Giant distributed optical-field enhancements from Mie-resonant lattice surface modes in dielectric metasurfaces

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Abstract: High-index dielectric nanoparticles can support strong localized Mie scattering resonances of both electric- and magnetic-dipole character. Compared to the plasmonic excitations of similar metallic nanostructures, these resonances have the distinct advantage of negligible absorption losses at the expense, however, of significantly reduced optical-field-intensity enhancements. To address this limitation, here we investigate their coherent superposition across neighboring nanoparticles in suitably designed periodic arrays via coupling to lattice surface modes. Numerical simulations show that the resulting excitations can provide giant spatially-averaged field enhancements (distributed across the entire surface of the array) with ultranarrow spectral linewidths, particularly in arrays embedded within a symmetric dielectric environment. These systems are therefore ideally suited for applications involving tailored light-matter interactions with extended-area active layers, such as surface-enhanced sensing, spectroscopy, fluorescence, and photochemistry.

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1. Introduction

The scattering of light by small particles of highly subwavelength dimensions is a subject of great fundamental and practical interest [1], which has received substantial renewed interest in the past several years in the broader contexts of plasmonics and nanophotonics. The ability of metallic nanoparticles (NPs) to support localized surface plasmon resonances (LSPRs) of highly enhanced local field intensity is well established, and has been widely investigated for applications in surface-enhanced spectroscopy, biochemical sensing, photochemistry, and optoelectronics [2]. More recently, Mie scattering resonances of high-index dielectric nanostructures have emerged as an equally promising photonic platform for similar applications [3–5]. When the incident wavelength is tuned to these resonances, dielectric NPs can also produce “hot spots” of enhanced optical field intensity, albeit typically not as strong as those of similar plasmonic nanostructures. At the same time, as long as the electronic bandgap of the NP dielectric material is sufficiently large compared to the incident photon energy, the resulting scattering resonances are essentially free of absorption losses, as opposed to LSPRs which notoriously suffer from extremely large nonradiative damping due to metallic ohmic losses. In addition, dielectric NPs can support localized resonances of both electric-dipole nature (as the fundamental LSPRs of typical metallic NPs) as well as magnetic-dipole character [6–14], which provide a promising route towards the realization of optical magnetism. Depending on the NP geometry, these electric-dipole and magnetic-dipole resonances (EDRs and MDRs, respectively) can also be made to overlap spectrally and therefore interfere with each other when excited at their mutual resonance wavelength. Under these conditions, dielectric NP arrays behave like reflectionless Huygens’ surfaces [15–18], which can then enable the development of complex waveform-shaping metasurface devices featuring extremely high transmission efficiency [19–21]. Applications of Mie resonances to enhanced light-matter interactions are also currently being investigated,
including the near-field control of fluorescence [22–29], Raman scattering [23], nonlinear harmonic generation [26,30], and biosensing [31].

Here we present a numerical study of the scattering resonances of periodic arrays of dielectric NPs with fundamental period equal, or comparable, to their EDR or MDR wavelengths (rescaled by the refractive index of the surrounding materials). In these metasurfaces, diffractive scattering of incident light at the same wavelength produces a lattice surface mode (LSM) propagating along the plane of the array, which can then interfere constructively with the localized excitations of the individual NPs. As a result, a coupled scattering resonance is produced featuring particularly narrow spectral lineshape and significantly increased field intensities in the immediate vicinity of the NP array. This effect is based on the Rayleigh-Wood anomaly which is well known in the general context of diffraction gratings [32,33]. An analogous situation is also obtained in periodic arrays of plasmonic NPs, where similarly narrow LSMs coupled to LSPRs have been predicted [34,35], measured [36–41], and applied to several useful functionalities including sensing [42], enhanced spontaneous emission [43–46], and lasing [47].

In all-dielectric systems, the coupling of LSMs and localized NP excitations has been considered in prior theoretical [48,49] and experimental [50] studies of the extinction spectra of periodic arrays, as a means to produce narrow geometrically tunable features in the optical response (reflection and transmission). More recently, the directional control and spectral shaping of light emission with similar arrays has also been reported [29]. The present work is focused on the optical-field-intensity enhancements produced by coupled LSM/Mie resonances in the near-field vicinity of the NPs. Rigorous full-wave simulations are used to quantify these enhancements and investigate their spectral properties, spatial distribution, and dependence on the surrounding dielectric environment. The key conclusion is that giant optical field intensities distributed across the entire metasurface (as opposed to concentrated within nanoscale hot spots) can be obtained, with spatially averaged enhancements as large as several 100s. Quality factors of a few 1000s are also computed for these resonances, limited by the phase mismatch between LSMs propagating in the media immediately below and above the NPs. As a result, these Mie-resonant LSMs are ideally suited for the control of light-matter interactions in extended-area active layers, with the important added benefit (compared to plasmonic systems) of negligibly small absorption losses.

