NARROW BAND EMISSION FROM LITHOGRAPHICALLY DEFINED PHOTONIC BANDGAP STRUCTURES IN SILICON: MATCHING THEORY AND EXPERIMENT*

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ABSTRACT

The authors previously reported discovery of narrow, thermal emission bands from symmetrically patterned features etched into silicon wafers [1]. Emitted wavelengths corresponded to the geometrical size and spacing of the lithographically defined features. In this paper, we report further results that show the measured absorption peaks for such patterned surfaces match theoretical calculations of the complete electrodynamic problem solved using the Transfer Matrix Method (TMM). Calculations were used to optimize pattern geometry to obtain high-power emission in a single, narrow spectral band. Improved experimental performance was achieved with addition of a thin, patterned metal layer on top of the silicon. This more complex geometry was more clearly modeled by including surface plasmon resonances. Data and calculations are presented for variations with feature size, etch depth, substrate resistance, and rounding of feature corners. These results augur a new class of tunable infrared emitter devices with hundreds of milliwatts of power in a narrow spectral bandwidth.

INTRODUCTION

The optical properties of photonic bandgap structures have attracted recent interest. [2,3] When electromagnetic waves with wavelength on the order of the period of the dielectric array propagate through this structure, the light interacts in a manner analogous to that for electrons in a periodic symmetric array of atoms. The structure exhibits allowed and forbidden extended states, a reciprocal lattice, Brillouin zones, Bloch wavefunctions, etc. [4,5,6] These photonic crystals, have been developed as transmission/reflection filters, low-loss light-bending waveguides, and for inhibiting spontaneous emission of light in semiconductors which could lead to zero-threshold diode lasers [7].

Metal grid structures are recognized as spectrally selective filters at microwave, millimeter and far infrared wavelengths [8,9,10] and more recently, at optical wavelengths [11]. One result is that the transmission curves exhibit a relatively narrow bandpass that is related to the geometrical spacing of small features. Secondly, the transmission patterns are accurately predicted by modeling the interactions between surface plasmons and incident photons.

Ion Optics currently manufactures and distributes infrared radiation sources for spectroscopic applications[1]. Our application for narrow line, photonic bandgap sources is their considerable power advantage for portable, battery operated systems compared to existing filtered, broad-band emitters.

EXPERIMENTS and RESULTS

We describe two experiments with matching theoretical calculations. First is a TMM calculation of the electric and magnetic fields surrounding a dielectric (silicon) with a regular periodic structure (crosses etched into the surface) compared to experimental results. The second experiment is a comparison of theoretical and experimental results for a series of square pits etched into a silicon wafer covered with a thin layer of gold. Emittance from this geometry as a function of azimuthal angle is described by the interaction of surface plasmons with photons, keeping in mind that by Kirchoff's law, emittance and absorbance are equivalent.

A pattern of crosses (4.1 microns long, 1.9 microns wide across a leg, with 1.0 micron separation between adjacent crosses) was etched into a thick silicon substrate. Sharp corners of cross pattern were rounded during photolithography of very fine features. Optical properties were measured at room temperature by FTIR(dotted line in figure 1). Reflectance, transmittance and absorbance of the 3-dimensional multilayer stack were calculated using TMM simulations on a multi-processor parallel computing system (Stepped line in figure 1). A coarse grid of 5 THz was used to evaluate the general features.

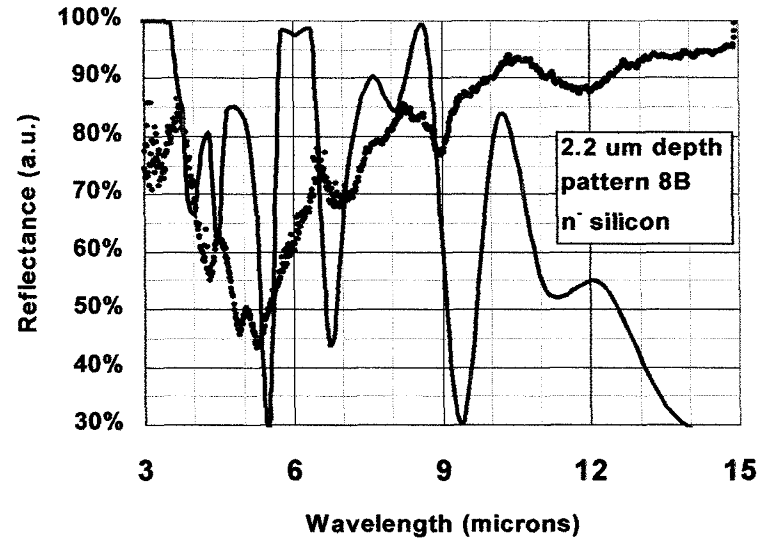

Figure 1 Measured absorption (dots) and calculated (line) data.

