THREE-DIMENSIONAL ALUMINA PHOTONIC BANDGAP STRUCTURES: NUMERICAL SIMULATION AND FABRICATION BY FUSED DEPOSITION OF MULTIMATERIALS

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Abstract

Three-dimensional photonic bandgap (PBG) structures using alumina (Al_2O_3) as the high permittivity material were modeled and fabricated. A finite element method and a real-time electromagnetic wave propagation software were used to simulate and design the layered PBG structures for their use in the microwave frequency range. The modeling obtained a 3-D photonic bandgap in the 16-23 GHz range. Fused deposition of multimaterials (FDMM) technology was then used to manufacture PBG structures. FDMM provides a computer-controlled process to generate 3-D structures, allowing high fabrication flexibility and efficiency. These PBG structures are potential candidates for applications in advanced communication systems.

I. Introduction

Photonic bandgap (PBG) crystals are periodic dielectric structures that alternate high and low permittivity materials in order to obtain an electromagnetic stop-band in a desired direction. PBG crystals were proposed in the late 1980's and since then there has been extensive theoretical and experimental work devoted to this new field [1]. The dielectric or metallic periodic structure gives rise to a forbidden band of frequencies, or photonic bandgap, which essentially changes the electromagnetic wave propagation properties through the structure. These structures have received increasing interest in recent years because of their capability to confine electromagnetic (EM) waves in all three spatial dimensions [2,3]. A variety of applications are possible, such as thresholdless lasers, high quality-single mode LEDs, microwave antennas, light diodes, an all kinds of optical circuits have been suggested, and some have already been demonstrated [4].

For the microwave/millimeter wave region, in which our interest is focused, applications involve control of signal propagation, quiet oscillators, frequency selective surfaces, narrow band filters, and antenna substrates. For the latter case, if a conventional substrate is used, then most of the antenna radiation is emitted into the substrate (since it has a higher dielectric constant than air). Much of this radiation is trapped inside the substrate because of total internal reflection. As a consequence of this, not only more than 50% of the radiated energy is lost, but also heat dissipation and temperature effects arise in the substrate. Instead, if an appropriate PBG substrate is selected, then all of the energy can be directed towards the radiating direction (total reflection by the PBG structure), thus improving the antenna directivity and eliminating the substrate heat dissipation. There have been many reports for the application of PBG structures as antenna substrates [5,6]. Our research will focus on the design 3-D PBG structures fabricated by FDMM that may have applications in the millimeter-wave band.

The main feature of PBG structures is their capability to affect the radiative dynamics within the structure so that there are no electromagnetic modes available within the dielectric. The periodically arranged atomic lattice of a semiconductor gives rise to allowed values of energy that an electron can have at the valence band and at the conduction band, with an energy bandgap separating the two. The optical analogy to this situation is a periodic dielectric structure with alternating high and low values of permittivity, which gives rise to a photonic bandgap. Photons with an energy within this interval cannot propagate through the structure. The periodicity of the PBG structures may be 1, 2 or 3-dimensional, producing 1-, 2- or 3-D photonic bandgaps, respectively. Different two-dimensional and three-dimensional PBG structures have been proposed in the literature [2-7]. 2-D structures with predicted and experimentally verified photonic bandgaps, include a square or a triangular lattice of cylindrical air rods in a higher permittivity material, while the first experimentally verified 3-D structure was the one proposed by Yablonovitch and fabricated on air spheres drilled on alumina plates [7].

Many groups have performed research in photonic structures using alumina as the high permittivity dielectric material [9-12]. The use of anodic porous alumina formed by anodization of aluminum in an appropriate acid solution has attracted attention as a starting material for 2-D PBG structures with typical dimensions in the nano- or micrometers, since this process is a typical example of a naturally occurring ordered structure [9-11]. Also, Feiertag *et al.* developed a microfabrication technique for building 3-D PBG structures using x-ray lithography with bandgaps in the infrared region [12]. These structures have a lattice constant of 85 μm and are made of 22 μm diameter rods.

