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Rough metal and dielectric layers make an even better hyperbolic metamaterial absorber

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Abstract: We numerically investigate the influence of roughness in layer thicknesses on the properties of hyperbolic metamaterials (HMMs). We show that random spatial variation of dielectric and metal layer thicknesses, similar to what occurs during actual structure fabrication, leads to dramatic absorption increase compared to an ideal, smooth-layer HMM; the absorption increases more strongly when roughness is induced throughout the HMM rather than in its surface layer only. Hence, we have found that moderate surface roughness does not deteriorate the HMM functionality, at least in absorption-related applications, thus eliminating the challenge of ultrasmooth metal layer fabrication. More severe roughness can also prove useful in the design of inexpensive HMM-based broadband absorbers.

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1. Introduction

Hyperbolic metamaterials (HMMs) are electromagnetic materials with extreme optical anisotropy that have different signs of main permittivity tensor components (for example, $\varepsilon_x = \varepsilon_y < 0$, $\varepsilon_z > 0$). For such materials the dispersion equation is hyperbolic [see Fig. 1(a)]
where \( \mathbf{k} = (k_x, k_y, k_z) \) is the wavevector and \( k_0 = \omega/c \) is the wavenumber in vacuum. Consequently, waves with very large wavevectors \( k \gg k_0 \), which cannot normally exist in isotropic or slightly birefringent dielectrics, can propagate in HMM. HMMs attracted a lot of attention due to their interesting physical properties (hyperlensing [1], existence of Dyakonov surface plasmons [2] and high-\( k \) (bulk) plasmons [3]) and various HMM applications have been proposed, including imaging, sensing, radiative decay and thermal radiation engineering [4–6].

\[
\frac{k_y^2 + k_z^2}{\varepsilon_x} - \frac{k_x^2}{|\varepsilon_{xy}|} = k_0^2,
\]

(1)

Consequently, waves with very large wavevectors \( k \gg k_0 \), which cannot normally exist in isotropic or slightly birefringent dielectrics, can propagate in HMM. HMMs attracted a lot of attention due to their interesting physical properties (hyperlensing [1], existence of Dyakonov surface plasmons [2] and high-\( k \) (bulk) plasmons [3]) and various HMM applications have been proposed, including imaging, sensing, radiative decay and thermal radiation engineering [4–6].

![Fig. 1. (a) An isofrequency contour of the HMM is hyperbolic. The inset shows an example of HMM – a layered metal-dielectric structure. (b) A schematic view of “superabsorption” effect. High-k waves scattered from an inhomogeneity on an HMM surface can couple to high-\( k \) HMM bulk plasmons.](image)

It has been also shown that the light scattered by an inhomogeneity (e.g. plasmonic nanoparticle) on the HMM surface is predominantly captured by the HMM, which significantly increases the absorption of light [7,8]. These HMM “superabsorbers” can find applications in radiation engineering and defense technology. Unlike other suggested absorbers (interference-based Salisbury screen [9], interplay of magnetic and electric resonators [10], anechoic-chamber-like gradual absorbers [11] etc.), the HMM superabsorption effect is based on a different physical principle: it is another consequence of the hyperbolic dispersion, namely, the fact that high-\( k \) spatial harmonics created by light diffraction at an inhomogeneity [see Fig. 1(b)] can be wavevector-matched with the bulk plasmons in the HMM. Recently, this principle was verified experimentally by observing increased absorption when the surface of a smoothly fabricated HMM was intentionally roughened by grinding [12].

In an ongoing quest towards a successful implementation of a multilayer HMM, the biggest challenge has been the fabrication of a large number of nanometer-thin smooth layers, which requires costly and time-consuming techniques such as atomic layer deposition. Conventional layer deposition techniques (evaporation or sputtering) introduce roughness in every layer that accumulates with increased thickness of fabricated structure. Relaxing the requirements on how smooth the layers in HMMs must be for the material to retain its properties may lower the cost of HMM-based applications dramatically, so studying the effects of layer roughness in multilayer HMMs has a very high practical relevance.

In this article we check how the accumulating roughness influences the absorbance of a multilayer HMM. We show that natural roughness in the bulk of an HMM is not detrimental to its functionality as an absorber; on the contrary, it can increase the absorbance compared to an ideal HMM with roughness only on the surface.

