Localization in shuffled-lattice random-fill structures

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Here, we demonstrate that stop-gaps can arise in "shuffled-lattices" dielectric structures even for maximally possible degree of disorder in such structures. Sharp minima of densities of states are observed in spectral regions corresponding to band gaps of unperturbed structures. Stop-gaps do survive even when shuffled-lattice sites are randomly filled with scatterers.

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It is known already for quite a long time that band gaps and sharp changes in transmission/localization length in non-absorbing dielectric structures are not the exclusive privilege of the perfect order. One does not need to have a crystalline self-translated structure as was initially professed in pioneering works of E. Yablonovich[1] and S. John.[2] They are not even optimal for having the largest band gaps [for example, for two-dimensional (2D) the optimal structures are quasiperiodic ones with long-range orientational, but not translational, order[3–5]]. To add more, fractal structures, such as one-dimensional (1D) Fibonacchi[6,7] or Cantor lattices[8,9] also demonstrate band gaps. Finally, even highly amorphous structures such as random continuous networks of dielectric rods can exhibit band gaps. Recently, it was shown that such a three-dimensional (3D) random diamond lattice (termed "an amorphous diamond") exhibits completely isotropic complete band gaps even larger than gaps of the perfectly periodic diamond structure.[10,11] The example of the amorphous diamond is especially interesting since it shows that careful introduction of randomness can lead to enhancement of the desired spectral features of the structure. Generally, interplay of randomness and order in structures of dielectric scatterers is quite complicated. For example, for finite structures, moderate random deviation in size/shape and positions of scatterers might either inhibit or enhance transmission in regions of the band gap of the perfectly periodic structure.[12–14] In 1D case, it is even possible to inhibit transmission in a desired frequency region by introducing an appropriate correlation.[15] A strong uncorrelated form or position disorder tend to obliterate spectral structure associated with interference from individual scatterers (in particular, Bragg gaps).[13,16] However, when correlations are present, the result can be quite unexpected.

In this work, we demonstrate that for certain kinds of structures even a maximally possible randomness does not obliterate spectral features associated with band gaps. To illustrate the concept, let us start with studies of localization in the simplest 1D structures. We assume that the stack is formed by two different kinds of intermittent layers: the first one (the layer A) has the refractive index n_a and the second one (the layer B) has the refractive index n_b, the permeability of both layers is taken to be unity. We take that widths of A layers remain constant and equal to a, but these layer positions are subject to random perturbations; thicknesses of jth B layer are defined as $b_j = b + \delta_j^b$, where the average thickness of B layers is b. The localization length, $\mathcal{L}$, for 1D case is calculated using a standard definition:[17] $\mathcal{L}^{-1} = -\langle \ln |T|/l \rangle$, where $|T|$ is the amplitude transmission coefficient and l is the total length of the stack, $l = \sum_{j=1}^{N}(a + b_j)$, N being the number of both A and B layers; $\langle \ldots \rangle$ denotes configurational average. For 1D structures, the transmission coefficient, T, can be calculated in a standard manner using the transfer matrix formalism.[18] Here, we consider a normal incidence.

First of all, let us consider the case when the random perturbations of distances between A layers are uncorrelated. For simplicity sake (and without much loss of generality), we take random perturbations of B layers widths to be distributed homogeneously in the interval $[-\Delta/2, \Delta/2]$. Intuitively expected results one can see in Fig. 1: for a perturbation with the amplitude Δ much smaller than the average distance b, one has a pronounced minimum of the localization length in the frequency region of the band gap of the ideal structure. When the perturbation amplitude increases, the localization length outside the gap decreases, inside the gap and in the vicinity of the gap it increases.[14] For large Δ, the gap is flattened out. Now let us consider the case when thicknesses of the neighboring B layers are correlated in such manner that A layers are shuffled randomly within defined intervals [see Fig. 1(a)], i.e., one has $b_{j+1} = b - \delta_j + \delta_{j+1}$, where random perturbations δ_j are independent (and taken to be homogeneously distributed in the interval $[-\Delta/4, \Delta/4]$). Immediately, one sees that the localization length minimum corresponding to the band gap of the ideal nonperturbed structure is affected in much smaller degree than in the case of uncorrelated B layer widths. For moderate Δ, the minimum is only slightly changed, for larger Δ, it becomes shallower but is neither shifted nor smeared. Even for maximal possible disorder there is a sharp dip in the localization length [see Fig.1(c)]. Even more, if the cells of the shuffled lattice are randomly filled with scatterers, the minimum is also surviving the maximal possible position disorder. In Fig. 1(d), it is shown that random filling with 0.75 probability makes the minimum narrower and shallower than for the completely filled shuffled lattice. However, the gap remains rather sharp.