Jin *et al.* made microwave measurements on a 2-D octagonal quasiperiodic photonic crystal made of an array of 23 x 23 rows of alumina cylinders [8]. The diameter of the alumina cylinders was 6.12 mm, so the filling fraction was ~49%. The authors demonstrated that there is a bandgap between 8.9 and 10.5 GHz, that the position and width of the bandgap does not depend on the incidence direction, and that it can appear even if the array's dimensions are lowered to 11 rows of cylinders. Because of these characteristics, this photonic quasicrystal seems to be more suitable for waveguide applications than as a periodic photonic crystal. For this purpose waveguides were fabricated by removing 3 rows of cylinders, leaving a 15.7-mm wide empty path from one side of the array to the opposite one, which was approximately half of a wavelength at the gap center. The results show that the efficiency of straight and bending guides is high.

Different materials have been used as the high permittivity dielectric and usually air is used as the low permittivity counterpart. Currently, fabrication of the PBG crystal starts with the bulk of the material fabricated and cut into spheres or rods and then manually arranged to form the structure, or machined in order to form the necessary air gaps. Alternatively, the use of semiconductor materials has been suggested (such as GaAs) with further anisotropic etching for the fabrication of the structure [13,14]. The difficulty associated with the fabrication of such structures, especially the ones with the 3-D periodicity, lies in the complexity of the structures involved. The size of the structure can also be a drawback for PBGs designed for the visible light regime, where the periodic lattice has to be of the order of nanometers, which makes it difficult to realize with the practical technology currently available.

Fused Deposition of Ceramics (FDC), or its variation for multimaterials (FDMM), presents several advantages for the fabrication of the PBG periodic structures for use in the microwave region, since the minimum part shapes are in the order 0.5 mm. The main advantage of this technique is the rapid prototyping of the complex design, which means that the geometry and the dimensions of a sample can be easily modified by the use of a CAD software. FDMM makes it possible to build PBG structures up to frequencies close to 100 GHz.

In this paper, we present the application of a novel fabrication technique, fused deposition of multimaterials (FDMM), to the manufacturing of PBG structures in order demonstrate their feasibility. The advantage of FDMM is the rapid prototyping of the design by the use of a CAD software and the near-net shape fabrication of the samples. While other fabrication processes make bulk pieces of the dielectric material and then cutting, drilling and/or etching is required to remove the bulk materials in order to fabricate the alternating high and low dielectric constant materials, FDMM only deposits the desired material in the fabrication procedure of the structure and is also able to fabricate PBG devices that cannot be made otherwise in a single fabrication process.

II. Experimental Procedure

The modeling was based on a finite element shareware Fortran program written by the Photonics Research Team of Imperial College (London, UK), which was adapted to this research in order to incorporate the specific structures that were modeled. This program uses the Transfer Matrix concept to solve Maxwell's equation in a complex geometry [15,16]. The input to this program are the geometry of the periodic structure as well as the frequency, ω, (or energy) of interest. For each step of ω, the corresponding wavevectors are calculated and thus the dispersion relationship can easily be obtained. Time-domain modeling was also performed using the High Frequency Structure Simulator (HFSS) commercial software from Ansoft Corporation, (Pittsburgh, PA). This is a powerful program that can perform real-time simulation of the wave propagation though 2- or 3-D dielectric or metallic periodic structures of any complex geometry. The program reflects the total electromagnetic (EM) field intensity in the region of interest and is capable of carrying out the real-time vector analysis of the EM field propagation in any structure.

The structure geometries that we have modeled with these approaches are shown in Table 1. The size of the unit cell and, in consequence, the spacing between bars and the geometry of the cross-section of each bar of the structure, was chosen so that the bandgap would lie in the 15-95 GHz frequency range. Alumina was used as the high permittivity dielectric material (relative permittivity, ε_r=9.6) and air as the low permittivity one.

