

Fabrication and Characterization of Large-Area 3-D Photonic Crystals

F. B. McCormick, J. G. Fleming, S. Mani, M. R. Tuck, J. D. Williams, C. L. Arrington, S. H. Kravitz, C. Schmidt, G. Subramania, J. C. Verley, A. R. Ellis, I. El-kady, D. W. Peters, M. Watts, W. C. Sweatt, J. J. Hudgens
Sandia National Laboratories
PO Box 5800, MS 0603
Albuquerque, NM 87185-0603
Voice: 505.284.1209
fbmccor@sandia.gov

Abstract—Full bandgap^{1,2} (3D) photonic crystal materials offer a means to precisely engineer the electromagnetic reflection, transmission, and emission properties of surfaces over wide angular and spectral ranges. However, very few 3D photonic crystals have been successfully demonstrated with areas larger than 1 cm². Large sheets of photonic bandgap (PBG) structures would be useful, for example, as hot or cold mirrors for passively controlling the temperature of satellites. For example, an omni-directional 3D PBG structure emitting only at wavelengths shorter than 8 microns will radiate only 7% of what a black body would at 200°K while radiating more than 40% at 400°K. 3D PBG materials may also find application in thermophotovoltaic energy generation and scavenging, as well as in wide field of view spectral filtering. Sandia National Laboratory is investigating a variety of methods for the design, fabrication, and characterization of PBG materials, and three methods are being pursued to fabricate large areas of PBG material. These methods typically fabricate a mold and then fill it with metal to provide a high refractive index contrast, enabling a full 3D bandgap to be formed. The most mature scheme uses Silicon MEMS lithographic fabrication means to create a mold which if filled by a novel tungsten deposition method. A second method uses LIGA to create a mold in PMMA, which is filled by electro-deposition of gold, copper, or other materials. A third approach uses nano-imprinting to define the mold, which is filled using evaporative deposition or atomic layer deposition of metals or other materials. Details of the design and fabrication processes and experimental measurements of the structures will be presented at the conference.

TABLE OF CONTENTS

TABLE OF CONTENTS.....	1
INTRODUCTION	.1
3-D PHOTONIC CRYSTAL DESIGN AND TOLERANCING	.2
FABRICATION AND CHARACTERIZATION	.4
MOLDED TUNGSTEN LITHOGRAPHY	.4
DEEP X-RAY LITHOGRAPHY (DXRL / LIGA)	6
MULTILAYER NANOIMPRINT LITHOGRAPHY (NIL)	7
SUMMARY AND CONCLUSIONS	8

¹ 0-7803-9546-8/06/\$20.00© 2006 IEEE

² Revision 4

INTRODUCTION

Photonic crystals have been a topic of intense research over the last 10 years, and photonic crystal-based applications are starting to reach maturity in fields such as bio sensing and fiber optics.¹ Photonic crystals can be thought of as the photonic analogues of semiconductors. When correctly designed, these engineered photonics structures can exhibit a photonic bandgap: a range of photonic energies which are forbidden to exist in this structure. Another way of considering this is that the density of allowed states of photons with energies within the bandgap goes to zero. It is also possible to increase the density of states, to engineer the absorption of the crystals. Photonic bandgaps have been measured in 1-D (similar to Bragg gratings), 2-D (a planar “slice” crystal), and 3-D synthetic crystals. For many applications full 3-D photonic crystals are desirable for their ability to “mold light” across a wide range of wavelengths and angles. Structures with full bandgaps are complex 3-D geometries, which exhibit particular symmetry elements. Symmetry elements which give rise to full 3-D bandgaps are the simple cubic and diamond and related symmetries such as face centered cubic^{ii,iii}. Full 3-D bandgap materials have been demonstrated which prohibit propagation of, and thus reflect, light at all angles across a spectral range greater than +/- 40% of the center wavelength. These 3-D bandgap materials also exhibit unique emission properties which do not follow Wien’s displacement law: their peak emission wavelength remains “pinned” regardless of the material’s temperature. These features may be used to advantage in space applications for hot & cold mirrors for temperature control, thermophotovoltaic power generation, broadband optical components, and improved performance IR scene generators and sensor calibration tools.

