3-D Silicon Photonic Lattices- Cornerstone of an Emerging Photonics Revolution

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JUL 21 1999
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ABSTRACT

Three-dimensional photonic lattices are engineered "materials" which are the photonic analogues of semiconductors. These structures were first proposed and demonstrated in the mid-to-late 1980's. However, due to fabrication difficulties, lattices active in the infrared are only just emerging. Wide ranges of structures and fabrication approaches have been investigated. The most promising approach for many potential applications is a diamond-like structure fabricated using silicon microprocessing techniques. This approach has enabled the fabrication of 3-D silicon photonic lattices active in the infrared. The structures display band gaps centered from 12μ down to 1.55μ .

Keywords: Photonic lattice, MEMS, Infrared, Photonic bandgap.

1. INTRODUCTION

The drive for miniature photonic devices has been hindered by our inability to tightly control and manipulate light. Moreover, photonics technologies are typically not based on silicon and, up till now, only indirectly benefited from the rapid advances being made in silicon processing technology. In this work, we overcome the disadvantage of silicon inherent in its electronic structure by using Si processing to create a 3-D silicon photonic lattice. This advance has been made possible through the use of a combination of MEMS (MicroElectroMechanical Systems) and IC (Integrated Circuit) fabrication technologies and may enable the development of a wide variety of entirely new photonic devices and the significant penetration of Si and MEMS processing into photonics.

The ability to confine and control light in three dimensions would have important implications for quantum optics and quantum-optical devices: the modification of black-body radiation, the localization of light to a fraction of a cubic wavelength, and thus the realization of single-mode light-emitting diodes, are but a few examples¹⁻³. Photonic crystals, the optical analogues of semiconducting crystals, provide a means of achieving these goals. The photonic band structure, Figure 1, results when light encounters a well-defined repeating arrangement of materials with differing refractive indexes, see for example Figure 2. This behavior is entirely independent of the electronic properties of the material making up the lattice, as long as it does not strongly adsorb. When correctly designed and fabricated, such structures can exhibit the property that photons with the bandgap energy can not penetrate the lattice, regardless of their angle of incidence. The existence of photonic bandgaps was proposed over a decade ago and was quickly demonstrated at millimeter wavelengths using macroscopic repeating structures made of machined alumina rods. However, since the critical dimensions of the lattice scale with the wavelength of the light, a reduction in wavelength to the infrared requires structures with minimum feature sizes on the order of a micron, Figure 3. As a result, until now, fabrication difficulties have stymied research in this area.

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Figure 1: Calculated band structure of a diamond lattice-like structure.

Figure 2: Oblique scanning electron micrograph showing a 7 layer photonic lattice fabricated in polysilicon with bandgap between 10 and 15 μ .

In this paper, we shall briefly summarize the various designs of 3-D photonic bandgap structures. We shall then outline the various fabrication approaches proposed to date, concentrating particularly on a silicon processing based approach which lends itself to integration with MEMS and Si processing^{4,5}. We will then provide experimental details of the properties of these artificial materials and outline their potential applications.

Figure 3: Plot of minimum feature size versus mid-gap wavelength for a diamond-like lattice. For mid gaps of 1.5 μ , the minimum feature size is $\sim 0.2\mu$. The batch fabrication of Si electronic devices with these minimum feature sizes has been demonstrated using commercially available tools.

2. DESIGNS

Yablonovitch⁶ and John⁷ first proposed the photonic lattice concept in 1987. In general, the idea was to modulate photons in a manner similar to the way electrons are modulated in a semiconductor. This is achieved through a periodic variation in refractive index. A pseudo-gap was first demonstrated in a macroscopic FCC (face centered cubic) structure with spherical air-atoms⁸. A design based on diamond symmetry was proposed by Ho *et al.*^{9,10} This design consists of a series of dielectric rods all aligned parallel to each other with a pitch equal to roughly half the wavelength of the mid point of the bandgap gap. The next layer is laid on top of, and orthogonal to, the first. The third level is aligned parallel with the first, but translated by a distance equal to half the pitch. The fourth level is parallel to the second, but is again translated by a distance of half the pitch. The structure then begins to repeat itself, Figure 2. This design mimics the way in which chains of atoms are lined up along the $\langle 110 \rangle$ directions in a diamond lattice. The resulting structure has a face-centered-tetragonal (FCT) lattice symmetry of which FCC is a special case. This design will be considered in most detail here since it lends itself to fabrication and has a full 3-D