The fabrication of the PBG structures was performed using the multimaterial deposition equipment designed and fabricated at Rutgers University, which is described elsewhere [17]. The feedstock materials used for the FDMM process were composites consisting of an alumina-loaded filament and ICW-06 wax (Stratasys, Inc., Eden Prairie, MN). To fabricate the alumina filament, the A152-SG alumina powder (Alcoa, New Milford, CT) was coated with a surfactant by mixing 150 g of alumina in 30 g/L of stearic acid (in toluene) and milling the mixture for 4 h. The slurry was then filtered in order to remove the solvent. The powder was dried in air and the loss on ignition test at 550 °C for 1 h indicated that the adsorption of stearic acid was 1.9 wt.%. The dried and coated alumina powder was mixed with a thermoplastic binder (ECG-9 composition, developed at Rutgers University [18]) inside a Haake System-9000 high-shear mixer (Haake-Fisons, Paramus, NJ) with a twin-roller blade mixing bowl operating at 100 rpm. The alumina powder volume fractions were 60 and 62 vol.%. The compounded alumina-binder system was then extruded at 90 °C into continuous filaments several meters long through 1.78-mm diameter nozzle using the same system but with a single screw extruding attachment.

Using the input from the PBG modeling, a CAD file was made in order to fabricate the structure using the FDMM equipment. The geometry of the PBG structure designed required the use of a supporting media under the alumina square rods. For this purpose, ICW-06 wax was used. The part was fabricated by the successive deposition of wax and alumina in a layer-by-layer manner. The alumina filament was extruded through a liquefier heated to 130 °C and provided with a 500 μm nozzle. The wax filament was extruded through a similar liquefier heated to 72 °C and with a 500 μm nozzle. The liquefier was moved by the CAD/CAM system through a predefined tool path.

To avoid the bending of the alumina bars while performing the binder-burn-out (BBO) process, it was necessary to remove the wax so that it could be replaced by a temperature resistant support material. The wax removal was performed in a furnace by placing the as-fabricated part for 10 min at a temperature of 110 °C. The de-waxed structure was then filled with zirconia powder and then subjected to the BBO cycle by heating it to 550 °C for 1 h, immediately followed by a partial sintering at 1050 °C for 1 h. The 100 to 350 °C range of the BBO cycle was carried out at 10 °C/h in order to avoid any excessive degassing of the sample from the calcination of the organic components that might structurally affect the structure. Finally, sintering was carried out at 1600 °C for 1 h.

III. Results and Discussion

3.1 Design and Simulation of PBG Structures

The objective of the theoretical simulation of the PBG structures is to solve Maxwell's equations inside the desired geometry. If it is assumed that the solution for the magnetic field is a superposition of plane waves, these equations can be reduced to a system of finite difference equations, which can be solved using standard numerical methods. As previously indicated, our simulation used two different computational methods to investigate the PBG structure. The first one, the Fortran-code software, was used to reformulate Maxwell’s equations on a lattice by dividing the space into a set of small cells with a coupling between neighboring ones [14]. Then, it calculated the propagation of the EM fields through a periodic dielectric structure in layer-by-layer manner by means of a transfer matrix [15]. The transfer matrix discretizes Maxwell's equations in a simple cubic lattice.

The transfer matrix can then be used to evaluate the bulk dispersion and transmission through a finite thickness slab of the material, since its eigenvectors are the solutions for the electric and magnetic field at each point for a given frequency ω. Then, from the eigenvalues, the band structure, k=k(ω), can be readily calculated. Since the transfer matrix T defines how waves cross a slab of the material, the transmission coefficients can also be calculated. The input to the program is the geometry of the periodic structure as well as the frequency, ω, (or energy) of interest. For each step of ω the corresponding wavevectors are calculated and thus the dispersion relationship can be obtained.

The Transfer Matrix method was applied to calculate the energy bandgap for different alumina structures with rectangular and cylindrical rods as shown in Table 1 and Figures 1 and 2. We demonstrated that the filling ratio (*i.e.*, the ratio between the volume of material in the unit cell and the total volume of the unit cell) and the dielectric constant ratios are the major factors that affect the bandgap existence and the width of the bandgap frequency. The lattice constants of the structure determine the starting frequency and the width of the bandgap. The shape of the dielectric rod is not important, and the rod can be either of a high permittivity material surrounded by air or it can be made of air rods embedded in a dielectric material. The frequency of the bandgap scales linearly with the unit cell length, which is defined by the size and the space between the rods. This is due to the linearity of Maxwell's equations.