However, many of these applications require large coverage areas, and while 1-D and 2-D photonic crystal developments are progressing into product applications, few full-bandgap 3-D photonic crystals have been demonstrated, and the sample sizes are often measured in the 100’s of μm², rather than in m². To address this gap, Sandia National Laboratory is investigating a variety of methods for the design, fabrication, and characterization of PBG materials.

Three methods are being pursued to fabricate large areas of photonic crystals. These methods typically fabricate a mold and then fill it with metal to provide a high refractive index contrast, enabling a full 3D bandgap to be formed. The most mature scheme uses Silicon MEMS lithographic fabrication means to create a mold which if filled by a novel tungsten deposition method. A second method uses LIGA to create a mold in PMMA, which is filled by electro-deposition of gold, copper, or other materials. A third approach uses nano-imprinting to define the mold, which is filled using evaporative deposition or atomic layer deposition of metals or other materials. This paper will provide an overview and status of this work.

3-D PHOTONIC CRYSTAL DESIGN AND TOLERANCING

This work has pursued both a general survey and theoretical understanding of the design forms and materials and a study of the manufacturability and tolerance analysis of the specific forms selected as vehicles for our fabrication experiments. Photonic band gap formation can be understood as a "synergic interplay" between the microscopic scattering resonance from the dielectric material contained in a single unit cell of the photonic crystal and the macroscopic resonance dictated by the geometrical arrangement of the repeating unit cells of the dielectric microstructure. A photonic band gap is facilitated only if the geometrical parameters of the crystal are such that both the microscopic and macroscopic resonances occur at precisely the same wavelength and both of these scattering mechanisms are independently quite strong. Because the photonic band gap manifests itself as a band in cermet topologies (disconnected scattering centers) and as a cutoff in network topologies (connected scattering centers), the general rule of thumb is that network topologies will express more resilience to fabrication errors as there is only one fundamental band edge to deal with versus two in the case of cermet topologies.

We have created design matrices for relevant photonic structures shown in Figure 1, identifying "global" designs based on topology and symmetry of the high dielectric material, as well as for specific photonic crystal design tradeoffs. The relative ranking (1=best, 3=worst) is a "snapshot" of our present theoretical understanding; to be confirmed in our parallel experimental work.

Design	Scalability	Fab. Tolerance Sensitivity	Manufacturability
Cermet Cubic Topology	Limited only by Fab	3	2
Network Cubic Topology	Limited only by Fab	2	1
Diamond Cermet Topology	Limited only by Fab	2	3
Diamond Network Topology	Limited only by Fab	1	2
Face Centered Tetragonal Network Topology	Limited only by Fab	2	1

Design	Scalability	Fab. Tolerance Sensitivity	Manufacturability
Cubic Array of Cubes	Limited only by Fab. min. feature size and aspect ratio	3	2
Logpile	Limited only by Fab. min. feature size and aspect ratio	1	1
Tilted Logpile	Limited by LIGA masks	1	1
Holographic Diamond Structure	Limited by infiltration capability and uniformity of the film	3	3
Twisted Rod Structure	Limited by Glancing Angle Deposition Repeatability and Accuracy	2	3

Figure 1. Design matrices for PBG structures.

ELECTROMAGNETIC SIMULATION APPROACHES

Photonic bandgap (PBG) structures are complex electromagnetic structures to simulate. Still, various rigorous numerical techniques can be used to do so, including Eigenmode Expansion (EME), Method of Moments (MOM), and Finite-Difference Time-Domain (FD-TD). Each of these techniques has strengths and weaknesses, and applied research projects at Sandia develop and use all of these approaches to design and tolerance PBG structures.

The eigenmode expansion technique, as the name implies breaks down the fields into the 2D cross-sectional modes. The full 3D field distributions are then developed by matching the boundary conditions with the available modes. The advantage of the EME technique is that if the layers are repeated, as they often are in PBG structures, the scattering matrix can be used over and over to quickly arrive at a solution. When few layers are required or when repeated layers are able to be used, the full 3D field solution can be developed very rapidly. However, if the structures do not fit neatly on rectilinear coordinates, (e.g. circles, spheres etc.) then many slices are required to decompose the problem which greatly increases the required number of calculations and the simulation time.