bandgap. Similar designs have been generically described as "wood-pile" structures ¹¹. A related structure has been proposed by workers at MIT and consists of a series of offset plates inter-attached by a series of columns ¹². A different design, which more closely mimics the arrangement of atoms in the diamond structure, has also been proposed ¹³. Another structure which is similar, but which can not be fabricated in the same manner on the macroscopic scale is a simple cubic structure ¹⁴. An interesting "triple-hole" structure has also been demonstrated ¹⁵.

During the evolution of these designs a number of rules of thumb have been developed. Successful lattice designs have large contrast in refractive index, a high degree of symmetry, and interconnected regions of high index material. While the theory describing the properties of these structures has now been well developed, it will not be considered here. However, it should be noted that it is possible to completely describe these properties using Maxwell's equations. However, though the equations can be solved, the problems are of a complex vector form requiring detailed code and extensive computational capabilities. Because of these difficulties, most research groups tend to concentrate their efforts on a single structure for which they have developed and refined the code.

3. FABRICATION

Over the past decade, several of the designs proposed above have been fabricated. Since the dimensions of the lattice scale with the wavelength of light, it is possible to fabricate active millimeter regime structures using macroscopic processes. In this fashion the "Iowa" state structure has been demonstrated, among others ¹⁰. The problem in reducing the dimensions of the lattice to the more technologically interesting infrared is that the minimum feature sizes approach the micron regime, Figure 3.

The first approach to this problem was the "triple-hole" technique of Yablonovitch ¹⁵. In this approach, a series of three holes are bored into the substrate through a surface mask. The holes are not perpendicular to the substrate; instead they are at an angle of 35 degrees from the normal, with each hole rotated 120 degrees one from another. The end result is a series of interconnecting holes with a high degree of symmetry. Since each hole is drilled through the same top-surface mask, only one photolithography level is required. Using e-beam techniques it is possible to obtain the minimum feature sizes required for the structure to be active in the infrared. However, while this approach was extremely innovative, it requires nonstandard processing and the performance of the structures did not meet expectations, possibly due to distortions of the hole shape and the gradual, cumulative, deviation from ideality inherent in such a approach.

Another fabrication approach demonstrated by Noda ¹⁶ involves the use of wafer bonding. In this approach, etching, wafer bonding and selective etching build up the layers making up the structure. Alignment is achieved using interference techniques. The advantage of this unconventional approach is that it enables the use of traditional III-V materials.

A completely different approach is the use of artificial opals. In this approach, close packed layers of mono-sized spheres are laid down to form either the structure or mold ^{17,18}. The advantage of this approach is that large volumes of material should be achievable relatively cheaply.

Yet other fundamentally different approaches have been the use of deep x-ray lithography to form a complex 3-D mold ¹⁹, and the use of two-photon polymerization ²⁰. The large variety of different fabrication techniques reflects both the difficulty of fabrication and the interest in these structures.

The approach we have taken in our work ^{4,5} has been to employ the structure extensively studied in the millimeter regime by Iowa State University ^{9,10}, and fabricate it using modified silicon processes. In the work described here, the width of the rods was targeted initially at 1.2 μ , the height of the rods was targeted at 1.6 μ and the pitch of the rods was targeted at 4.2 μ . In our more aggressive structure the width was targeted at 0.18 μ , the height at 0.22 μ and the pitch at 0.65 μ . The bandgap size is determined by the dielectric contrast of the two different materials that constitute the 3-D structure and by the filling fraction of the higher dielectric constant material. The index contrast in our case is between polysilicon and the

surrounding air and is therefore $\sim 3.6:1$, or in the case where the sacrificial silicon dioxide has not been removed, $3.6:1.46$.

Two different processes were developed in the course of this work. The first process combined a series of mold definition, mold filling, and CMP (chemical mechanical polishing) steps to create parts with a minimum feature size of 1.2μ . The second process allowed us to fabricate parts with minimum feature sizes of 0.18μ . This was performed on a stepper with a 0.5μ limit of resolution and involved a complicated series of fillet processing, reactive ion etching and CMP. In both cases processing proceeded in a layer-by-layer fashion. The first process is schematically rendered in Figure 4.