Table 1. Simulation prediction of PBG structure.

PBG Structure	**Diameter or side dimension (mm)**	**Pitch (mm)**	**Filling ratio**	**Bandgap (GHz)**	$\omega_{gap}/\omega_{midgap}$
Cylindrical Al_2O_3 rods in air	0.625	1.25	0.39	55-75	30%
Cylindrical air rods in Al_2O_3	0.625	1.25	0.39	48-57	17%
Cylindrical Al_2O_3 rods in air	0.521	2.084	0.19	69-95	32%
Square Al_2O_3 rods in air	2	8	0.25	15-22	38%
Square Al_2O_3 rods in air	1	4	0.25	32-46	36%
Square Al_2O_3 rods in air	3	8	0.375	14-19	30%
Square air rods in Al_2O_3 rods	3	4	0.75	32-46	36%

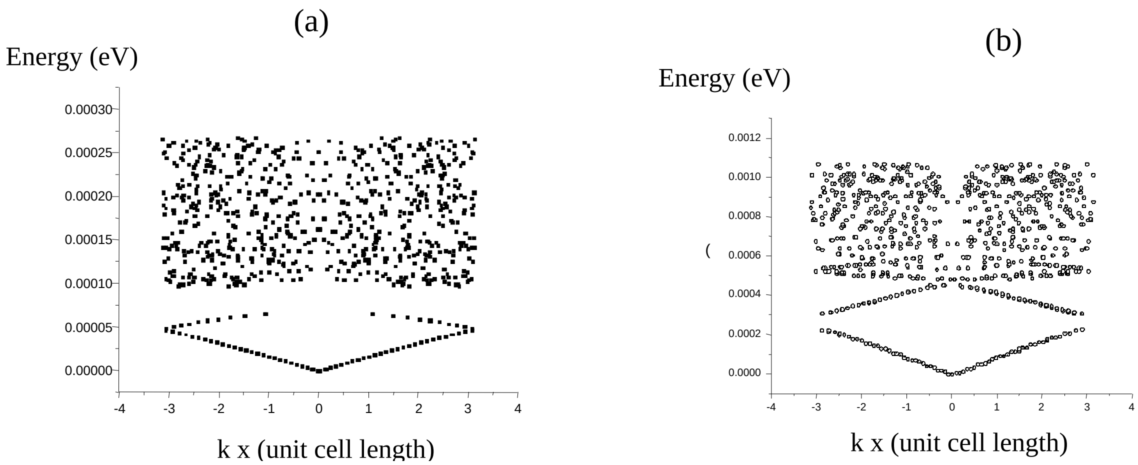

Figure 1. E(**k**) diagrams showing the band gap in alumina structures with (a) square cross-section rods (2 x 2 mm) and (b) cylindrical rods (0.625 mm diameter).

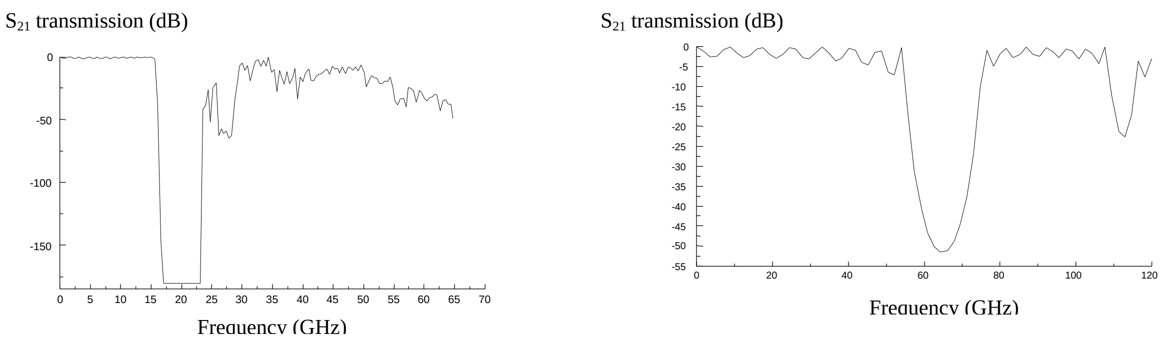

Figure 2. Transmission loss of the alumina structures (a) square cross-section rods (2 x 2 mm^2) and (b) cylindrical rods (0.625 mm diameter).