The method of moments is another highly accurate technique for simulating electromagnetic structures. This approach uses equivalent current sources in order to match boundary conditions. The 3D field is then arrived at by considering the summed radiation of all the current sources. The MOM technique is especially useful for structures that are widely separated because it is not necessary to grid the whole space in order to develop a solution. It is also generally a highly accurate technique, so it can be used for almost any electromagnetic problem.

Both EME and MOM solve the electromagnetic problem in the frequency domain. In contrast, the Finite-Difference Time-Domain method solves the problem in the time domain. FD-TD is simply a discrete implementation of Maxwell's equations. The entire simulation space is

discretized, and a short electromagnetic pulse is launched into the simulation domain. Overlaps and discrete Fourier transforms are typically taken at the input in order to isolate individual spatial mode and frequency components. The simple nature of the implementation results in a very direct approach to the electromagnetic problem. However, discretizing the entire space often causes the technique to be relatively slow. In order to efficiently solve PBG structures, periodic boundary conditions must be implemented. Doing so complicates the approach significantly. Moreover, solving metallic structures, especially in the near infrared, further complicates the technique, as the temporal response of metals in this regime is not well defined.

TOLERANCING OF PHOTONIC CRYSTAL GEOMETRIES

Tolerancing is a necessary and important part of design, as slight deviations from the original design are unavoidable in fabrication. Modeling these fabrication tolerances for different structures allows us to determine whether significant changes to the optical properties may occur due to process variation. Critical parameters may be identified and further design can aim to lessen the possible impact of that device parameter.

For example, the logpile structure was toleranced using a transfer matrix method for solving Maxwell's equations. The logpile design had a period of $1.8\mu\text{m}$, with $0.5\mu\text{m}$ bar widths. Figure 2 illustrates the difference in the reflectivity for varying degrees of misalignment for E and H polarizations. Figure 3 illustrates the effect of changes in bar width on the reflectivity. In all cases significant variation can be seen below the bandgap, particularly for the alignment tolerance. For the case of alignment error, a shift in the bandgap itself is evident, with a monotonic movement of the bandgap to longer wavelengths as the misalignment error increases. Above the bandgap, as the wavelength increases, the effect of misalignment and bar width variation is minimal. It should be noted that while 100% misalignment is plotted in these graphs for completeness, it is not expected that typical fabrication error would near this value. In the Sandia MEMS process, likely misalignment for the logpile is typically well within 20% of perfect alignment. In Figure 2, the 0%, 10%, and 20% error curves for both polarizations are nearly indistinguishable. For longer wavelength devices, where structure dimensions are larger, the percentage of error in alignment should be even less. Therefore we expect a minimal effect on the optical properties due to misalignment for structures we may likely fabricate.