Data	Calculation
2.55	4.03
3.20	4.48
5.15	5.50
7.05	6.74
7.80	8.10
8.95	9.38
11.80	11.11

Table 1 Peak Location (µm) For Measured and Calculated Absorption in Figure 1.

Initial calculations showed spectral features at wavelengths shorter than 10 microns. These were found to be due to high frequency resonances resulting from coherent reflections from the wafer's back surface. Back-surface reflections were suppressed in further calculations by gradually changing the index of refraction of silicon from 3.4 to a value of 1 in 36 layers. [In the real world, the back surface of the silicon wafer is as-cut, then etched so reflections are scattered.] This change stabilized the numerical results, with reduced statistical fluctuations.

The calculated results for absorbance were compared to measured data at room temperature (Figure 1). The wavelengths of absorbance maxima in this figure are listed in Table 1. The agreement between experiment and the model is good. Differences are attributed to:

- the calculation computed absorption only every 0.5 microns in wavelength
- calculation used very sharp geometrical figures, experiment had rounded corners
- calculation did not include a reflective surface coating important at long wavelengths

Changing the index of refraction used for silicon in the near front surface region did not change the height nor central wavelength of the largest minima peak; but it did alter the wavelength for the smaller satellite peaks. This shows that the large peak results from a resonance in the low dielectric material (air) while smaller peaks are resonances in the dielectric.

The second experiment used a simpler geometry: etched squares, at varying size and spacing (Figure 2). TMM calculations indicated that this geometry should give a desired singular, large absorbance peak. Samples shown in Figure 2 were etched 5 microns deep. The silicon surface is covered by 500nm of gold. The corners of the pattern are rounded due to diffusion-limited etching during the RIE process. All holes were supposed to be square but the smallest size, 2.0μm lattice spacing, is nearly a perfectly round hole.

Results for room temperature absorbance at normal incidence (bottom) and emittance measured at 325°C (top) are compared in Figure 2. The data imply that preliminary measurements of absorption at room temperature is a good predictor of emission at higher temperatures for the same angle of measurement. Note that the emittance minima at about 4μm in all cases is a measurement artifact caused by absorption in the coupling fiber optic cable.