Our second approach was to solve Maxwell's equations in time-domain. For this purpose, the High Frequency Structure Simulator (HFSS) software was used. The wave-guide simulator method was used to calculate the EM wave distribution in the propagation direction (z-direction). The unit-cell concept is also applied in the simulation so that the structure is assumed to repeat in the x-y plane. The inputs for the program were the geometry of the structure, which is defined in terms of its unit cell, the monochromatic source and the boundary conditions at the surface edges. The structure used was of rectangular alumina rods of 2 x 2 mm^2 cross section, with a pitch separation of 8 mm between rods. The structure exhibits a bandgap starting around 14.7 GHz with a bandgap width of 8 GHz. Figure 3(a) shows the wave distribution at a frequency below the bandgap (12 GHz) and that the structure behaves as a homogeneous material with an effective permittivity between that of air and alumina. Figure 3(b) shows that, at frequencies inside the bandgap (16 GHz), the material behaves like a Bragg reflector, *i.e.*, all the incident energy is reflected. The transmission coefficient calculated by the HFSS program has the same bandgap range as that shown in Figure 2(a) using the T-matrix approach.

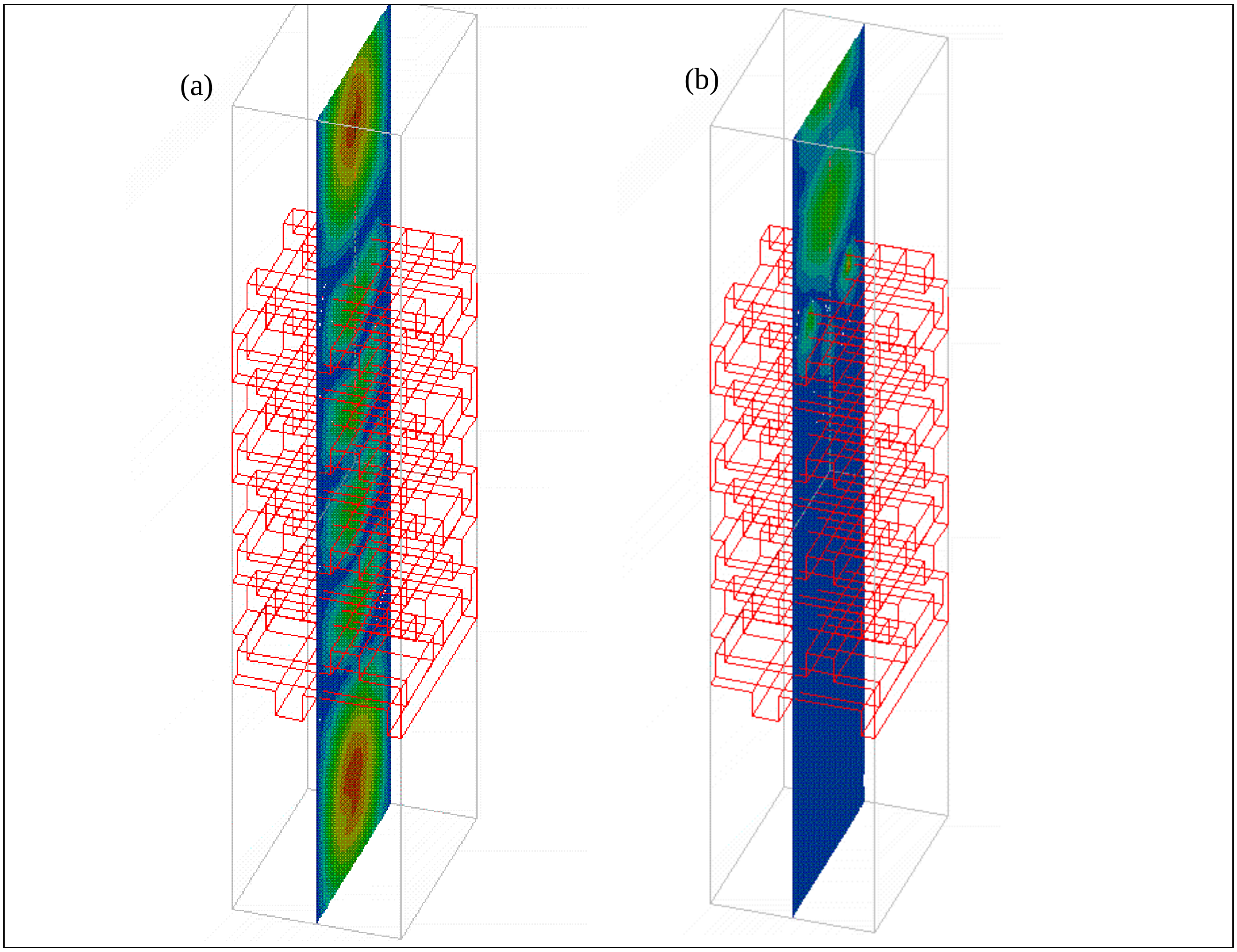

Figure 3. Electrical field distribution in the propagation direction of the PBG structure made of rectangular alumina rods of 2 x 2 mm^2 cross section, with a pitch separation of 8 mm between rods, at (a) 12 GHz (below the bandgap) and (b) 16 GHz (inside the bandgap).

3.2 <u>FDMM Fabrication of PBG Structures</u>

In order to test the FDMM process in the fabrication of the PBG structures listed in Table 1, it was decided to fabricate the 3-D logpile-type structure with alumina bars and air gaps. Each alumina bar was 28 mm long, with a 2 x 2 mm^2 square cross-section, and separated by a pitch of 8 mm. The bars are stacked in an alternating manner, parallel to each other in each layer, and perpendicular to the direction of the immediate neighboring layers. For every second layer, there is a shift in the position of the rods by half lattice constant (every fourth layer is identical, so that a unit cell is constituted by 4 rows of bars). This can be visualized better in Figure 4, which shows the CAD drawing of the unit cell structure fabricated.