2. Structure and method

The specific metasurface geometry investigated in this work consists of a square-periodic array of Si nanocylinders supported by a SiO$_2$ substrate and embedded within a polymeric cap layer [Fig. 1], although the same ideas can be extended to other periodic arrays of different symmetry, NP shape, and materials. These NPs can support pronounced Mie resonances, which have already been studied extensively in the case of non-diffracting arrays [11,14,17] (i.e., with periods $\Lambda$ well below the EDR and MDR wavelengths). The diameter $D$ and height $H$ of the nanocylinders are initially fixed at 490 and 170 nm, respectively, selected to produce strong tunable resonances across the near-infrared spectral region as the period is varied. For the refractive index of the cap layer we use $n_{\text{cap}} = 1.49$, corresponding to the commodity polymer poly(methyl methacrylate) (PMMA). For practical applications involving surface-enhanced light-matter interactions, PMMA can provide a convenient host or supporting material for the chemical species involved in the interaction process (e.g., fluorescent sources or sensing analytes). In addition, its refractive index is closely matched to that of the SiO$_2$ substrate (about 1.45 near 1550 nm), which is favorable to maximize the LSM-mediated coupling of localized resonances of distant NPs as discussed in the following.

In the simulations presented below, the metasurfaces are illuminated with a plane wave at normal incidence having linear polarization along a lattice vector of the array (the $x$ direction in Fig. 1). The local intensities of both electric and magnetic fields $|E|^2$ and $|H|^2$ are computed throughout the simulation region and normalized to those of the incident light. The resulting
electric-field-intensity enhancement is then averaged over all positions on a monitor plane parallel to the NP array across a unit cell, and plotted as a function of free-space wavelength to determine the metasurface scattering resonances. We consider both the plane through the center of the NPs and the planes at a near-field distance of 5 nm above and below their top and bottom surfaces, respectively. Insight into the nature of each resonance (MDR versus EDR) is obtained by plotting the enhancements in electric- and magnetic-field magnitudes $|E|$ and $|H|$ at the resonance wavelength as a function of position over the same monitor planes.

All simulations were carried out with a numerical solver based on the finite difference time domain (FDTD) method (FDTD Solutions by Lumerical), with a built-in model for the complex permittivity of Si and SiO$_2$ based on Ref. 51. In each calculation, the computational region consisted of a single unit cell of the NP array, with periodic boundary conditions along the $x$ and $y$ directions (as defined in Fig. 1), and perfectly matched layers (PMLs) along the $z$ direction. All relevant computational parameters including mesh size and run time were carefully optimized through extensive convergence tests. The use of periodic boundary conditions effectively produces infinite array dimensions. The peak field-intensity enhancement and spectral linewidth of the coupled LSM/Mie resonances are then limited by the refractive-index mismatch between the substrate and cap layer (again as discussed below).

3. Results and discussion

While the focus of this study is on the coupling between LSMs and dipolar Mie resonances, we begin by considering for reference a non-diffractive array with 700-nm period. The spatially-averaged electric-field-intensity enhancement spectra of this metasurface feature two pronounced peaks at 1198- and 1270-nm wavelengths [Fig. 2(a)], corresponding to the NPs’ MDRs and EDRs, respectively. This assignment is confirmed by the field-magnitude maps on the monitor plane through the center of the NPs, shown in the insets of the same figure. In the case of the shorter-wavelength resonance (left insets), the magnetic field $|H|$ (which is predominantly oriented along the $y$ direction) displays a single intensity maximum inside each NP, which therefore behaves like a magnetic dipole. Correspondingly, the electric field $|E|$ circulates around the magnetic field (mostly on the $x$-$z$ plane), leading to a two-lobe intensity pattern on the monitor plane. The opposite behavior is observed at the longer resonance wavelength (right insets), consistent with the field distribution of an $x$-oriented electric dipole centered at each NP. The general situation just described is in good agreement with prior work on similar arrays of Si nanocylinders [11,14,17]. In both resonances, significant electric-field intensity is also observed at the boundaries between adjacent unit cells of the array, mostly in the direction transverse to the $E$-field polarization, arising from the near-field (non-diffractive) coupling between neighboring
Fig. 2. (a) Electric-field-intensity enhancement spectra of a 700-nm-period array, averaged over three different horizontal monitor planes (through the center of the NPs and at a distance of 5 nm above and below their top and bottom surfaces, respectively). Insets: field-magnitude enhancement maps (on the middle monitor plane) of the resonance peaks at the indicated wavelengths. The area of each map corresponds to a unit cell of the array, and the circles indicate the NP boundaries. (b), (c) Same as (a) for a 1035-nm- and 1500-nm-period array, respectively. Right inset of (c): in-plane-averaged electric-field-intensity enhancement plotted as a function of position of the monitor plane along the $z$ axis, for the LSM/EDR resonance peak shown in this panel (E), and for the LSM/MDR resonance peak of panel (b) (M). The $z = 0$ plane in this plot runs through the center of the NPs. The dip in the M trace at the NP location is due to the MDR character of the corresponding resonance, whose electric field is mostly localized near the NP boundaries.