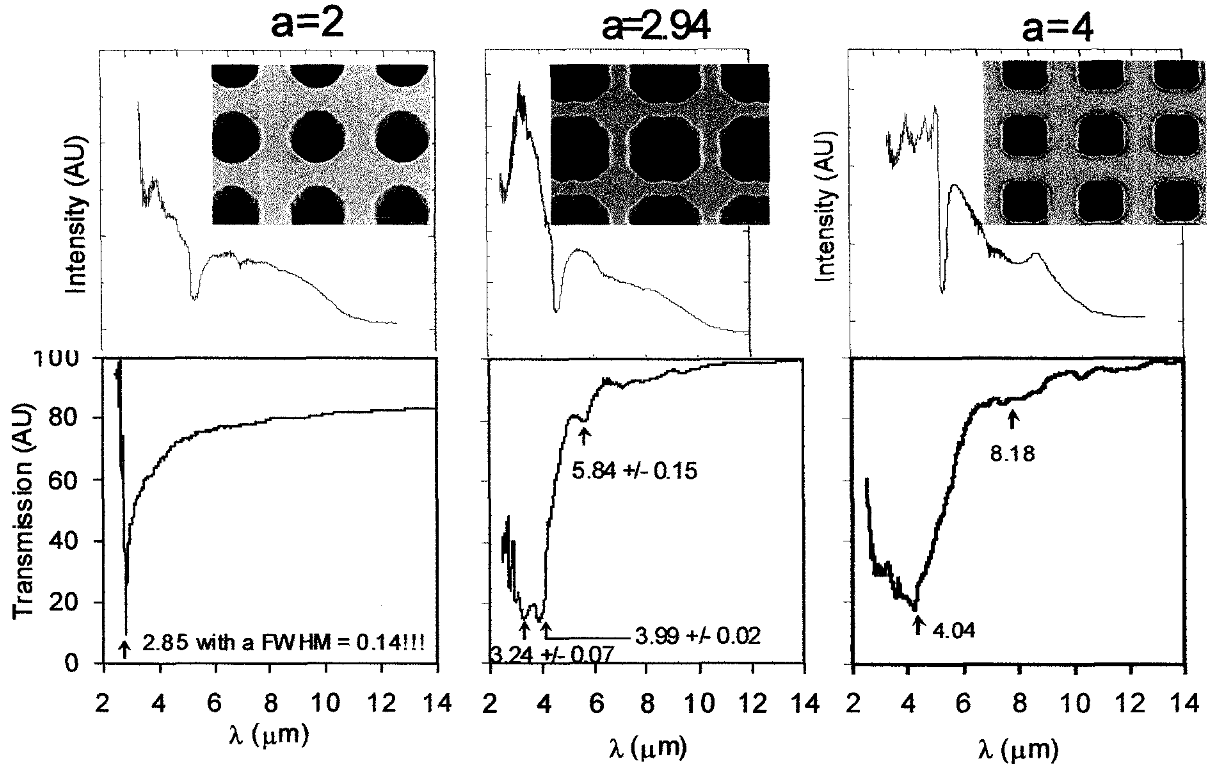

Figure 2 Measured emission (top) at 325°C and absorption at room temperature (bottom) for varying surface geometry shown in inset. Top surface coated with thin gold. Center-to-center spacing given at top of graphs. Emission minima at 4.6 μm is an artifact. There are fewer peaks with narrower FWHM compared to data in Figure 1 for the cross pattern.

The calculation of absorption by TMM was repeated for the smallest pattern shown in Figure 2, a 2μm lattice spacing for holes one micron diameter etched 5μm deep into silicon. The top metal layer was assumed to be one micron thick (finite element grid could not accommodate actual thinner film). Surface plasmon resonance calculated per reference 11 was used as a boundary condition to fix charge on the upper surface. Results show a sharp curve as do measurements, but at varying wavelength due to the change in film thickness. Peak wavelength will increase as the metal thickness is adjusted.

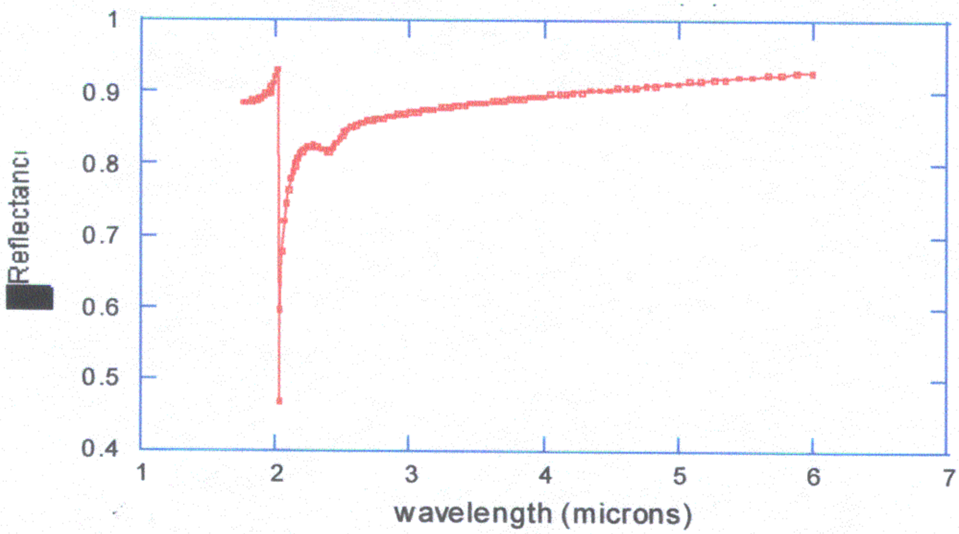

Figure 3 Calculated reflectance from sample a=2 (Figure 2) using TMM including surface plasmon modes. Metal layer is simulated by one micron thick layer.

The emission and absorption patterns from samples shown in Figure 2 change with viewing angle. The patterns change with angle from the normal to the plane of etch pits, and they also vary with angle relative to the axes of the geometrical pattern. Figure 4 shows the data for one sample. As the viewing angle increases, the wavelength shifts only slightly, while the relative intensity of different peaks changes substantially. Let phi be the azimuthal angle measured from the normal to the sample surface (z-axis) passing through the center of a line of square etch pits (x-axis), then the absorption peaks correspond to surface plasmon resonances. Resonance points, calculated from the work of Ebbensen for thin metal foils, are plotted in Figure 5 as curved lines.[12] The center line is for the lattice parameter (-1.-1) relative to the geometrical pattern. Top and bottom are (-1,0) and (0,-1) respectively. At 45° the latter two lines join as expected.