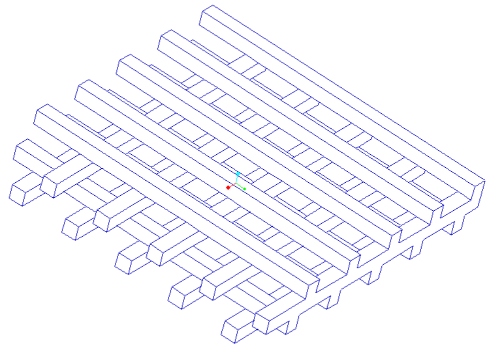

Figure 4. CAD drawing of the unit cell of the PBG structure fabricated by FDMM. Each alumina bar is 28 mm long, with a 2 x 2 mm^2 square cross-section, and separated by a pitch of 8 mm.

The FDMM fabrication of the PBG structures was made with the multimaterial deposition equipment using alumina-loaded and wax (ICW-06) filaments as feedstock materials. The fabrication was made by the successive deposition of the filaments in a layer-by-layer manner, finishing each layer before proceeding to the following one. The main problem encountered was the lack of adhesion of the alumina to the underlying wax layer. The deposition parameters (deposition speeds and mass flows) were adjusted to overcome this problem, thus improving the adhesion of the two materials so that the successive layers were able to deposit appropriately. Figure 5 shows an as-fabricated PBG structure with the wax support totally surrounding it.

The BBO cycle procedure used was the same one as for the fabrication of other electroceramic materials made with this method [19]. The wax removal was optimized so that the alumina filament would not bend due to its own weight while the wax was flowing around. The optimum temperature for the wax removal was 110 °C and at, this temperature, it only required 10 min for the wax to flow and leave all hanging bars free of underlying wax. In the BBO/presintering cycle, the parts were immersed in zirconia powder in order to provide support for the overhanging alumina bars. This procedure proved to be effective for supporting the bars while not reacting with the structure. The removal of the zirconia was simple and was done using a flow of high pressure air. Following this, the sintering cycle densified the structure, leaving the finished structure shown in Figure 6.