The key to understand such survival of spectral features associated with the long-range order despite large random perturbation is the fact of shuffled lattices being an example of a hyperuniform structure.[19] The distribution of points in the d-dimensional space is hyperuniform if the variance of the point number in a sphere with the radius R grows as R^{d-1}. Whereas for uniformly random distributions of points (say, the

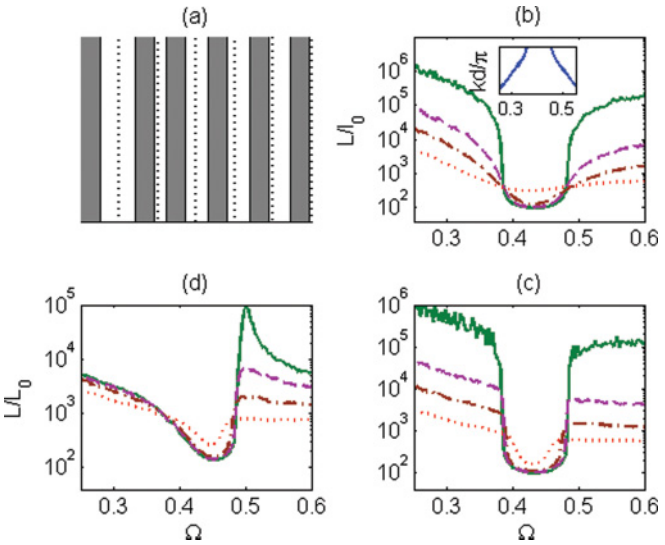

FIG. 1. (Color online) An example of 1D (a) "shuffled lattice" structure; dotted lines depict cell borders and gray blocks represent A layers. (b) The localization length $\mathcal{L}$ for the uncorrelated position disorder of A layers. The inset in (b) shows a band-gap diagram for the perfect structure demonstrating the position of the Bragg band gap. (c) $\mathcal{L}$ for the shuffled-lattice position disorder of A layers. (d) $\mathcal{L}$ for the shuffled-lattice position disorder of A layers with randomly filled cells; cells are filled with the probability 0.75. In (b)–(d), solid, dashed, dash-dotted, and dotted curves correspond to $\Delta = 1$, 6, 12, and $24l_0$, the structure of 1000 triple (B-A-B) cells was taken, $a = b = 12l_0$, refractive indices are $n_a = 1.458$ (as for silica), $n_b = 1$, $\Omega = (a+b)\omega/2\pi c$ is the normalized frequency and l_0 is the characteristic length scale; the incidence is normal.

Poissonian one) the variance grows as the volume of the sphere, and not as the surface area. Usual perfectly periodic structures, fractal ones, and the most recent example of an amorphous diamond are hyperuniform structures.[5,10,11,19] Uncorrelated position disorder breaks hyperuniformity, whereas even for the largest possible disorder the shuffled-lattice structure remains hyperuniform. It preserves long-range order,[20–22] i.e., interference effects, akin to those leading to formation of Bragg band gap, do survive. Naturally, the shuffled lattice with some scatterers randomly removed is also the hyperuniform one. In this case, one is also to expect preservation of the long-range order and collective interference effects. The consideration given above leads to a suggestion that preservation of the collective interference for the randomly filled shuffled-lattice structures will take place in structures of higher dimensions.