2. Methodology

Numerical studies are carried out in CST Microwave Studio [13]. A metal-dielectric multilayer infinitely extended in the \( x-y \) plane is modeled using the supercell approach. In the
z-direction the HMM consists of 5 pairs of metal (silver [14], Drude model, plasma frequency $1.37 \times 10^{16} \text{s}^{-1}$, collision frequency $1.4 \times 10^{14} \text{s}^{-1}$) and dielectric (alumina [15], refractive index 1.76) with thickness $T_0 = 10 \text{ nm}$ each. In the considered wavelength range (500-1000 nm), such HMM has $\varepsilon_x = \varepsilon_y < 0$, $\varepsilon_z > 0$. To simulate roughness, we divide the supercell into $5 \times 5$ regular square cells of the size $a \times a$ in the $x$-$y$ plane [Fig. 2(a)] and vary the layer thickness of each layer in each cell “column” separately [see Fig. 2(b)] according to the law $T = T_0(1 + \delta \xi)$, where $\delta$ is the “roughness parameter” and $\xi$ is a random number uniformly distributed between $-0.5$ and $0.5$. The structure starts from a flat substrate and thickness perturbation occurs in each layer, so the roughness of the structure accumulates with the layer’s number. From both sides the structure is surrounded by vacuum. Figure 2(c) shows examples of structures with varying $\delta$. We compute the absorbance $A = 1 - R - T$ for normal incidence for 5 random structures realization and then calculate the average and standard deviation. We limited ourselves in the simulations to 5 random realizations for the sake of keeping the reasonable amount of simulation time (the random metal-dielectric structure requires fine spatial meshing and is relatively large in size). Boundary conditions are the following: x-perfect electric, y-perfect magnetic, z-open. The lateral size of the considered cells $a$ (10, 30 and 100 nm) is much smaller than wavelength, so diffraction grating effects can hardly be observed.

3. Results

First, we perform numerical characterization by calculating the absorption spectra of the structures with increasing randomness $\delta$ for light incident from the flat side [Fig. 3(a)] or rough side [Fig. 3(b)] of the structure. We see that while the absorbance of the regular smooth HMM is small ($A = 0.03-0.04$, black line in Fig. 3), it monotonically increases as $\delta$ grows. The increase is much less pronounced for the light incident from the flat side since more light is reflected from the smooth surface of HMM; for $\delta = 50\%$ the absorbance is only about $A = 0.1$ at $\lambda = 600 \text{ nm}$. For rough-side incidence, the textured surface leads to much larger absorbance $A = 0.35$ at $\lambda = 600 \text{ nm}$ for $\delta = 50\%$, in agreement with earlier results [12]. We see that at the shorter wavelengths roughness has a greater overall effect, and that at these wavelengths absorbance becomes sensitive to roughness in the bulk of the structure rather than just at its surface.

An important role is played by the lateral size $a$ of the inhomogeneity. When increasing $a$ from 10 nm to 100 nm the absorbance decreases to almost regular HMM’s value [see Fig. 4(a) and 4(b) for randomness $\delta = 10\%$ and $\delta = 50\%$, respectively]. Interestingly, making the lateral inhomogeneity sizes smaller and more subwavelength (in the case of $a = 10 \text{ nm}$ it corresponds to $\lambda/100-\lambda/50$) results in larger absorbance. This rather counterintuitive fact confirms the importance of high-k waves scattered by small features on the surface and leaking into HMM.

Fig. 2. (a) Schematic of supercell division into $5 \times 5$ cells. (b) Cross-section of the structure showing accumulation of roughness from right to left. (c) Examples of structures made of 5 metal and dielectric layers with average thickness $T_0 = 10 \text{ nm}$ and randomness parameter $\delta = 0\%, 25\%$ and $100\%$.
Finally, in order to reveal the physical mechanisms behind the increased absorbance, and to distinguish the effects of randomness in the bulk vs. on the surface of the HMM, we compare our structure with accumulated randomness (R5 in Fig. 5) to the HMM with the same rough surface layer stacked with 4 ordinary smooth layers (R1O4). The results for the randomness $\delta = 10\%$ and $50\%$ are shown in the Fig. 5(a) and 5(b), respectively.

