Unavoidable variations in size and position of the building blocks of photonic crystals cause light scattering and extinction of coherent beams. We present a model for both two- and three-dimensional photonic crystals that relates the extinction length to the magnitude of the variations. The predicted lengths agree well with our experiments on high-quality opals and inverse opals, and with literature data analyzed by us. As a result, control over photons is limited to distances up to 50 lattice parameters (~15 μm) in state-of-the-art structures, thereby impeding applications that require large photonic crystals, such as proposed optical integrated circuits. Conversely, scattering in photonic crystals may lead to different physics such as Anderson localization and nonclassical diffusion.

The promise of full control over emission and propagation of light has led to a widespread pursuit of photonic crystals in recent years. Photonic crystals are dielectric structures in which the refractive index varies periodically over length scales comparable to the wavelength of light. For three-dimensional periodicities, such crystals promise a photonic band gap, i.e., a frequency range for which emission and propagation of light are completely forbidden. Ideally, photonic-band-gap crystals will form a backbone in which many photonic devices, such as ultrasmall waveguides, cavities, and light sources, are combined to create optical integrated circuits. This requires photonic crystals with negligible optical extinction over millimeter distances.

Tremendous progress has been made in the fabrication of photonic-band-gap materials of the required high-refractive-index materials, with low point and plane defect densities. Structural variations in size and position of the building blocks, however, are intrinsic to three- (3D) and two-dimensional (2D) photonic crystals alike, amounting to at least 2–7% of the lattice spacing in all current state-of-the-art photonic crystals. While displacements are well known in condensed matter, size polydispersity of individual unit cell building blocks, including roughness, is intrinsic to metamaterials such as photonic crystals. All such variations can ultimately be traced back to basic thermodynamic arguments, but are at present probably limited by materials science. These deviations from perfect periodicity cause scattering, and hence exponential attenuation of coherent beams propagating through photonic crystals over lengths \( \ell \), also known as the “(extinction) mean free path.” After propagating over a distance \( \ell \), a coherent light beam is converted to a diffuse glow that corrupts the functionality of any photonic integrated circuit. Conversely, short mean free paths open up physics related to diffusion of light and ultimately Anderson localization of light. Therefore, it is crucial to obtain the relation between the extinction length \( \ell \) and the structural disorder. In this paper, we derive such a relation and test it against available experimental results.

We consider extinction in photonic crystals due to scattering by size polydispersity and displacements from lattice sites of the structural units (size \( r \)) that compose the unit cell (lattice spacing \( a \)). Light scattering is caused only by the difference in refractive-index profile of the displaced, slightly polydisperse building blocks as compared to the ideally ordered structure. As illustrated in Fig. 1, this difference is a collection of thin shells of high- and low-index material. The polydispersity and displacements of the building blocks translate linearly into the shell thickness \( \Delta r \). Since in many photonic crystals, such as cubic (3D) or hexagonal (2D) structures, light transport is isotropic, we treat the ideal crystal as an effectively homogeneous medium with index \( n_{\text{eff}} \) equal to the volume-averaged refractive index. Within this framework, the inverse extinction length

\[
\frac{1}{\ell} = \rho \alpha_{\text{Rayleigh}} F
\]

is the product of three factors: Rayleigh’s extinction cross section \( \alpha_{\text{Rayleigh}} \) of each shell, the number density of shells \( \rho \), and a wavelength-dependent geometrical factor \( F \) which embodies corrections beyond Rayleigh scattering. Since the volume of each shell is proportional to its thickness \( \Delta r \), Rayleigh’s extinction cross section is proportional to \( (m-1)^2 \Delta r^2 \), where \( m \) is the index contrast relative to the background medium. Even though scattering by each shell is generally weak, the huge density \( \rho \) set by the number of structural units per unit cell causes the scattering mechanism to be important. For Rayleigh scatterers, in the low-frequency limit, the dimensionless factor \( F \) equals unity. For weakly scattering shells, the Rayleigh-Gans approach is suited to find \( F \).

We now focus on the extinction length in 3D photonic crystals that consist of spheres (mean radius \( r \)), such as opals and inverse opals where many data are available. Size polydispersity results in scattering due to thin spherical shells with a Gaussian distribution of thicknesses. The inverse extinction length \( \ell \) scales quadratically with the size polydispersity \( \Delta r \) and with \( m-1 \), since Rayleigh’s extinction cross section for a shell of thickness \( \Delta r \) reads \( \alpha_{\text{Rayleigh}} = \frac{\pi}{3} k_{\text{eff}}^2 \Delta r^2 \) (cf. Ref. 14), with \( k_{\text{eff}} \) the wave vector in

\[
\ell \sim \frac{3 \pi r^2}{k_{\text{eff}}^2 \Delta r^2}
\]
the effective medium. We find that the Rayleigh-Gans correction\(^1\)

\[
F(k\_\text{eff}) = 0.78 \frac{1}{(k\_\text{eff})^2} (1 + 0.09k\_\text{eff})
\]  