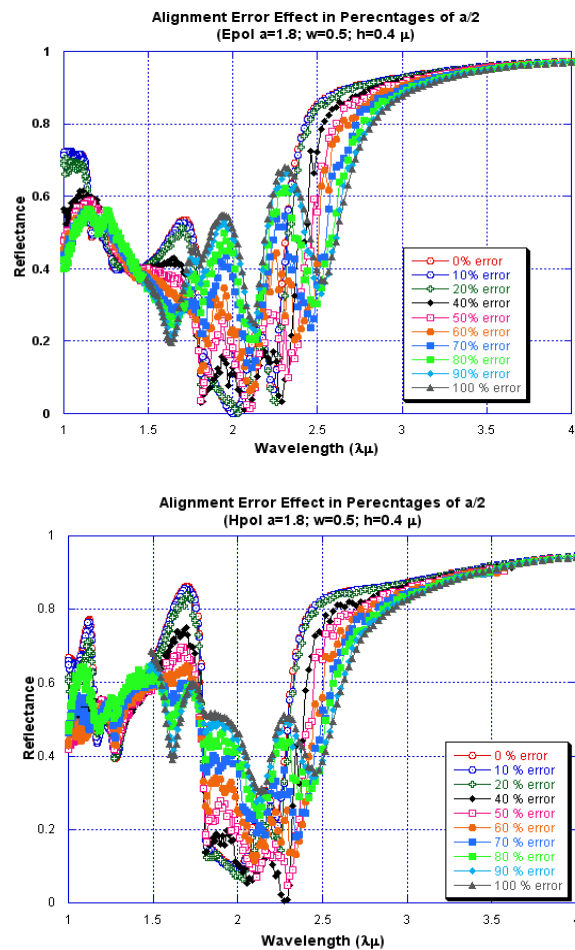


Figure 2. Alignment error effect on reflectivity for logpile geometry. E (left) and H (right) polarizations shown. Period = $1.8\mu\text{m}$, bar width = $0.5\mu\text{m}$ and bar height = $0.4\mu\text{m}$.

Likewise, the errors attributed to the deviation of the rod thickness from the ideal are plotted in Figure 3 do not significantly affect the location of the bandedge or the optical behavior for longer wavelengths. For short wavelengths a significant difference in the H polarization reflectance is observed.

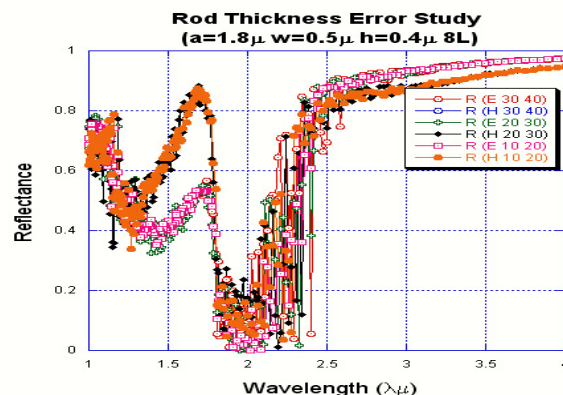


Figure 3. Effect on reflectivity of bar thickness variation for logpile structure with period = $1.8\mu\text{m}$, bar height =

0.4μm. Legend: (E 30-40) denotes E polarization with 30% to 40% error.

FABRICATION AND CHARACTERIZATION

Sandia National Laboratories has been exploring the design, fabrication, and application of PBG materials for the last 10 years, and has steadily developed the multidisciplinary infrastructure needed to reproducibly demonstrate full bandgap 3-D photonic crystals. This infrastructure includes multiple design codes for 3-D electromagnetic modeling of complex dielectric and real-metal structures, submicron tolerance mold fabrication and metal/dielectric deposition processes, and high-precision visible and infrared spectroscopic and radiometric characterization tools. By iterating this “design-fab-test” loop, we are attempting to examine the interrelated tradeoffs between the structural designs, the mold fabrication limits, and the required material sets associated with building PBG materials in large areas (see Figure 4).

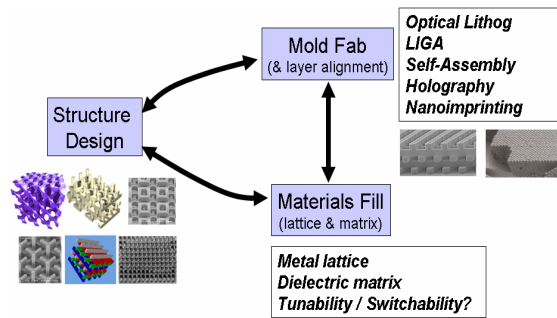


Figure 4. Large area 3D PBG materials require tradeoffs between, and optimization of the structural parameters, the mold fabrication technology, and the lattice material.

MOLDED TUNGSTEN LITHOGRAPHY

The complexity and small size of photonic crystal structures has slowed progress in this area due to the difficulty in fabrication. However using variations in MEMS processing we have found that it is possible to fabricate a wide variety of such structures.^{iv,v}

We have fabricated 3-D metallic (tungsten) photonic crystals and demonstrated broad full bandgaps at near to long infrared wavelengths, and emissivity peaks that do not shift with temperature, as in Figure 6. Moreover, within the photonic bandgap region of the crystal, the emissivity is very low. In this way, a photonic crystal can be designed as a high efficiency selective emitter. For cooling applications this implies that the wavelength of radiative emissions can be tightly controlled to certain wavelength regions.