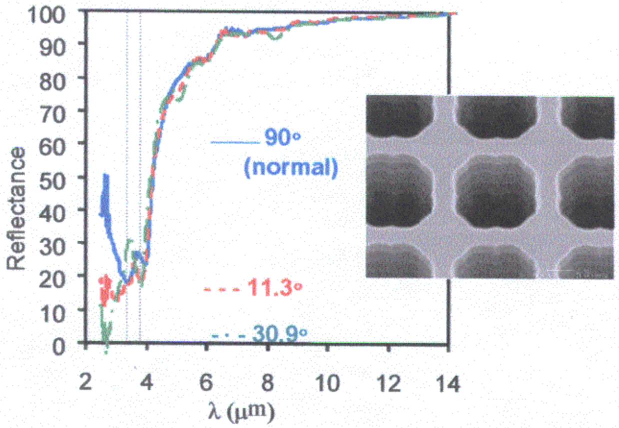

Figure 4 Reflectance data from sample 17A-001 taken with microFTIR at various angles of incidence.

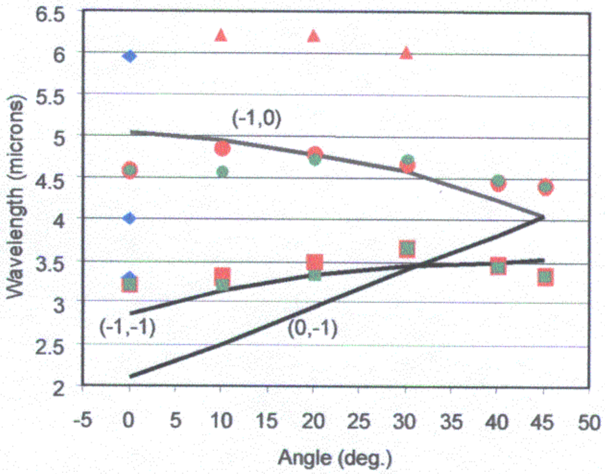

Figure 5 Variation of peak absorption wavelength as a function of azimuthal angle. Points are measured values, lines are calculated plasmon resonances.

All points are from measurements. Agreement for the (-1,-1) line is very good, and reasonable for the (-1,0) line. We do not know why the (0. –1) line is not present in measured data. Data at 6 microns seems to correspond to modes for underlying silicon from transfer matrix calculations that do not predict the other peaks seen in Figure 4.

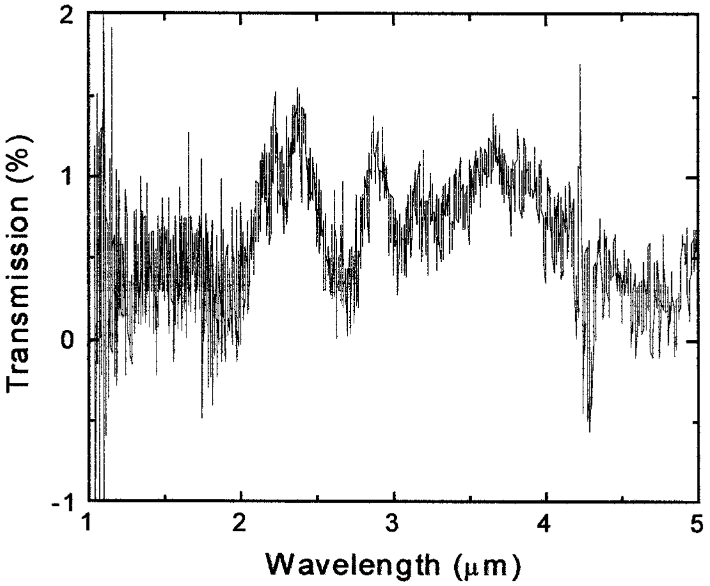

Figure 6 Transmission through 17A-001

The original paper on plasmon resonances calculated the effects of transmission through a thin metal film with a regular array of holes.[11] Are we measuring transmission through such a filter? Figure 6 shows measured transmission through sample 17A-001 (Figure 4) which is identical to a=2.94 from Figure 2. The absolute scale was calibrated from transmission through the same bare silicon wafer away from any metal coating and any surface etching. According to reference 11, the filter should transmit light at a level greater than that expected from geometrical shadowing, and instead it transmits much less light.

CONCLUSIONS

We have used photonic bandgap structures etched in gold-coated silicon surfaces to control emissivity vs. wavelength for these structures. The central wavelength of these peaks is proportional to the spacing of the geometrical patterns. Variation of wavelength with angle of observation can be directly related to the interaction of surface plasmons and photons, and to the finite element model of E-M fields in the underlying silicon. The surface metal film is not acting as a filter alone, independent of the etched structure in silicon. The possibility now exists to fabricate narrow-band thermal emitters with wavelength selected by features size and spacing as tuned light sources for spectroscopic applications.

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