NPs. Finally, the spectrum of Fig. 2(a) also contains two smaller and narrower peaks at shorter wavelengths (1013 nm and 1042 nm), which are displayed more clearly in the zoom-in near the bottom left corner of the figure. These wavelengths are in excellent agreement with the array period $\Lambda = 700$ nm multiplied by the refractive indexes of the substrate and cap layer, indicating that the corresponding resonances are LSMs induced by first-order diffraction of the incident light. In the present array, such LSMs are widely detuned from the NP localized resonances, and as a result their field-intensity enhancements are very limited.

If the array period $\Lambda$ is increased, the LSM free-space wavelengths increase proportionally. At the same time, both Mie resonances are also red-shifted [52] (which may be attributed to the aforementioned transverse inter-NP near-field coupling), but at a slower rate. At a period of about 1035 nm, the (cap-layer) LSM catches up with the MDR at a free-space wavelength of 1547 nm, and as a result the corresponding resonance peak in the field-intensity enhancement spectra is dramatically increased and narrowed [Fig. 2(b)]. The hybrid nature of this excitation is clearly illustrated by the maps shown in the left insets. Inside each NP, the electric- and magnetic-field-magnitude distributions exhibit a single node and antinode, respectively, consistent with magnetic-dipole behavior. At the same time, nearly linear fringes oriented perpendicular to the $x$ direction are also observed across the entire unit cell, suggesting a strong LSM contribution originating from the $(\pm 1, 0)$ diffraction of the incident light. [Here we are using the standard notation $(p, q)$, where $p$ and $q$ are integers, to indicate the diffraction process by which the $x$ and $y$ components of the incident-light wavevector are shifted by $2p\pi/\Lambda$ and $2q\pi/\Lambda$, respectively.] In contrast, no similar features oriented perpendicular to the $y$ direction are observed in the same maps. Since oscillating magnetic and electric dipoles predominantly radiate in the direction perpendicular to their moment (i.e., in the $x$ and $y$ directions on the plane of the array for the NP MDRs and EDRs, respectively), this observation confirms the purely magnetic origin of such LSM, which represents a unique property of the metasurfaces under study. For the same array geometry, a separate EDR is also observed at longer wavelength (1605 nm), whose field-magnitude maps (right insets) retain the same general features described above for this type of excitation.
If the period is increased to 1500 nm, again for the same NP diameter and height, the LSM is further red-shifted to overlap with the EDR at a free-space wavelength of 2234 nm. As a result, the EDR peak in the field-intensity enhancement spectra [Fig. 2(c)] becomes significantly narrower and stronger than for any other values of \( \Lambda \). The corresponding field-magnitude maps are shown in the left insets: a two-lobe magnetic-field pattern inside each NP is observed together with fringes perpendicular to the y direction, consistent with a LSM originating from (0, ±1) diffraction driven by \( x \)-oriented electric dipoles. It should also be noted that the MDR peak is no longer clearly resolved in the spectrum of Fig. 2(c), which can be partly attributed to the rather small fill factor of the NPs in this array (where \( \Lambda \) is significantly larger than \( D \)), so that any localized NP resonance makes a proportionally small contribution to the spatially averaged field intensities. In addition, because the MDR in this array occurs at a wavelength shorter than the period \( \Lambda \), it can also be expected to be significantly weakened by diffractive coupling into radiation.