(2)

reduces the well-known fourth-power Rayleigh increase of extinction to a nearly quadratic dependence on wave vector.\(^1\)\(^6\) We have checked the validity of our result using the exact Mie solution for spherical shells. Although for \(m > 2\) and \(k\_\text{eff} > 1\) the Rayleigh-Gans result underestimates the extinction loss compared to Mie theory, the Mie model reproduces the quadratic scaling with frequency and shell thickness. Our model captures the effect of both polydispersity \(\Delta r/r\) and displacements \(\Delta u/r\): calculations of \(F\) show that both effects are similar in magnitude, and can be combined by taking an effective shell thickness \(\Delta r + 0.5\Delta u\). From now on, \(\delta R\) indicates effective shell thicknesses normalized by the shell radius. An essential result of our paper is that given the current fabrication accuracies of \(\delta R \sim 5\%\), the maximum extinction length \(\ell\) is only 50 lattice spacings in high-index crystals at relevant frequencies.

Enhanced backscattering measurements obtained earlier by us have allowed us to determine the mean free path\(^5\) \(\ell\) in synthetic opals, i.e., fcc crystals of close packed polystyrene spheres with \(n = 1.59\) and \(n\_\text{eff} = 1.45\).\(^1\)\(^7\) In Fig. 2(a), we plot \(\ell\) for a wide normalized frequency range, obtained with \(\lambda = 632, 685,\) and 780 nm, and many different \(a\). We see that \(\ell\) decreases from 100\(a\) for frequencies below first-order diffraction, to 5\(a\) at the highest frequencies, where we have converted the wave vector from the scattering model to the frequency scale \(a/\lambda\) typical of photonic crystals. The data and our model agree well on both the observed decrease of \(\ell\) with \(a/\lambda\) and the magnitude of \(\ell\), which confirms that extinction is due to nonuniformities and displacements of the spheres, assuming \(\delta R = 5\%\). This value matches well with the cumulative effect of polydispersity \(\sim 2\%\) and rms displacements of spheres from their lattice sites (\(\lesssim 3.5\%\) of the nearest-neighbor distance), as independently determined by small-angle x-ray scattering.\(^1\)\(^8\) In contrast, the data refute the often assumed Rayleigh \(\omega^4\) dependence.\(^4\)\(^,\)\(^5\) The degree of extinction is also inconsistent with the common assumption that scattering is due to point defects, e.g., missing spheres:

FIG. 1. (Color) (Schematic) Any 2D or 3D real photonic crystal is an ordered stack of building blocks with a spread \(\Delta r\) in their average radius \(r\), each slightly displaced (displacement \(\Delta u\)) from the lattice sites. The real structure is the sum of the perfect crystal and the difference between the real and perfect structures. This difference is a collection of thin shells that each scatter weakly. Due to their high number density, the shells dominate the scattering loss.

FIG. 2. (Color) Symbols, mean free path (Ref. 15) \(\ell\) in units of \(a\) versus normalized frequency \(a/\lambda\) in polystyrene opals (a) and titania inverse opals (b). Open symbols in (b) were obtained by averaging for each \(a/\lambda\) total transmission spectra for many samples with different \(a\). The blue shaded area indicates the standard deviation. In the stop gap (orange bar), total transmission is reduced in excess of \(\ell/L\) due to Bragg reflection of the input beam. This affects the data in this limited range. Previous data show that \(\ell\) is unaffected if the frequency is tuned through a gap (Ref. 17). In both (a) and (b), the extinction length agrees well with the model (1) and (2) with \(\delta R \sim 5\%\) (red curves). Green curves represent scaling of \(\ell\) with \(\omega^4\), and illustrate the failure of Rayleigh scattering models.

From the cross section of a sphere\(^1\)\(^4\) we calculate that the observed scattering would require a density of missing spheres larger than 0.13\(a^{-3}\), an order of magnitude larger than the estimated density\(^6\)\(^,\)\(^9\)\(^,\)\(^1\)\(^9\) 0.01\(a^{-3}\).