These 3D tungsten photonic crystals are fabricated using a modified 6” wafer silicon MEMS process developed at Sandia^{vi}. In the first step, a layer of silicon dioxide is deposited, patterned, and etched to create a mold. The mold is then filled with a 500-nm-thick tungsten film and planarized using a chemical mechanical polishing process. The process is repeated several times. At the end of the process, the silicon dioxide is released from the substrate and the sample is a freely standing thin film. These films can remain attached to the silicon substrate, but are robust enough to also be lifted from the substrate and handled separately.

In this process, the starting material used are 6 inch diameter silicon wafers (Figure 6). On a single wafer a particular pattern with a total area of ~2cm² will be repeated effectively identically ~60 times. A single experimental run will typically yield ~6 wafers.

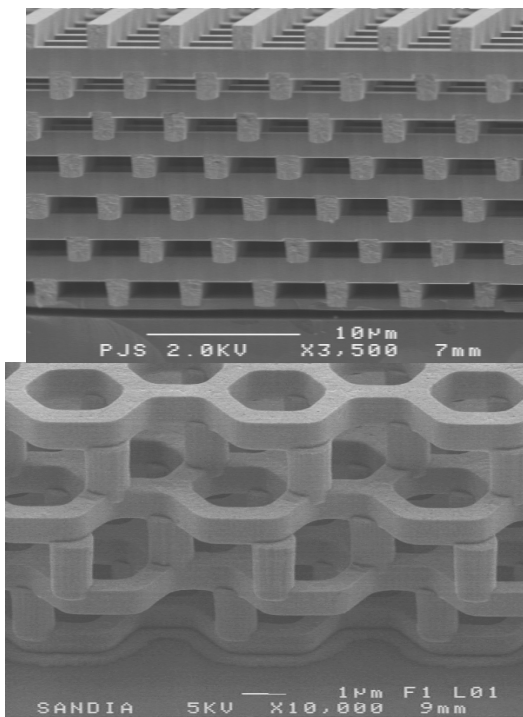


Figure 5. Examples of 3-D photonic crystals fabricated at Sandia.

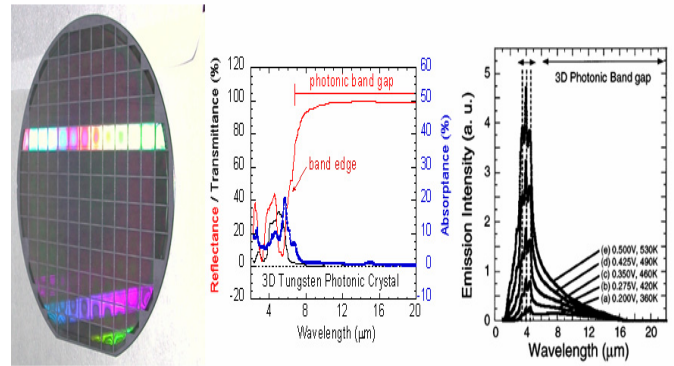


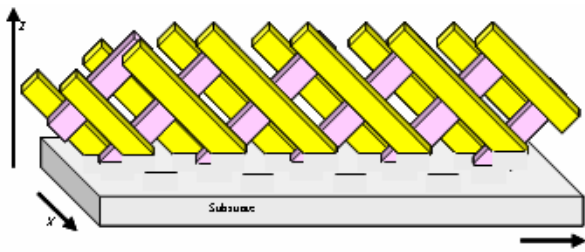
Figure 6. Tungsten 3D PBG material fabricated using Sandia's modified MEMS process: 6" PBG wafer and typical optical properties.

DEEP X-RAY LITHOGRAPHY (DXRL / LIGA)

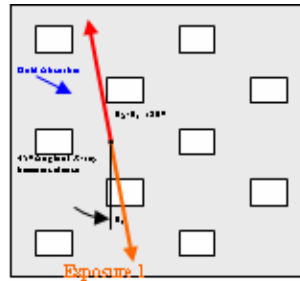
The LIGA microfabrication technique offers a unique method for fabricating 3-dimensional photonic lattices. These “tilted logpile” lattices have a similar structure and band gap to Sandia’s “logpile” structure except that the orientation of the logpile structure is rotated 45 degrees out-of plane (see Figure 7(a)). Gold, rather than Tungsten, is used as the matrix material, since it can be readily electrodeposited into small high aspect ratio patterns, retaining the index contrast required to achieve the full photonic band gap.

