Light transport through amorphous photonic materials with localization and bandgap regimes

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We propose a framework that unifies the description of light transmission through three-dimensional amorphous dielectric materials that exhibit both localization and a photonic bandgap. We argue that direct, coherent reflection near and in the bandgap attenuates the generation of diffuse or localized photons. Using the self-consistent theory of localization and considering the density of states of photons, we can quantitatively describe the total transmission of light for all transport regimes: transparency, light diffusion, localization, and bandgap. Comparison with numerical simulations of light transport through hyperuniform networks supports our theoretical approach.

Photonic bandgaps (PBG) and light localization fundamentally alter a dielectric material’s wave transport properties [1 2]. In 1987 Yablonovitch proposed that crystal lattices composed of high and low index dielectric materials can lead to forbidden propagation in certain electromagnetic frequency bands [3]. More recently, researchers demonstrated the existence of bandgaps also in two- and three-dimensional disordered, amorphous dielectrics based on numerical simulations and experiments [4 13]. In particular, disordered ‘hyperuniform’ photonic materials raised a lot of attention [11]. Several groups showed that these materials could exhibit isotropic complete photonic bandgaps nearly as wide as the corresponding crystal structure [4 4]. Bandgaps in amorphous dielectrics have renewed interest in strong Anderson localization (SAL) of light and other transport regimes in those materials. We, with others, proposed a transport phase diagram to organize numerical and experimental data [12 14]. However, recent three-dimensional finite-difference time-domain (FDTD) simulations have also shown that existing theoretical models cannot describe the transition between the localization and bandgap regimes [15], calling for a new and improved theoretical approach. In this letter, we introduce a theoretical model based on the self-consistent theory of localization (SC-theory) of a semi-infinite medium [15 18], together with an exponential direct reflection coefficient. We show that our model is capable of describing the transmission of light through amorphous photonic materials over the entire range of frequencies, encompassing all transport regimes.

Ballistic and diffuse transport of light. The transmission of light through non-absorbing disordered dielectrics is usually described by single scattering and multiple scattering, which turns into photon diffusion for many scattering events. For a wide slab, thickness L, the total transmission coefficient T(L) is given by a ballistic contribution, \( T_b(L) = e^{-L/\ell} \), with a scattering mean free path \( \ell \), a diffusive part \( T_d(L) \) set by the transport mean free path \( \ell^* \) and a crossover term considering the conversion of incident photons to diffusive photons via multiple scattering [19 20]. For optically dense samples (\( L \gg \ell^* \)), neglecting surface reflectivity, the diffusive total transmission coefficient is

\[
T_d(L) \simeq \frac{1 + z_0}{2z_0 + L/\ell^*} \left( 1 + z_0 \right)^{-1} \left( 1 + \frac{\ell^*}{L} \right),
\]

where \( z_0 \) is the extrapolation length ratio, a constant of order unity [19 22]. The scattering length \( \ell \) and the transport mean free path \( \ell^* \) are linked by the scattering anisotropy parameter \( g = \langle \cos \Theta \rangle d\sigma/d\Omega \) with \( \ell^*/\ell = 1/(1 - g) \). For very small scatterers, or for the case of stealthy hyperuniformity, the differential scattering cross section becomes zero, \( d\sigma/d\Omega \sim (\ell^{-1})^2 \equiv 0 \), resulting in transparency with \( T = 1 \) independent of \( L \) [13 23 24].

Anderson localization of light. Strong Anderson localization (SAL) is an interference effect in multiple scattering of waves leading to exponentially attenuated diffuse transmission through a slab. SC-theory describes SAL by introducing a position-dependent light diffusion coefficient \( D(z) \), where \( z \) denotes the distance from the surface of a wide slab [19 25]. One needs to solve an implicit equation that contains the average “return probability” which is increased in the presence of SAL and in turn reduces \( D(z) \) from \( D(0) \) at the interface to zero deep inside the medium [17 18]. To this end we replace \( L/\ell^* \) in Eq. (1) and write:

\[
\frac{L}{\ell^*} \rightarrow \frac{L}{\ell^*} \equiv \frac{1}{\ell^*} \int_0^L \frac{D_B(z)}{D(z)} dz
\]