Figure 4: There are a number of possible modifications to this basic flow, for example the patterning of the as-deposited poly, or the filling of trenches between poly lines. In every case the elimination of previous level topography by CMP is critical.

The first step is the deposition of a film of silicon dioxide on the surface of the wafer with a thickness equal to that of the desired height of one layer of the lattice [A]. Photolithographic patterning and etching through the oxide down to the substrate [B] then forms a mold. The mold is then filled with a deposition of polysilicon [C]. The polysilicon can then be chemically mechanically polished back to the original oxide surface [D]. There is excellent, $\sim 100:1$, CMP selectivity between the polysilicon and the silicon dioxide. Alternatively, topography permitting, the polysilicon thickness can be made equal to the layer thickness. In this case, patterning this film forms the second layer. Gaps between the rods can then be filled with silicon dioxide. The silicon dioxide is then planarized by CMP. A thin silicon nitride layer on top of the polysilicon is used as a CMP stopping layer. Though not used in this process flow, CMP slurries with selectivity's of $\sim 1:100$ between SiN and SiO_2 are available ²¹. In our case, an observed selectivity of $\sim 6:1$ was found to be sufficient. The entire process can then be repeated to add additional layers. In either case, the use of CMP to maintain planarity is critical. The CMP process ensures that topography introduced in one layer does not propagate into subsequent levels. In this manner, the number of levels is limited only by the generation of stress on the wafer. At the end of the process, the silicon dioxide can be selectively removed using a HF based solution to increase the refractive index contrast. Since the structure is highly interconnected and stiff there are no problems with stiction. Also, since the performance of the device only depends on a contrast in dielectric constants, the resistivity of the polysilicon and the contact resistance between layers are immaterial. Figure 2 shows a 7 layer structure fabricated using this process.

As examples of the flexibility of this approach we have used it to fabricate not just the "Iowa State" ^{9,10} structure, but also the "MIT" structure ¹² and the "90-degree" Iowa State structure. An example of the MIT structure fabricated using this approach is given in Fig. 5. In this case, the MIT design was broken up into its component slices and the slices were then fabricated sequentially, with CMP being used to ensure planarity. We have experimentally demonstrated that this structure also has a photonic bandgap. This particular structure is of sufficient complexity that it is virtually impossible to fabricate and test on a macroscopic scale. Another technologically interesting design is the 90-degree Iowa State structure. One of the distinguishing characteristics of 3-D lattices is that the bandgap exists for all angles of incidence of light. This is predicted theoretically, however, it is experimentally difficult to demonstrate for the "zero degree" case, in which the incident light is parallel to the substrate surface. Furthermore, this structure can not be readily fabricated on the macroscopic scale and tested in the millimeter regime. However, using the layer-by-layer fabrication approach, it is possible to again break up the 90-degree Iowa State structure into separate slices and then assemble them in a layer by layer fashion using the process outlined above. The end result is shown in Figure 6. Testing of this structure is experimentally straightforward and a gap is

indeed found. We have also applied this approach to the simple cubic design ¹⁴ and a variety of the “wood pile” structures ¹¹, Figure 7.

Figure 5: Oblique view cross section through the first three levels of the MIT structure ¹² fabricated using the layer-by-layer technique. This complex structure would be difficult to fabricate using macro-machining techniques.

Figure 6: Top view scanning electron micrograph of a “Iowa State” structure fabricated using the layer-by-layer approach. The fabrication of this structure enabled us to demonstrate experimentally the existence of a full 3-D photonic bandgap. Such a structure is difficult to fabricate on the macroscopic scale.

Figure 7: Oblique view scanning electron micrograph of a “wood pile” structure ¹¹ fabricated using the layer-by-layer technique.