The lattice is patterned using deep X-ray lithography (DXRL) to create a series of intersecting channels in PMMA. Deep X-ray lithography is a proximity exposure technique in which a gold absorber is used to mask the X-ray exposure of PMMA. The mask, shown in Figure 7(c),

and the resist-coated substrate are held fixed with respect to one another and scanned across a collimated X-ray beam generated by a synchrotron light source. The PMMA mold for this design is generated with two shuttered exposures repeated one after another without releasing the mask from the substrate. A series of tilts and rotations of the mask and substrate together between exposures provides the proper exposure angles required to generate the pattern without any fine alignment of the pattern during the entire fabrication process. This technique makes it possible to create large area molds for gold electrodeposition without alignment errors or multiple exposure runs. Once exposed, the substrate developed to reveal the electroplating mold required to generate the lattice. Gold is then electrodeposited into the mold uniformly to eliminate the need for polishing such a fine structure. After plating, the resist is stripped to reveal the “tilted logpile” structure (shown in Figure 8).



(a)



(b)



(c)

Figure 7. Fabrication of LIGA PBGs: (a) Illustration of the tilted logpile design (b) X-ray mask design illustrating the tilt and rotations required for the logpile (c) optical picture of DXRL mask.

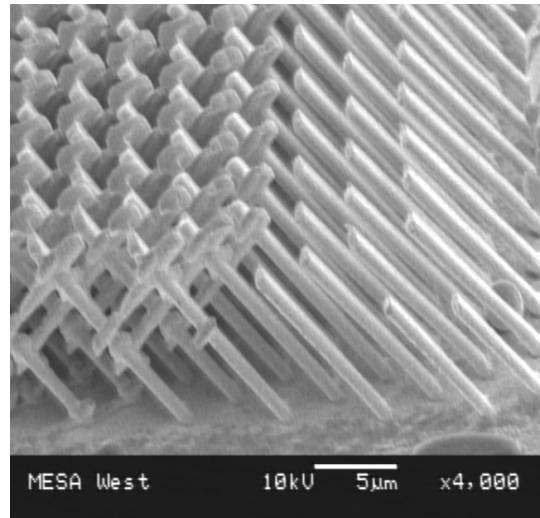
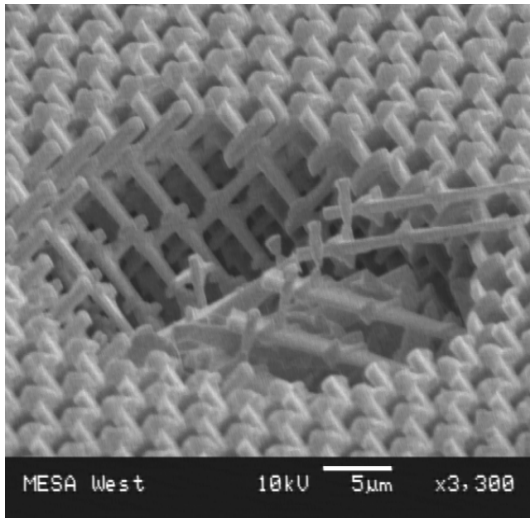


Figure 8. “Tilted logpile” PBG material fabricated in gold using the LIGA technique.

Optical reflectivity measurements shown in Figure 9 indicate the presence of a photonic band gap in the electroplated lattice. However, the sizes of crystals currently produced are too small to observe an ideal PBG effect without scattering from the edges of the pattern. These scattering effects are thought to be observed as ripples observed in the data above 6 μm and the reduction of reflected light observed in wavelengths longer than 12 μm .