where \( D_B = v_E \ell^*/3 \) denotes the (Boltzmann) light diffusion coefficient for a speed of light \( v_E \). Far from the localization regime \( D(z) \equiv D_B \) and \( L \equiv L \) [19 20 25]. For localization in a semi-infinite medium the SC-theory solution is \( D_\infty(z) \simeq D(0) e^{-2z/\ell^*} \), where \( \xi \) denotes the localization length. By interpolation, for a slab of finite thickness Van Tiggelen et al. proposed \( D(z) \simeq D_\infty(L/2 - |L/2 - z|) \) [17 18]. Due to the mirror symmetry relative to the center of the slab at \( z = L/2 \)
Direct coherent reflection.– Previous studies argued that
tems sizes are limited, and a study of the critical regime
deveiates. In realistic numerical simulations, the sys-
tem \( T \) the transmission probability
pends on the transport mean free path
of the single scattering angular distribution and only de-

reasoning of Magkiriadou et al. that the intensity of light
reflection, fundamentally altering the way scattered pho-
provides an even stronger, coherent mechanism for direct
the opening of a gap in amorphous photonic materials
scattering reflection. Compared to structural coloration,
for a matching wavelength, results in enhanced single
tonic glasses leads to coherent collective scattering that,
for photonic glasses \([27–29]\). Short range order in pho-
tical glasses is limited. For low frequencies, stealthy hyperuniform materials
show transparency. For weak or moderate scattering, light
transport is 'diffusive' followed by strong Anderson 'locali-
sation' (SAL) with transitions at \( \nu \) and a band-gap regime
('PBG') around \( \nu \). Closer to the gap the reduced density of
states influences localization, shaded areas. The mid-gap fre-
quency is \( \nu_G \sim 0.50 \), in agreement with the Bragg condition in a corresponding crystal \( \lambda = a/\nu' \sim 2a \).

we can take the integral in Eq. (2) from \( z \in [0, L/2] \),
\[
L = 2 \int_0^{L/2} \frac{D_B}{D(0)} e^{2z/L} dz
\]
and find
\[
T_d (L) = \frac{1}{2} \frac{1}{L_{9/7}} \left( e^{L/\xi} - 1 \right) = \frac{L_{9/7}}{\xi D_B} e^{-L/L_{9/7}}
\]
(3)

At the localization transition ('mobility edge'), the full
SC-theory, for a finite thickness \( L \), predicts a critical
power-law decay \( T_d \sim 1/L^2 \), instead of an exponen-
tial \([13]\). The onset of this power-law is captured by
Eq. (3), which can be seen by expanding \( e^{L/\xi} - 1 = L/\xi + (L/\xi)^2/2 + (L/\xi)^3/6,... \), but for thick slabs, \( L/\xi \gtrsim 3 \),
it deviates. In realistic numerical simulations, the sys-
tems sizes are limited, and a study of the critical regime
is beyond the scope of the present work.

**Direct coherent reflection.–** Previous studies argued that
the transmission probability \( T (L \gg \ell^* ) \) is independent of the single scattering angular distribution and only de-
pends on the transport mean free path \( \ell^* \), as expressed by
Eq. (1) \([13] [19] [21]\). More recent work, driven mainly by the
renewed interest in structural coloration, showed the im-
portance of explicitly adding a single scattering reflection
term in the presence of correlated disorder, for example,
for photonic glasses \([27][29]\). Short range order in pho-
tonic glasses leads to coherent collective scattering that,
for a matching wavelength, results in enhanced single
scattering reflection. Compared to structural coloration,
the opening of a gap in amorphous photonic materials
provides an even stronger, coherent mechanism for direct
reflection, fundamentally altering the way scattered pho-
tons convert into diffuse photons, Figure 1. We follow the
reasoning of Magkiriadou et al. that the intensity of light
directly reflected scales with \( \sigma_d e^{-z/\ell} \), where \( \sigma_d \) denotes the
direct reflection cross section and \( \sigma \) the total scattering
cross section. The direct reflection from layers close to
the surface is higher and the reflected intensity from inside
the sample decreases exponentially as the coherent beam attenuates \([27]\).
Simultaneously, direct reflection reduces the probability density for the creation of dif-
fuse photons within a distance \( z \) into the slab which now scales as \( \left( 1 - \frac{2\mu}{\sigma} \right) e^{-z/\ell} \) \([15][19]\). For \( \sigma_d = \sigma \), the reflection
coefficient \( R_0 = \frac{2\mu}{\sigma} = 1 \) and all light is coherently reflected in the limit \( L \gg \ell \). For \( \sigma_d < \sigma \) a propor-
tional amount \( T_d = 1 - R_0 = 1 - \frac{2\mu}{\sigma} < 1 \) can couple to the
diffuse up- and downstream of photons. Consequently,
the total transmission coefficient is lowered to
\[
T (L \gg \ell^*) = T_0 \times T_d (L)
\]
(4)

