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Optical properties of two-dimensional polymer photonic crystals after deformation-induced pattern transformations

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The photonic band structure and optical transmittance of two-dimensional periodic elastomeric photonic crystals are studied computationally to understand the effects of large strains on optical properties of the structures. The large compressive deformation patterns of the two-dimensional periodic structure studied by Mullin and coworkers [Mullin, T., Deschanel, S., Bertoldi, K., Boyce, M.C., 2007. Pattern transformation triggered by deformation. Physical Review Letters 99(8), 084301] are first reproduced using hyperelastic material models for the elastomer SU-8. Finite element analysis is then used to solve Maxwell's equations to obtain light transmittance through both the undeformed and deformed structures; simultaneously the wave equation resulting from the appropriate two-dimensional form of Maxwell's equations is solved as an eigenvalue problem to obtain the band structure. The deformation-induced shift in transmission spectrum valleys for different bands is calculated, and the changes in the width of these reflectance peaks are also obtained. The band structure calculation shows that there are no complete photonic band gaps as expected for the low dielectric contrast system. However, the effect of the observed reversible, symmetry-breaking deformation pattern is to uncouple many of the photonic bands in all three high symmetry directions, i.e. Γ–X, X–M, and Γ–M. New non-degenerate deformation-induced optical modes appear in both the real space transmittance spectra and the band structure with lower reflectance values. Analyses of the deformation pattern, the optical mode shapes, and the photonic band structure reveal that localized regions of large rotation are responsible for the significant changes in optical transmittance. The results have practical importance for the design of strain-tunable optomechanical materials for sensing and actuation.

1. Introduction

One-dimensional periodic photonic structures were studied by Lord Rayleigh in as early as 1930 (Rayleigh, 1930). Such structures have found use for a long time in the form of multi-layer dielectric stacks used commonly in reflective coatings, for example. The photonic crystal area underwent rapid development particularly after the seminal papers by Yablonovitch (1987) and John (1987), in which the physics of spontaneous emission and the theoretical existence for structured photonic materials were presented. Two-dimensional (2D) photonic crystals were studied after the successful fabrication of one such structure in the optical near-infrared range by Krauss et al. (1996). Theoretical and numerical developments in

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characterizing such 2D periodic structures include a method for calculating band structures of 2D structures as in Plihal et al. (1991), band gap calculations below infrared wavelengths in 2D structures as in Lem and Moroz (2000), study of 2D photonic slabs (Johnson et al., 1999), etc. Experimental fabrication and analysis of photonic crystal slabs are conducted in Dulkeith et al. (2005) and Foteinopoulou et al. (2001) with developments for applications such as wave splitters (Borel et al., 2005), polarization detectors (Wu et al., 2004), and waveguides (Loncar et al., 2000a, b). Other types of 2D photonic crystals include photonic crystal fibers, which are alternatives to optical wave guiding fibers (Broeng et al., 1999). Two-dimensional photonic crystals with tunable properties have also been developed. Permittivity or permeability tuning (Figotin and Godin, 1998), strain tunability (Kim and Gopalan, 2001; Li et al., 2004), and tunability by infiltrated liquid crystals (Leonard et al., 2000) are some different techniques of developing tunable 2D photonic structures.

Soft-material photonic crystals are also being used to develop tunable sensing devices. Strain-based sensing devices using such polymer-based photonic crystals are developed in Arsenault et al. (2006). A pH-based tunable three-dimensional sensor is developed using hydrogel materials by Lee and Braun (2003). The prospects for new applications using such strain- or deformation-based sensors require understanding of the complicated deformation behaviors in such two- and three-dimensional photonic crystals. By comparison, the mechanical properties of cellular structures have been studied earlier (Gibson and Ashby, 1997) for the purposes of developing light weight foams and lattices. However, for soft-material photonic crystal structures it becomes imperative to understand the coupling of the optical properties to the mechanics of structural deformation, and to understand changes in mechanical and birefringence properties of the soft material (Treloar, 1975) under large deformation. Towards this objective, it was recently noted that interesting bifurcations and pattern transformations occur in typical 2D periodic structures fabricated using elastomers under compressive deformation modes (Triantafyllidis et al., 2006). It should be noted that different fabrication techniques such as replica molding (Choi et al., 2006) and laser-based interference lithography (Zhang et al., 2008), for example, are used to fabricate such elastomer-based periodic structures; the details of the fabrication methods may influence the mechanical and optical properties as well.