Our second, more aggressive, process is outlined in Figure 8. In the first step of the process, a thin film of polysilicon is deposited having the thickness of the desired final height of the line, 0.22μ . The polysilicon is then capped with a thin film of silicon nitride which acts as a combination etch and CMP stop [A]. The sacrificial step material is then deposited [B]. A plasma enhanced CVD (chemical vapor deposition) silicon dioxide is used in this step. The layer is then photopatterned. Since the minimum dimension is attained using the fillet process the minimum stepper feature size is now only slightly smaller than that of the pitch of the array, 0.65μ . After photo patterning, the oxide is anisotropically etched to just above the level of the silicon nitride layer [C]. Following patterning, the oxide is densified using a 1050 C , 20 second rapid thermal anneal in a nitrogen/ oxygen mixture. A 30 second wet etch in a room temperature 6:1 (Ammonium fluoride: Hydrofluoric acid) mixture is then used to isotropically remove $\sim 0.1\mu$ of silicon dioxide [D]. This was done to ensure that the silicon nitride was exposed and to slightly relax the minimum feature requirement of the photolithography. Polysilicon was used to form the fillet. Since the deposition process

has excellent step coverage, the width of the fillet was essentially the same as the thickness of the film deposited [E]. The polysilicon was then etched in a high-density plasma source system using a HBr/O_2 chemistry [F]. Following fillet formation, the sacrificial oxide is stripped in 6:1 mixture [G]. The fillet was then used as a mask for the etch of both the underlying silicon nitride and silicon dioxide layers. The silicon nitride was isotropically etched in a 180 C bath of refluxed phosphoric acid [H]. The underlying polysilicon was etched in a high-density plasma system using a HBr/O_2 chemistry [I]. Since the height of the polysilicon fillet is greater than that of the layer being etched, the fillet itself serves as the mask. The next critical step in the processing involves the use of CMP to maintain planarity. The first step was to fill the gaps between the lines of poly silicon with a 0.3μ deposition of silicon dioxide [J]. This was done using a plasma enhanced TEOS (TetraEthOxySilane) process commonly used in back end IC technologies. The wafers were then planarized back to the silicon nitride-stopping layer using CMP [K]. Again, CMP processing is critical since it prevents the topography generated in the first levels from being replicated in each subsequent level. At this point, the entire process is repeated to form the subsequent layers of the structure. After completion of the desired number of layers, the silicon dioxide between the polysilicon lines may be removed in a concentrated HF/water solution with excellent selectivity between polysilicon and silicon dioxide. The parts are now ready for testing. As will be seen below, these parts display a band gap between 1.35 and 1.95μ . Figure 9 gives an example of a four-layer structure.

Figure 8: Schematic process flow for the fabrication of structures with minimum feature sizes on the order of 0.18μ using a stepper with a minimum feature size of 0.60μ . Further processing details are given in the text.

Figure 9: An oblique view of a cross section through a device formed by fillet processing. Due to the aggressive nature of the requirements on feature size and alignment the end result is not as well defined as the less aggressive part. However, as will be seen below, these defects had relatively little effect on the performance of the structure.

To date, we have found the performance of these devices to be relatively insensitive to most processing parameters. Level-to-level alignment can deviate by as much as 10% as can layer width and height without seriously compromising performance. However, care must be taken to ensure that neighboring levels make physical contact if the silicon dioxide is to be removed at the end of the process.

4. TESTING

The existence of a bandgap in these structures was determined from optical transmission and reflection measurements. Since light with the bandgap energy is forbidden, it is not able to penetrate the lattice and is instead reflected. To test the transmission properties of the 12μ mid-gap devices we used a standard, room temperature, Fourier-transform infrared measurement system with a broad spectral response from 2.5 to 25μ . The more aggressive device was tested with a similar system with a spectral range from 1 - 3μ . Before measurement, the back of the Si substrate was polished to a smoothness of better than 0.3 microns to avoid significant light scattering. The sampling beam was collimated to within a 10 degree divergence angle and had a spot size of $\sim 3\text{mm}$. Unless otherwise noted, the infrared light is incident along the stacking direction of the 3-D photonic crystal and was unpolarized. To find the absolute transmittance, a reference spectrum from a bare Si wafer coated was first obtained along with the signal spectrum taken from a wafer with a 3-D photonic crystal built on it. By ratioing the signal to the reference spectrum, the system's detector response was normalized, thereby eliminating the small unwanted absorption and other losses in the silicon substrate.