We see that the absorption for both R5 and R1O4 greatly exceeds that for ordinary smooth-layered HMM, so we confirm that the first rough layer is the most important and gives the largest increase in absorbance\textsuperscript{12}. However, we also see that the absorbance for R5 is generally larger than that for R1O4, so the roughness in the inner layers of the HMM is beneficial rather than detrimental for the overall absorbance. This also makes us conclude that the leakage channels that an HMM provides for high-k waves are largely preserved when the inside layers contain roughness.
4. Discussion and conclusions

It is of crucial importance for the hyperbolic dispersion ($\varepsilon_x < 0$, $\varepsilon_y < 0$, $\varepsilon_z > 0$) that the metal layers are continuous (which gives negative $\varepsilon_x$, $\varepsilon_y$) and separated from each other by dielectric spacers (which gives positive $\varepsilon_z$). In random HMMs with severe roughness, the outermost layers can eventually break up into clusters. Two cases are then possible. For large enough metal filling fraction, the metal “platelets” from neighboring layers can get into contact with each other, forming a continuous random sponge-like mesh conductive in all x-, y- and z-directions. In such a case, hyperbolic dispersion can hardly be preserved. The structure may, however, be a good absorber, both due to a smooth “tapered transition” from the outer medium to an HMM beneath it (randomly placed particles in the longitudinal direction can be regarded as material with gradually increasing metal filling fraction), and due to localized plasmonic resonances that trap light and absorb it eventually. The role of such localized states can be noticed by comparing the absorbance of rough HMMs with that of just a single rough outermost layer (R1) with no HMM below, as seen in the insets of Fig. 5. We see that the peaks apparently originating from localized plasmonic resonances correspond to the local maxima of R5 and R1O4 absorbance.

On the other hand, in the case of small metal filling fraction, platelets from various layers may simply be randomly distributed in the dielectric matrix. Then, absorbance may again be large due to localized plasmonic resonance and light scattering in the composite medium. Moreover, randomly distributed platelets can provide not only electric dipole resonances, but also (since two platelets separated with a dielectric spacer is a cut-wire pair forming a magnetic resonator) magnetic dipole and higher-order multipole resonances.

In the general case of a random HMM-based absorber, all these effects may be present simultaneously, as depicted in Fig. 6. First, light reflection is suppressed due to gradual “tapered” transition in the superficial layers of the random HMM. Then, light interacts with localized plasmonic resonators (electric, magnetic, higher-order multipoles) in heavily corrugated or clustered underlying layers, either absorbing the light directly or coupling it into high-k bulk HMM modes of lower-lying inner layers. These continuous but still randomly
corrugated layers absorb even more light, both by supporting high-\( k \) waves and by containing random cavities for them, where these bulk waves can oscillate and then be absorbed.

We should emphasize that no matter how random the metamaterial is the first continuous layers (counting from the flat substrate) always possess hyperbolic dispersion, while the outermost layers may or may not be “hyperbolic”. Therefore it may happen that it is no longer possible to introduce meaningful effective parameters applicable to the whole metamaterial.

![Diagram of HMM with labeled parts: tapered transition, localized resonances, hyperbolic dispersion.](image)

**Fig. 6.** The random HMM is very complex in a general case and various physical mechanisms can contribute to light absorption: reflection cancellation due to tapered air-HMM transition, localized plasmonic resonances and coupling to the high-\( k \) waves in the HMM.

One should keep in mind that the numerical model of a random hyperbolic metamaterial studied here is relevant for fabrication but still relatively simple. Obviously, in real fabrication we obtain not only longitudinal (thickness) variation, but also random variation of lateral particles sizes. Moreover, chemical composition of the constituents may vary randomly, too. Interesting effects can be observed in such complex system as random HMM, for example, Anderson localization of high-\( k \) waves.

Even such a simple model, however, shows us important indications. First of all, we confirm that roughness increases absorbance, shorter waves feeling the roughness stronger than longer waves. Second, smaller lateral roughness size results in larger absorbance, which is a counterintuitive but specific feature of HMMs where smaller rough features can excite larger-\( k \) waves. Third, and perhaps most importantly, not only the top rough layer but also the underlying rough layers play an important role in absorbance. The entire system is interesting and complex, as it combines several distinct absorption mechanisms together (Fig. 6).

The first conclusion that one can make is that absorbance in HMMs is very sensitive to the layers roughness and even small roughness (\( \delta = 10\% \) corresponds to thickness variation \( \pm 5\% \)) can increase absorbance by 2 times.

The second, much more optimistic, conclusion is that one should not put much effort into optimizing the fabrication to obtain ultra-smooth metal and dielectric layers for the HMM to act as an absorber. Naturally occurring disorder actually helps, so contrary to the common belief we can state that rough metal and dielectric layers, such as those that occur during conventional deposition techniques, make an even better hyperbolic metamaterial absorber.

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