Mullin et al. (2007) demonstrate using finite element analysis that an elastomeric periodic structure under large compressive strain shows interesting symmetry-breaking deformation patterns. Such pattern transformations are also observed in three-dimensional hydrogel-based inverse opal photonic sensors (Lee and Braun, 2003). This behavior is attributed to elastic instabilities in the interconnecting ligaments of the microstructure and is completely reversible. Subsequently Bertoldi and Boyce (2008) study the effect of compressive strains on such structures by conducting phononic band structure calculations. They calculate the changes in phononic band gaps (i.e. frequencies at which no elastic waves can propagate through the structure) and also changes in gap widths due to the deformation-induced pattern transformations.

In this work we study the effect of such pattern transformations on the optical characteristics of photonic crystals consisting of square lattices of circular holes in an elastomer matrix. We first analyze the deformation of the material, and then compute optical properties for the deformed structure; we do not consider the effect of incident light on the mechanical behavior, which would be negligibly small for the material we consider. Our final objective is to develop an understanding from the analysis of such pattern transformations in 2D structures that may be applied to study the functional effects of transformations in more complicated three-dimensional structures (Lee et al., 2006).

2. Model development

2.1. Model to simulate large deformation in SU-8 based two-dimensional photonic crystal

In this section nonlinear elastic models to study pattern transformations in 2D photonic crystals made of SU-8 elastomer are developed. Two model structures are analyzed: one, a complete non-repeating structure consisting of a 9×9 array of circular holes of radius r spaced periodically, with lattice constant a_0 in both Cartesian directions shown schematically in Fig. 1a; and the other, a 2×2 array of the same circular hole geometry shown in Fig. 1b, but with periodic boundary conditions to eliminate boundary effects associated with the finite 9×9 domain. The deformation of the first model structure (the complete photonic crystal) is subsequently analyzed by comparative real space optical transmittance calculations through the undeformed and deformed structures. The pattern transformations in the second model structure (the periodic unit cell case) are studied by performing comparative photonic band structure calculations between the undeformed and deformed structures.

The structures have a hole radius to lattice constant ratio of $r/a_0 = 0.44$. The structural material SU-8 is characterized by nonlinear finite elastic behavior as observed from the tensile experiments in Feng and Farris (2003). The behavior of such materials, displaying finite elastic behavior and near incompressibility, is typically described using hyperelastic material models. The neo-Hookean hyperelastic model is used here because it is appropriate for moderate strains before locking stretches are reached by the straining material (Boyce and Arruda, 2000). The neo-Hookean model is also useful for calculating stresses because the Gaussian approximation for the statistical mechanical model of photoelastic properties, as will be discussed later, uses the same neo-Hookean formulation (Treloar, 1975). The strain energy density in this formulation is given by $W = C_{10}(I_1-3)+(1/D_1)(J-1)^2$ where $C_{10} = \mu/2$ and $D_1 = 2/K$, where μ is the shear modulus, K the bulk modulus, I_1 the first invariant of the stretch tensor, i.e. $I_1 = \lambda_1^2+\lambda_2^2+\lambda_3^2$, and J the volume change ratio (Boyce and Arruda, 2000). Feng and Farris (2003) also provide detailed experimental evaluation of thermomechanical properties of the SU-8 elastomer. Following the results from that work we take the Young's modulus of SU-8 to be 2.4 GPa as obtained for a sample