The absolute transmission and reflection spectra of light propagating along the $\langle 001 \rangle$ direction of the 3-D photonic crystal, that is, normal to the substrate, is plotted as a function of wavelength in Figures 10 and 11. Between 10 and 14μ , a strong transmittance dip is observed, signifying the existence of a photonic bandgap in the 3-D structure. Since light with these wavelengths can not penetrate the lattice it is reflected, indicated by an increase in the reflectance spectrum, Figure 10,11. A similar phenomenon is illustrated in Figure 12 for the transmittance through a crystal with midgap at 1.5 microns fabricated using the fillet process.

Figure 10

Figure 11

Plots of transmittance and reflectance through a 5 layer, 12μ midgap structure. There exists a dip in transmittance, which corresponds with an increase in reflection indicating the existence of the bandgap in the structure.

Figure 12 also shows the manner in which the bandgap develops with the addition of layers. To date the most layers we have fabricated are 12 for a structure with a midgap centered at 6μ . Figure 13 shows the transmission spectra of the 7-layer lattice shown in Fig. 2. In general, there appears to be roughly a factor of 2 reduction in transmission for every layer of lattice added.

Figure 12: A plot of transmission as a function of wavelength for 3 and 4 layers of crystal with gap centered at 1.5μ . The development of the gap with the addition of layers can be clearly seen.

Figure 13: Plot of transmission amplitude as a function of wavelength for the structure shown in Fig.2. At a wavelength of 11μ there is $\sim 98\%$ attenuation. At this wavelength there is minimal absorption of light by the polysilicon. The lattice itself is only 10.5μ thick.

One of the distinguishing characteristics of the 3-D photonic lattice is that the bandgap is preserved regardless of the angle of incidence of light. This property is experimentally demonstrated in Figure 14.

Figure 14. Plot of transmittance as a function of angle for a structure with mid-gap at 12μ . Unlike a diffraction grating, the photonic band-gap exists for all angles of incidence.

5. POTENTIAL APPLICATIONS

While still in its infancy, this technology has great potential. In our work we have demonstrated that the lattice building blocks can be fabricated in the infrared and optical ($1.5\ \mu$) wavelengths using widely available and supported Si fabrication equipment. Even these simple structures have interesting physical properties, they are efficient dielectric mirrors and they no longer demonstrate typical black body emission²². In our work we have also demonstrated the ability to fabricate cavities with volume less than one cubic wavelength²³ this has important implications for the fabrication of single mode LED's and lasers. High Q cavities have also been demonstrated at millimeter wavelengths²⁴. These cavities are the result of structural defects introduced into the lattice. The defects can either be additive, (the periodic addition of a line or line segment) or subtractive (the periodic removal of a line or a line segment). To date, we have been able to demonstrate similar cavities in the infrared with Q's of up to 300²⁵. This is sufficient for many laser applications. Knowledge of the influence that such structural defects can have on the lattice can also be used to design efficient three-dimensional waveguides. In this application, the light propagates through the lattice by travelling along a string of intentionally introduced defects. This is a fundamentally different process than the traditional approach to waveguides, which relies on a gradation in refractive index and is restricted as to the maximum bending angle. Using the photonic lattice approach, 90 degree bends have been demonstrated in 2 dimensional structures at millimeter wavelengths,²⁶. While waveguides in 3-D photonic crystals have not yet been demonstrated, we are confident, based on the 2-D result, that such guides with 90 degree bends are possible.

The early work in this area^{6,7} was motivated by a desire to find a way to modify the spontaneous emission of light during various physical processes. This behavior is expected by theory and has been partially demonstrated by the modification of the black body emission spectra²². It may be possible to use this property to greatly increase the emission efficiency of a very narrow range of wavelengths in what would normally be a inefficient, broad band emission spectra, such as the emission of erbium in Si based materials. If such a property can be demonstrated, it may lead to the development of silicon-based lasers and LED's, that are active at optical communication wavelengths. This could herald the evolution of low cost, complex, electronic and photonic components existing on a single chip and based upon a common set of materials and fabrication processes.

6. ACKNOWLEDGEMENTS

These parts were fabricated at Sandia National Laboratories Microelectronics Development Laboratory. The authors especially acknowledge the efforts of Tony Farino, Brad Smith, Dale Hetherington and Pat Shea. This work was supported by the United States Department of Energy under contract DE-AC04-94AL85000. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy.

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