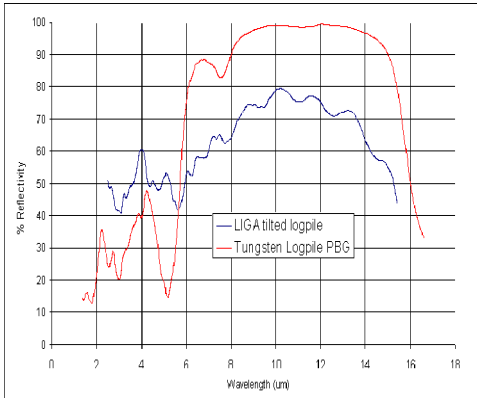


Figure 9. Initial data from small area tilted logpiles fabricated using LIGA.

MULTILAYER NANOIMPRINT LITHOGRAPHY (NIL)

Nanoimprint lithography is a ultra-high resolution patterning technique similar to the methods used for DVD and CD disk production. We are pursuing NIL as a path for fabricating large areas of the deep-submicron mold structures needed to implement visible wavelength PBG materials. NIL tools are maturing rapidly, with several vendors offering products capable of imprinting sub-100nm features over 6" wafer areas.^{vii} Tools exist which simultaneously offer sub-50nm resolution and sub-10nm 3 \square multilayer alignment capability.^{viii} Preliminary experiments have been performed which demonstrate roll-to-roll nanoimprinting and offer the potential for very large scale and inexpensive manufacture of nanoimprinted structures.^{ix} The path we are following is to develop multilayer lithography, alignment, and plating techniques for IR wavelength PBGs, then transition to nanoimprint lithography (NIL) as a means to achieve visible PBGs. PBGs fabricated for the IR have > 1 μm feature sizes amenable to contact lithography similar to NIL, but which can be done with readily available contact mask aligners. This approach provides rapid prototyping for flexible investigation of polymer filler materials, alignment techniques, and electroplating studies. Two mask sets have been developed to fabricate both a gold logpile design similar to our MEMS-fabricated tungsten logpile crystals, and a cubic-array-of-cubes design.

We have fabricated the cubic-array-of-cubes design using our rapid prototyping approach with 3D lattices of gold cubes separated by BCB as the polymer filler material. An example of the optical reflection spectra for our initial 2-layer structure is shown in Figure 10. As a filler material, the polymer needs to have compatible optical and material properties to create the PBG and operate effectively in the desired LWIR wavelengths. It has to demonstrate high optical transparency and low absorption in the operating range while remaining compatible with the fabrication process. It has to be easy to prepare and spin on a wafer scale for thin film applications while remaining inert to attacks from most processing chemicals. It requires low water absorption and a high enough transition temperature to maintain dimensional stability through processing and over the long term. Finally it needs to adhere well to gold and the substrate with or without an adhesion promoter without affecting the optical properties of the lattice. Polymers under consideration included Cyclotene 3022 (BCB), cyclo-olefin polymers such as Zeonor 1020R, Zeonex E48R, and Topas, Appear polynorborene polymers, polyethylene and polymethylmethacrylate (PMMA). PMMA was excluded because its water solubility was too high for stable feature size/shaping over the long term. Zeonex E48R was rejected because it reticulated after spinning on a wafer making it unsuitable for our continuous thin film applications.

This rapid-prototyping contact-lithography approach has provided a platform for investigating new structures, materials, and multilayer alignment techniques critical for a successful transition of these designs to visible wavelengths using nanoimprinting approaches.

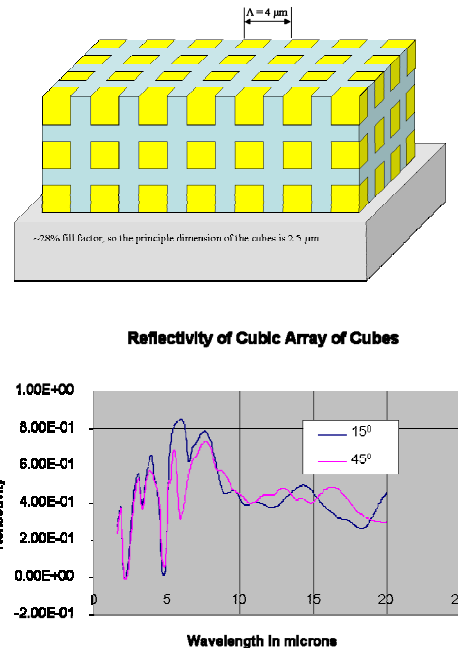


Figure 10. Schematic of the cubic-array-of-cubes structure and initial experimental results.