(a) (b) (c)

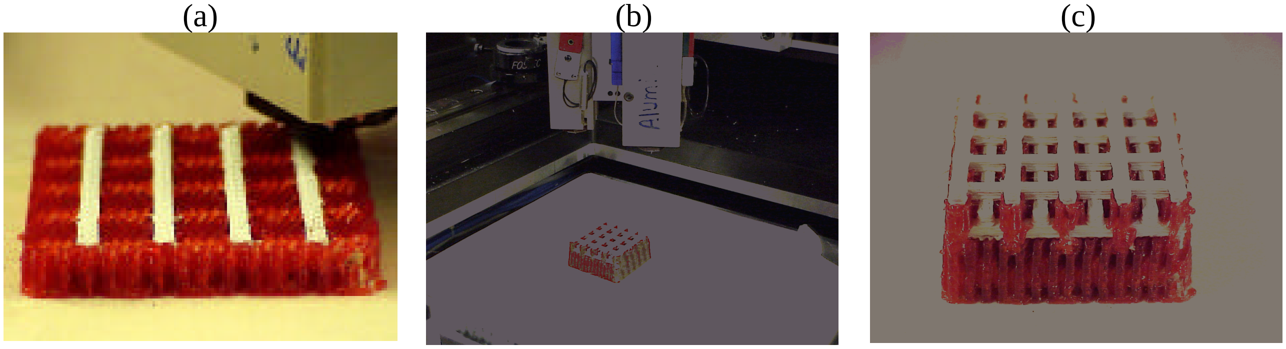

Figure 5. (a) FDMM fabrication of PBG structure showing the deposition of the alumina loaded material (white) and the ICW-06 wax (red). (b) The finished PBG structure and the two liquefiers of the FDMM system. (c) The finished FDMM structure (before thermal treatments).

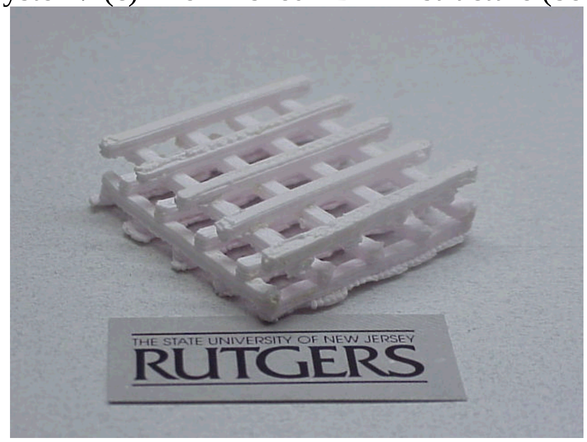

Figure 6. Structure fabricated by FDMM after sintering at 1600 °C for 1 h.

IV. Conclusions

Photonic bandgap (PBG) structures were designed and modeled in order to have possess a bandgap in the microwave frequency region. Computer simulation was performed using the T-Matrix and time-domain approaches. The results with both methods resulted in the appearance of a bandgap in the required frequency region. The modeling demonstrated that the photonic bandgap can be predicted in a structure of a given geometry and material, thus allowing the engineering of PBG structures for specific applications.

SFF has demonstrated its feasibility as a manufacturing tool to realize complex 3-D PBG structures that can be applied in the microwave frequency region. Alumina structures were fabricated using a continuous alternating multi-material deposition approach, using wax as a supporting agent in order allow the placement of the rods in long supportless areas. The successful removal of the wax, and the use of zirconia as a support agent during the BBO and presintering cycle, allowed the further sintering of the structure with minor changes in the part geometry. FDMM is found to be a promising tool for the fabrication of PBG crystals in the microwave frequency range.

Further work is required in the microwave characterization of the PBG structures in order to compare the modeling results with experimental ones.

Acknowledgments

This project has been sponsored by the New Jersey Commission of Science and Technology under the Research Excellence Program. We wish to acknowledge the helpful assistance provided in this research by Mr. Ferdus Safari and by Mr. Kian Elsayed.

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