We include an approximate expression for \( T (L) \) covering
the entire range of \( L \) in the Supplemental Material, Eq. (S1).

**Numerical transport simulations.–** To check the model
predictions, Eq. (4), we performed FDTD simulations using
the open source MIT Electromagnetic Equation
Propagation (MEEP) package on a computer cluster \([13]\).
We generate hyperuniform network structures, Fig. 2 (a), using a custom-made code based on a 10,000-particle jammed seed pattern taken from ref. 32, volume filling fraction $\sim 0.64$. Jammed, random close sphere packings display nearly hyperuniform behaviour at large length scales 103, 104. All units are given relative to the diameter $a$ of the spheres of the seed pattern. Next, we perform a Delaunay tessellation of the seed pattern. The tessellation divides the pattern into tetrahedra. We connect the centres of mass of the tetrahedra with dielectric rods, creating the desired tetravalent network structure 6, 7. We apply a silicon refractive index $n = 3.6$ and a volume filling fraction of $\phi = 0.28$. We cut the digital box into slices to obtain slabs of different thicknesses $L \leq 18a$, footprint $18a \times 18a$. In the MEEP simulation, we apply periodic boundary conditions perpendicular to the propagation axis and we add perfectly matched layers (PML) at both ends of the simulation box acting as absorbers. We send a pulse of linearly polarized light and record the Poynting vector on a monitor located behind the structure. The transmission coefficient $T(L, \nu')$ is defined as the ratio of the transmitted power to the incoming power. In total we study twenty three sample packings display nearly hyperuniform behaviour at large $\xi/a < 37$ at $k\ell = (k\ell)_c = 4.1$ and at $\nu' \approx 0.53$ for $k\ell = (k\ell)_c = 2.85$, Figure 4 (b). We only consider values $\xi/a < 18$ (smaller than the system size). The agreement between theory and data is remarkable. However, we find better agreement with the dimensionless $\xi/a$ compared to the originally suggested $\xi/\ell$. Moreover the expression for $\xi$ does not consider the DOS. In a recent dissertation 37, Monsarrat derives a slightly different formula for the localisation length from SC-theory that explicitly accounts for the DOS and does not scale with $k\ell^*$ in the nominator: $\xi/\ell^* \propto 1/[\pi \rho (k\ell^*)^2]$. This expression agrees well with our data for $\xi/\ell$ if we again use $\ell^* = \ell$ and replace $k\ell$ by $k\ell^*$, 38, as shown in the Supplemental Material, Fig. S2. Note that the influence of the density of states on $\xi$ is small since $\rho < 1$ only in a regime where $k\ell/(k\ell)_c \ll 1$. 

**Density of states and coherent reflection.** It seems plausible that the normalized density of states (DOS) is responsible for the observed direct reflection since, for a full bandgap, we know that the DOS is zero and $R_0 \equiv 1$. Here we consider the DOS normalized by the density of states of the ‘homogeneous’ medium 6, 15. In and near the bandgap the coherent beam’s intensity and the z-dependent local density of states (LDOS) decay exponentially to their bulk values over a distance of a mean free
FIG. 4. Frequency dependence of the transport parameters determined from the fit to the FDTD data \( T (L) \), as described in Fig. 3 (a) Reduced mean free path \( k \ell = 2 \pi \ell / \lambda = 2 \pi \nu \ell / a \). (b) Localization length \( \xi / a \). Lines show the scaling prediction from SC-Theory, \( \xi / a \propto (k \ell)^2 / (1 - \left[k \ell / (k \ell)_c\right]^4) \), with \((k \ell)_c \approx 4.1 \) (black line) and \((k \ell)_c \approx 2.85 \) (orange line) and a prefactor of order one. The different transport regimes are indicated at the bottom. (c) Red solid squares: \( T_0 = 1 - R_0 \), compared to numerical calculations of the DOS \( \rho \) (open symbols). The DOS-data has been reproduced from ref. [6] (circles) and ref. [15] (open triangles). The arrows indicate the frequencies for the data shown in Figure 3.