SUMMARY AND CONCLUSIONS

Several approaches under investigation at Sandia National Laboratories show promise as fabrication paths to large areas of full 3D photonic bandgap materials. Such materials may potentially be useful for space applications such as platform thermal control (cold/hot mirrors), TPV power generation, omnidirectional spectral filtering, and IR scene generation or calibration.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DEAC04-94AL 85000.

REFERENCES

- ⁱ For an overview, see for example: J.D. Joannopoulos, R.D. Mead, J.N. Winn, Photonic crystal: Molding the flow of light, Princeton University Press (Princeton, 1995), or K. Sakoda, Optical Properties of Photonic Crystals, Springer Verlag (New York, 2001).
- ⁱⁱ K.M. Ho, C.T. Chan, C.M. Soukoulis, R. Biswas, M. Sigalas, Solid State Communications, **89**[5], (1994).
- ⁱⁱⁱ S.Y. Lin, J.G. Fleming, R. Lin, M.M. Sigalas, R. Biswas, K.M. Ho, J. Op. Soc. Amer. B, **18**[1], (2001).
- ^{iv} Lin, SY; Fleming, JG; Hetherington, DL; Smith, BK; Biswas, R; Ho, KM; Sigalas, MM; Zubrzycki, W; Kurtz, SR; Bur, J., "A three-dimensional photonic crystal operating at infrared wavelengths", Nature; 16 July 1998; vol.394, p.251-3.
- ^v Fleming, JG; Lin, SY; El-Kady, I; Biswas, R; Ho, KM, "All-metallic three-dimensional photonic crystals with a large infrared bandgap", Nature; 2 May 2002; vol.417, p.52-5.
- ^{vi} S. Y. Lin, J. G. Fleming, E. Chow, J. Bur, K.K. Choi, and A. Goldberg, Phys. Rev. B **62**, R2243 (2000).
- ^{vii} See, for example: <http://www.nanonex.com/>,
<http://www.molecularimprints.com/>,
<http://www.suss.com/main.php>,
http://www.obducat.com/sida_71.asp,
- ^{viii} See
<http://www.molecularimprints.com/Products/I250page.html>
- ^{ix} H. Tan, A. Gilbertson, S.Y. Chou, "Roller nanoimprint lithography," J Vac Sci Tech B 16 (6) 3926-3928 Nov-Dec 1998.

BIOGRAPHY

Presenting author:

Frederick B. (Rick) McCormick received his BSEE, MSEE, and PhD degrees from University of Washington, Georgia Institute of Technology, and Heriot-Watt University (Edinburgh), respectively. His career has focused on the design and development of novel optical microsystem products, typically incorporating microoptics, array optoelectronics, and high speed digital and RF electronics. He was a staff member at AT&T Bell Laboratories until 1994, developing optical switching system prototypes using GaAs/AlGaAs MQW modulators (S-SEEDS) and VCSEL arrays. From 1994-2000 he built and staffed the systems division of Call/Recall, Inc., an R&D startup developing 3D optical data storage products using 2-photon absorption recording and parallel access fluorescent readout. In 2000, he joined Emcore, helping build and staff the Fiber Optics division, then, as Director of Product Development, leading the product design and development efforts for four parallel optics/VCSEL transceiver products with data rates up to 40Gbps, and finally reporting to the CTO as Director of Fiber Optic Technology. In mid-2003, he joined Sandia's Integrated Microsystems department, where he led several projects integrating advanced optical technologies into national security related products. In the Fall of 2004 he became the team leader for the Applied Photonics Microsystems group within the Photonic Microsystems Technology department, which pursues novel applications of optical MEMS, photonic crystals, silicon photonics, biophotonic and other optical sensors, and optical signature control. He has over 80 publications in the above areas, including 4 book chapters and 16 patents & patents pending. He is a member of IEEE and OSA.

All of the sixteen coauthors of this paper work in the Microsystems Enigneering, Science and Applications center at Sandia National Laboratories in Albuquerque, New Mexico. Please see:

<http://www.sandia.gov/mstc/>