To demonstrate that it is indeed so, let us consider a simple example of the dielectric structure composed of a finite square lattice of square rods in the air [an example of its shuffled and randomly filled version one can see in Fig. 2(a)]. We assume that the shuffling is performed by random shifting of rods from the center of the jth cell by the vector $\vec{r}_j = \delta_j^x \vec{n}_x + \delta_j^y \vec{n}_y$, where $\vec{n}_{x,y}$ are unit vectors in directions of x and y axis, $\delta_j^{x,y}$ are independent random perturbations taken to be homogeneously distributed in the interval $[-\Delta, \Delta]$, where $\Delta \leqslant L - a$, L being the period of the lattice and a is the side of the square rod. We investigate a projected localized density of states (PLDOS) in the frequency region of the first

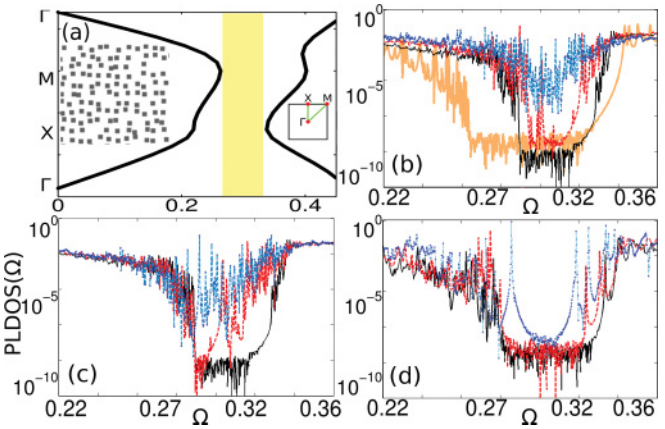

FIG. 2. (Color online) (a) A part of band-gap diagram for the perfect square lattice corresponding to the first Bragg gap; right inset shows the path through the first Brillouin zone; on the left inset is an example of a shuffled square lattice structure with 10% of scatterers missing. A maximal possible degree of shuffling disorder is considered. (b) Examples of the PLDOS for TM field averaged over 50 realizations of the structure. Thick and thin solid lines correspond to regular structure and the shuffled structure; dashed and dash-dotted lines correspond to "overshuffling" when scatterers can be moved outside the cell by $0.25a$ and $0.75a$; a is the scatterer side. (c) Examples of the PLDOS for TM field averaged over 50 realizations of the structure and (d) corresponding to single realizations of the structure are shown. Solid lines correspond to the shuffled structure with all filled cells; dashed and dash-dotted lines correspond to 5 and 10% average missing cells in the same structure; the structure is 20×20 cells. Refractive index of the square scatterers is, as for silicon, 3.42. Greens function is calculated in the geometrical center of the structure. $\Omega = L\omega/2\pi c$ is the normalized frequency.

band gap of the unperturbed structure [its band diagram in this region is shown in Fig. 2(a)]. For simplicity sake, we consider only TM waves (results for TE waves are quite similar). The PLDOS for the frequency ω at the point $\vec{r}$ can be defined in the standard manner as $\rho(\omega,\vec{r}) = \frac{2|\vec{d}|^2\omega}{\pi c^2}\vec{n}_d \cdot \mathrm{Im}[\overleftrightarrow{g}(\vec{r},\vec{r},\omega)] \cdot \vec{n}_d$, i.e., the PLDOS is the imaginary part of the macroscopic dyadic Green function convoluted with unit vectors $\vec{n}_d$ in the direction of the vector of the emitter's dipole moment $\vec{d}$, where the dyadic Green function is defined from the solution of the following inhomogeneous wave equation for the electric field:[23]

$$-\frac{1}{c^2}\epsilon(\vec{r})\frac{\partial^2 \vec{E}(\vec{r},t)}{\partial t^2} + \nabla \times \nabla \times \vec{E}(\vec{r},t) = \mu_0 \frac{\partial \vec{J}(\vec{r},t)}{\partial t},$$
$$\vec{E}(\vec{r},t) = \int_{-\infty}^{+\infty} dt' \int dr' \overleftrightarrow{g}(\vec{r},\vec{r}',t-t')\mu_0 \frac{\partial \vec{J}(\vec{r}',t')}{\partial t'}, \quad (1)$$