path \( \ell \ll \xi \). In the bulk the mean LDOS is equal to bulk DOS \( \rho (\nu') \) and thus for \( L \gg \ell \) we expect \( T_0 (\nu') \approx \rho (\nu') \). Hasan et al., as well as Skipetrov, argued similarly when discussing finite-size effects in photonic crystals where the incident beam’s coherent intensity \( T (z) = 1 - R (z) \) and the LDOS decay exponentially. For a crystal the decay length is the Bragg length \( L_B \). Koenderink et al. discussed the attenuation of the coherent beam for the case of disorder in photonic crystals.

In Figure 4 (c) we compare the results for \( T_0 (\nu') \) from the fit to numerical simulations of the normalized optical density of states (DOS) \( \rho (\nu') \), published earlier by Hui Cao and co-workers [6] and by us [15, 34] using identical design parameters for the hyperuniform dielectric networks shown in Figure 2 (a). We find indeed \( T_0 (\nu') \approx \rho (\nu') \).

Origins of the bandgap.—Some remarks concerning the bandgap’s origins are in order. This work shows that resonant scattering in the presence of correlated disorder leads to destructive interference in the forward direction and enhanced single scattering reflection. Backscattering can also be induced by single scattering resonances [12]. This microscopic picture of preferential backscattering is supported, at least up to the lowest order, by recent diagrammatic calculations [43, 44]. Zhang-Stillinger and Torquato argued that another structural property is essential for forming a band gap. Uniformity and resulting bounded hole sizes (empty regions) prevent deep penetration of unscattered photons into the bulk of the material [35, 40]. They say that such structural “rigidity” confers novel physical properties to disordered systems, including the desired band gap. Qualitatively, stealthy hyperuniformity can provide both mechanisms. Stealthiness implies bounded hole sizes [15] and suppresses scattering at scattering angles \( \vartheta < \vartheta_c \) (\( q_0 = 2 k \sin (\vartheta / 2) < q_c \)) through collective scattering and destructive interference [11, 23]. For a quantitative microscopic assessment, however, higher-order scattering loops, beyond the collective scattering approximation, must be taken into account [43].

Summary and Conclusion—In this work, we study the transmission of light through hyperuniform, high refractive index networks using numerical simulations and theory. We propose adding a direct reflection term to the theoretical model describing light transmission through optically dense amorphous photonic materials. Combined with the results of the self-consistent theory of localization (SC-theory) for a semi-infinite medium, we derive a simple, closed-form analytical expression for the total transmission coefficient of optically dense slabs \( T_1 (L) \). Our model captures the optical transmission behavior between localization and the bandgap. Moreover, we rationalize that near and inside the gap, the reduced density of states is responsible for the coherent reflection and the attenuation of the coupling of the incident light beam to diffuse and localized transport. The quantitative agreement of our theory with numerical simulations suggests that it could be of considerable value for experimental studies. Moreover, this study shows that for an amorphous PBG material in the gap, the scattering mean free path \( \ell \) is equivalent to the Bragg length in a photonic crystal [34, 40]. This observation is essential, and the behavior is different from disordered photonic crystals, where the Bragg length is given by the periodically repeating environment and the scattering length by the degree of disorder [40, 44, 48, 49].

We thank Sergey Skipetrov and Arthur Goetschy for insightful discussions. The Swiss National Science Found-
Optics supported this work through the National Centre of Competence in Research 'Bio-Inspired Materials’, # 182881 (FS and LFP), projects number # 149867 (FS) and # 97146 (LFP).

