the intensity in the unperturbed structure; the intensity has been scaled to obtain a good fit. Left: silicon nitride tip; right: silicon tip.

## Conclusions

Two-dimensional calculations show that perturbing a defect grating with a thin silicon nitride or silicon tip shifts the resonance wavelength significantly, and may also perturb the shape (and thus the quality factor) of the resonance. The wavelength shift turns out to be almost directly proportional to the local light intensity at the location of the tip in the unperturbed structure. The silicon tip perturbs the shape of the resonance much more strongly than the nitride tip. These simulations confirm measurements reported in [1].

## References

[1] W.C.L. Hopman, K.O. van der Werf, A.J.F. Hollink, W. Bogaerts, V. Subramaniam and R.M. de Ridder, "Nano-mechanical tuning and imaging of a photonic crystal micro-cavity resonance ", *Optics Express*, vol 14, issue 19, pp. 8745-8752, 2006.

[2] M. Hammer, "Quadridirectional eigenmode expansion scheme for 2-D modeling of wave propagation in integrated optics", *Optics Communications*, vol 235 (4-6), pp. 285-303, 2004.