In these equations, $\varepsilon(\vec{r})$ is a position-dependent permittivity and $\vec{J}(r,t)$ is the source current. The Fourier domain dyadic Green function is $\overleftrightarrow{g}(\vec{r},\vec{r}',\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} \overleftrightarrow{g}(\vec{r},\vec{r}',\omega)$. The key to our approach is that the calculation of the Green function can be accomplished by solving Eq. (1) with the excitation current of the special form: $\vec{J}_{\mathrm{GF}}(\vec{r},t) = \Theta(t)\vec{d}(\vec{r}')\delta(\vec{r}-\vec{r}')/\mu_0$, where $\boldsymbol{\Theta}(t)$ is a unit step function, $\vec{d}(\vec{r}')$ is a dipole source at position $\vec{r}'$. Using this expression with Eq. (1), one gets that the electric field values equal to the time domain Green

dyadic values convolved with the source dipole: $\vec{E}(r,t) = \overleftrightarrow{g}(r,r',t) \cdot \vec{d}(\vec{r}')$. For our simulations, we have adopted this method calculating the time domain Green function by using a homemade FDTD Maxwell equation solver.[24] The results obtained are in full correspondence with the ones obtained with a fluxes-based method of PLDOS calculation.[25] Results for the PLDOS calculation one can see in Fig. 2 for the structure of 20×20 cells. One can see there examples of the PLDOS for an individual realization [see Fig. 2(d)] and examples of the PLDOS averaged over 50 realizations [see Fig. 2(c)]. For comparison, the PLDOS for the ideal unperturbed structure is shown in Fig. 2(b). Notice, that overshuffling (i.e., when scatterers can randomly move out of the cell) quickly destroys the gap [see Fig. 2(b)]. Even when the scatterer cannot move out of the nearest row of cells surrounding the given one, the gap is flattened out. But even maximal possible shuffling disorder does not lead to the degradation of the gap. Similarly to 1D case, the gap becomes narrower and the low-frequency band edge shifts rather pronouncedly toward higher frequencies. The PLDOS for different realizations of the structure differs mainly by the band edge shifts, so the PLDOS averaged over different realizations [50 for the examples considered in Figs. 2(b) and 2(c)] is quite similar to the PLDOS for a single realization. So, the PLDOS for the maximally shuffled lattice is rather close to the PLDOS for the unperturbed structure; the influence of the long-range order unbroken by shuffling is obvious. However, the shape of the field localized in the gap shows rather drastic difference. The field localized in the ideal structure has a symmetry defined by the lattice [see Fig. 3(a)]. Even a delocalized field has the same symmetry; if one places the monochromatic point isotropic source with the radiation frequency outside the gap in the center of the cell of the ideal structure, the field would leak in certain directions defined by the geometry of the structure.[26] But for the shuffled structure neither localized nor leaking fields exhibit any visible symmetry, and for different realizations, field profiles could be quite different. Simultaneously, the region of localization increases not very strongly in comparison with the ideal structure [see Fig. 3(b)]. One understands such behavior noticing that preservation of the long-range order does not mean a preservation of the local order. On a smaller scale the structure is essentially disordered. Thus one has a curious random cavity effect; the field is localized due to the long-range order, but the field profile can be quite arbitrary.

For the structure with some rods randomly missing, the difference between 1D and 2D cases is more pronounced. One can see in Fig. 2(d) that for an individual realization of the maximally shuffled structure, narrow peaks of the PLDOS arise in the gap region. For different realizations, positions of these peaks are different. In Fig. 2(c), it can be seen that for comparatively small percent of missing rods (5% in the depicted example) the gap in the averaged PLDOS still survives. However, already for 10% missing rods the gap is obliterated completely; peaks for different realizations of the structure are overlapping. The nature of these peaks in the density of states can be guessed by looking at the