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SUPPLEMENTAL MATERIAL

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Total transmission over the entire range of slab thicknesses. Durian’s two-stream theory for the propagation of light through a randomly scattering slab provides a simple expression for the total transmission coefficient covering the entire range of slab thicknesses from \( L = 0 \) to thick slabs [19, 20]. The theory was later reformulated and generalized in terms of a telegrapher equation [20] but the expression we use here is the same in both works. In his two-stream theory, Durian describes scattering photon transport by two concentration currents, an up- (forward) and down- (backward) stream. The theory takes into account ballistic, diffusive scattering and the cross-over regime where the incident photons are converted into diffuse photons. For classical scattering, e.g. in the absence of PBG and SAL, the theory describes transport in three dimensions more accurately than diffusion theory. Notably, it covers the cross-over regime to thin slabs and reproduces the expected \( T(L=0) = 1 \), neglecting (Fresnel) surface reflectivity at normal incidence (typically of a few percent). We can generalize the results by Durian ad-hoc by multiplying the multiple scattering term, Eq. (14) in ref. [19], by \( T_0 \). Using Eq. (S1), again with \( \ell^* \approx \ell \), we can describe the FDTD transport data for \( T(L/a, \nu') \) over the entire range of \( L/a \) as shown in Figure S1. The ad-hoc generalization appears to work well, but we note that to consistently merge SC theory with the theory by Durian, additional corrections appear as discussed in [15]. A full theoretical treatment is beyond the scope of the present work and shall be addressed in the future.

\[
T(L) = T_b + T_0 \times T_d \simeq e^{-L/\ell} + T_0 \left[ \frac{(1+z_0)}{2z_0 + L/\ell^*} \left( 1 - e^{-L/\ell} \right) - \frac{L/\ell^*}{2z_0 + L/\ell^*} e^{-L/\ell} \right]
\]

(S1)

![Figure S1](image-url)  
**FIG. S1.** Total transmission \( T(L, \nu') \) as a function of the reduced slab thickness \( L/a \) in log-log representation for two different frequencies \( \nu' \) in the localized and bandgap regime. Symbols denote the results from FDTD simulations averaged over 6 (thick slabs) to 15 (thin slabs) samples. The dash-dotted green line shows the curve fitted with Eq. (S1) over \( 7a < L < 18a \). a) \( \nu' = 0.462, \ell/a = 0.75, \xi/a = 3.6 \) and \( 1 - R_0 = 0.22 \), b) \( \nu' = 0.474, \ell/a = 0.62, \xi/a = 4.5 \) and \( 1 - R_0 = 0.09 \). The extrapolation length ratio is \( z_0 = 3.25 \), taken from ref. [15].

**Localisation length for the 3D case.** In a recent dissertation, Monsarrat proposes an expression for the localization length derived from SC-theory in 3D [37]:

\[
\xi/\ell^* = \frac{3}{2} \frac{1}{3/\pi - \rho (k\ell^*)^2}
\]

(S2)

Eq. (S2) explicitly considers the normalized DOS (\( \rho \)) and the localization length is expressed in units of \( \ell^* \). For a comparison to the values of \( \xi/a \) shown in Figure 4 (b), we again use \( \ell^* = \ell \) and replace \( k\ell \) by \( k\ell / (k\ell)^c \). Moreover, we assume \( \rho \equiv T_0 \) for the density of states, and thus all parameters are defined from the fit of Eq. (3) to the FDTD data.

\[
\xi/\ell \propto \frac{1}{3/\pi - T_0 (k\ell)^2}
\]

(S3)
We note that the influence of the density of states on $\xi$ is small since $\rho < 1$ only in a regime where $k\ell / (k\ell)_c \ll 1$.

FIG. S2. Localization length in units of the mean free path $\xi/\ell$ as a function of the dimensionless frequency $\nu' = a/\lambda$ (only data with $\xi/a < 18$ shown). Lines show the prediction from SC-Theory in three dimensions according to Monssarat [37], Eq. (S3) with $(k\ell)_{c,l} \simeq 4.1$ (black line) and $(k\ell)_{c,h} \simeq 2.85$ (orange line), input parameters from the FDTD fit and a prefactor on the order of one.

We use the same values of $(k\ell)_{c,l} \simeq 4.1$ (black line) and $(k\ell)_{c,h} \simeq 2.85$ as in Figure 4. In Figure S2 we compare the prediction by Eq. (S3) to the data for $\xi/\ell$ and find excellent agreement.