We have carried out experiments to probe scattering losses in photonic crystals with high photonic interaction strength, i.e., inverse opals in a TiO\(_2\) backbone. The strength of the interaction of a photonic crystal with light is gauged by the relative bandwidth \(S\) of the lowest order gap in the dispersion relation (see Ref. 1, p. 194). The generally pursued large interaction strengths require a large index contrast \(n_{\text{high}}/n_{\text{low}}\) and are thus associated with stronger scattering, due to the factor \((m-1)^2\) in Rayleigh’s cross section. While the magnitude of the nonuniformities is similar to those in
the wide range of crystals agree with 26. Fits to our model further show that extinction lengths for
dows. Similar exponents were recently also observed in Ref.
exponents
each data set shows that extinction does not increase accord-
2–5 %, as reported in Table I. The quantitative agreement of
=650–930 nm. To obtain the absolute magnitudes of the

Given the success of our model, we can now use it to
infer the general dependence of the extinction length \( \ell/a \) on
the photonic interaction strength \( S \) and the nonuniformity \( \delta R \).
In Fig. 3 we present both \( \ell/a \) and \( S \) that are calculated as a
function of index contrast \( (m-1) \). It is clear that the extinction
length decreases both with increasing photonic strength and
with increasing structural disorder. We also present the
experimental extinction data from Table I for fcc opals and
inverse opals, showing again a good agreement with our
model with \( \delta R > 4 \%
A photonic band gap requires interaction strengths beyond \( S=0.15 \); extinction lengths less than 20
lattice spacings are expected at the current level of fabrication
accuracy. Ultimately, one hopes to realize photonic crystals
that combine many optical functions. Recent technology
roadmaps foresee crystals containing \( \sim 10^4 \) optical functions
per mm\(^2\) (Ref. 2, p. 245), requiring negligible loss over more than
millimeter distances. From the general scaling of extinction
with nonuniformity we conclude that applications of
photonic-band-gap crystals in circuits require a formidable
extension of tenfold increased perfection in statistical fabrication accuracy to \( \delta R < 0.25 \%
, or subnanometer precision. Such an improvement is far beyond the current state of the art.\(^{1,2}\)

Although 3D photonic crystals potentially offer the best
platform for photonic crystal functionality, 2D photonic crystals
possess many of the desired properties with the advantage
of ease of fabrication. While the fabrication methods
are radically different, 2D photonic crystals suffer from
polydispersity and displacements of their unit cell building
blocks analogous to 3D crystals.\(^{7,8}\) To obtain the scattering
losses, we consider 2D crystals of infinitely long cylinders.
Now, Rayleigh’s cross section per unit length \( \sigma_{Rayleigh} = (3 \pi^2)(m-1)^2 / k_{eff} \Delta r^2 \) of thin cylindrical shells of thickness
\( \Delta r \) and radius \( r \) increases with the cube of the optical frequency.\(^{14}\) In the relevant range of cylinder radii, the
Rayleigh-Gans model causes the \( \omega^{-2} \) dependence of \( \ell \) in the
Rayleigh limit to be reduced to \( \omega^{-2.2} \) since\(^{16}\)

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For a hexagonal lattice of air cylinders in silicon with \( r/a = 0.45 \), typical for macroporous silicon crystals,\(^{27} \) we find \( \ell = 40a \) for frequencies near lowest-order stop gaps, assuming a nonuniformity \( \delta r \) of 5%. A much larger \( \ell \) is required for integrated circuit applications.

Many efforts currently focus on quantifying losses in 2D crystals made from high-index slabs on lower-index cladding layers, for which the nonuniformity \( \delta r \) is around 5%.\(^{1,7,8} \) Although the guided wave profile normal to the slab is not incorporated in our model, we believe that Eq. (3) yields a reasonable estimate of scattering due to nonuniformity of the air holes in such structures. Similar to 3D, applications that rely on large structures, such as 2D photonic crystal integrated circuits, require a considerable increase in fabrication accuracies beyond the current state of the art.\(^{1,2} \) These scattering losses add to widely studied out-of-plane scattering, which could serve to enhance nonlinear interactions.\(^{10} \) As a fascinating application is the possibility to localize light, which could serve to enhance nonlinear interactions.\(^{10} \) According to the usual Ioffe-Regel criterion, Anderson localization occurs when the mean free path is so strongly reduced that its product with the wave vector equals one: \( k\ell = 1 \). It has been proposed that in photonic crystals this challenging criterion is relaxed to \( k\ell = 1/\hat{\rho}_s \), with \( \rho_s \) the modification of the photonic density of states (DOS) relative to free space.\(^{29} \)

Scattering in photonic crystals opens opportunities to explore new phenomena in multiple scattering of light.\(^{11} \) Photonic crystals allow unique control over fundamental aspects, such as the transport velocity or anisotropies of light diffusion. A fascinating application is the possibility to localize light, which could serve to enhance nonlinear interactions.\(^{10} \) According to the usual Ioffe-Regel criterion, Anderson localization occurs when the mean free path is so strongly reduced that its product with the wave vector equals one: \( k\ell = 1 \). It has been proposed that in photonic crystals this challenging criterion is relaxed to \( k\ell = 1/\hat{\rho}_s \), with \( \rho_s \) the modification of the photonic density of states (DOS) relative to free space.\(^{29} \)

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