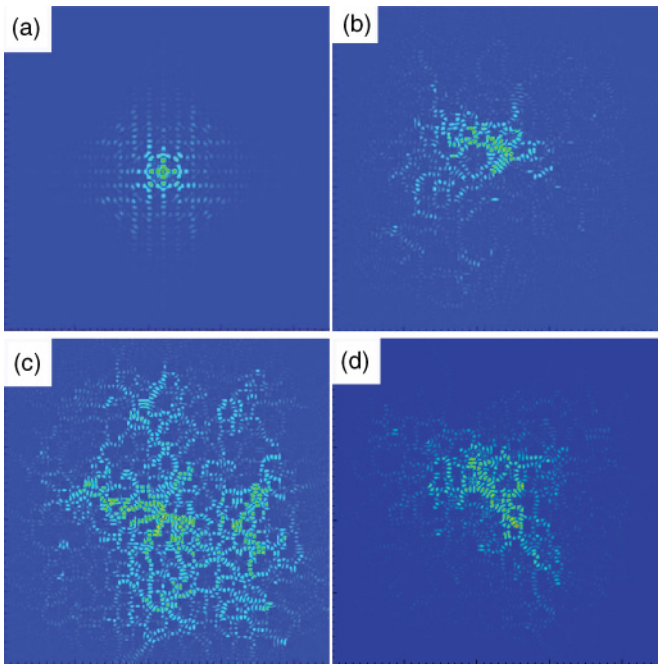

FIG. 3. (Color online) Examples of individual realizations of TM electric field distribution for the structure considered in Fig. 2. (a) The localized field distribution for the unperturbed square lattice. (b) The localized field distribution for the maximally shuffled lattice for the frequency corresponding to the gap [$\Omega = 0.27$ for Fig. 2(c)]. (c) The delocalized field distribution for the maximally shuffled lattice for the frequency corresponding to the edge of the gap ($\Omega = 0.35$). (d) The localized field distribution for 10% missing scatterers in the maximally shuffled lattice ($\Omega = 0.3$). Other data are as for Fig. 2.

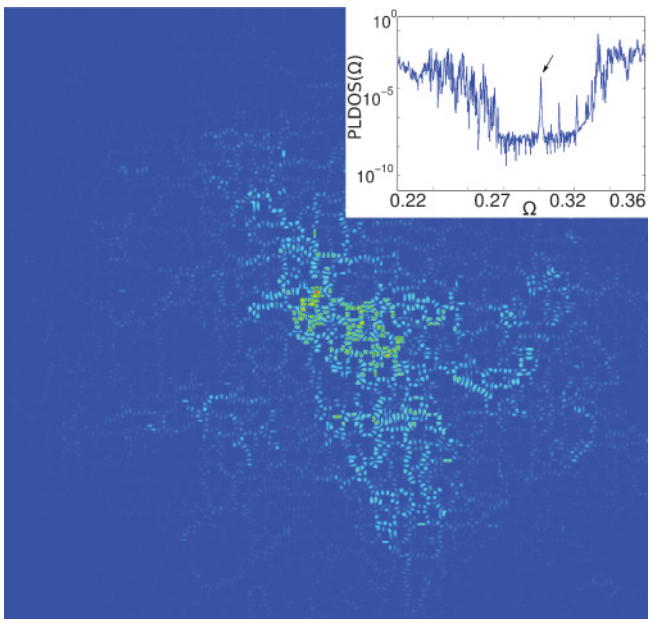

FIG. 4. (Color online) An examples of an individual realization of TM electric delocalized field distribution for the structure considered in Fig. 2 with 10% missing scatterers in the maximally shuffled lattice ($\Omega = 0.3$). The structure is 100×100 cells.The field intensity is given in respective units. Only the central part of the structure is shown, approximately 40×38 cells. The inset shows the frequency dependence of the PLDOS for such a structure; the arrow points to the frequency of the depicted field.

field profile corresponding to the center frequency of such a peak. An example is shown in Fig. 4. Here, the delocalization occurs due to occasional closeness of missing rods. The field concentrates in the regions of low permittivity. So, the chain of cavities is formed and the field can leak through this chain toward the edge of the structure. When the percentage of the missing rods increases, one has higher chances for formations of such a cavity chain. Notice that for a larger structure (for example, 100×100 shown in Fig. 4, see also the inset), peaks corresponding to the leaky modes arising in the gap are narrower than for smaller structures.

To summarize, we have shown that even maximally possible shuffling disorder occurring in the otherwise periodic lossless dielectric structures does not break band gaps arising due to collective interference effects, whereas usual uncorrelated positional disorder washes them out completely. We have demonstrated this effect on examples of 1D and 2D structures by calculating the localization length in the 1D case and the PLDOS for the 2D case. The shuffled-lattice structure is hyperuniform and is preserving the long-range order required for band-gap formation. This long-range order is not broken if some of the scatterers are missing; so, the band gap can survive even if some high-index layers or rods are randomly missing. It is interesting that for the shuffled lattice, the region of the field localization is not much larger than for the ideal unperturbed structure. However, the profile of the localized field can differ rather strongly for different realizations of the structure. Such a random cavity effect might find applications in nanophotonics and QED.

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