In the right inset of Fig. 2(c), the trace labeled E shows the spatially averaged electric-field-intensity enhancement of the LSM/EDR resonance of the same array, plotted as a function of position along the vertical direction. The trace labeled M shows similar data for the LSM/MDR coupled mode of Fig. 2(b). These plots illustrate the z-dependent spatial profile of the resonances under study. As expected, the region of high local-field intensity extends over a distance of several hundred nm from the NPs, on the order of the resonance wavelength in the surrounding media. The LSM/EDR mode of the array of Fig. 2(c) can also be seen to be less strongly confined in the plane of the NPs compared to the LSM/MDR excitation of Fig. 2(b), which is consistent with its larger resonance wavelength (for fixed NP dimensions) and thus can also explain its smaller peak enhancement.

The detailed impact of coupling dipolar Mie resonances to LSMs is quantified (for the NP design under study) in Fig. 3, where we plot the maximum value and spectral linewidth \( \Delta \lambda \) of the spatially-averaged electric-field-intensity enhancement peaks for both EDR and MDR as a function of the array period. These quantities were computed from the enhancement spectra on the monitor plane 5 nm above the top of the NPs, with the full width at half maximum of each resonance peak extracted with a Lorentzian fit. When the LSM and MDR are optimally coupled to each other [i.e., for \( \Lambda = 1035 \) nm as in Fig. 2(b)], the electric-field intensity is enhanced by a factor of 859, over 25 times larger than for the localized MDR of the same NPs in the 700-nm-period non-diffractive array of Fig. 2(a). Once again, it should be emphasized that this large field-intensity enhancement is an average value across the entire surface of the array (as opposed to a peak value at a hot spot), and the underlying resonances are broadly distributed across the whole unit cell [see top left inset of Fig. 2(b)]. Therefore, these metasurfaces are particularly well suited for the control of light-matter interactions over spatially extended layers, as opposed to carefully aligned nanoscale elements. For reference, significantly lower spatially-averaged field-intensity enhancements on the order of a few 10s have been computed for coupled LSM/LSPRs in periodic arrays of metallic NPs [41,45], although in a different wavelength region (\( \lambda < 1000 \) nm) which prevents a more direct comparison. The maximum local enhancement produced by the optimized array of Fig. 2(b) is about 4600, at four equivalent positions around each NP near the corners of the unit cell [see top left inset of Fig. 2(b)], again on the monitor plane 5 nm above the top of the NPs. At the same time, under the same optimal LSM/MDR coupling, the resonance linewidth is reduced to less than 0.5 nm at \( \lambda_0 = 1547 \) nm, corresponding to a large quality factor \( \lambda_0/\Delta \lambda \) of over 3000. This property (combined with the high field enhancements) is particularly attractive for sensing applications that rely on small spectral shifts induced by changes in the surrounding dielectric environment.

Similar results were obtained in simulations with different NP diameters and heights within the same square-periodic array geometry. As an illustration, in Fig. 4 we plot the center wavelength and spatially-averaged enhancement of the coupled LSM/MDR resonance as a function of NP
diameter (for fixed period $\Lambda = 1035 \text{ nm}$ and height $H = 170 \text{ nm}$). The value of $D = 490 \text{ nm}$ used in all calculations presented so far was selected to produce an LSM/MDR resonance peak at the representative target wavelength of 1550 nm. As $D$ is varied, a nearly linear shift in resonance wavelength is obtained (at a relatively weak rate). At the same time, large values of several 100s are computed for the enhancement factor over a broad range of values of $D$. These results are also quite relevant to the practical realization of the arrays under study, e.g., using electron beam lithography and reactive ion etching with standard Si-on-insulator (SOI) wafers. In such process, the NP diameter can be generally expected to be the most difficult to control geometrical parameter, and Fig. 4 shows that the coupled LSM/Mie resonances are relatively robust with respect to reasonable deviations from its target value. On the other hand, fabrication imperfections such as surface roughness and size inhomogeneity can produce a significant degradation in the peak enhancement and quality factor of these collective resonances, and therefore must be carefully minimized [a detailed discussion of suitable fabrication processes for dielectric metasurfaces can be found in Ref. 4].

![Fig. 3. Periodicity-dependence of MDRs and EDRs in dielectric NP arrays. (a) Maximum value and (b) spectral linewidth of the electric-field-intensity enhancement peak produced by each resonance (averaged over the horizontal monitor plane 5 nm above the top of the NPs).](image1)

Because of the diffractive nature of LSMs, the coupled resonances under study also exhibit a strong dependence on the direction of propagation of the incident light. To illustrate, we consider again the metasurface design of Fig. 2(b), where, under normal incidence excitation,

![Fig. 4. NP-diameter-dependence of the coupled LSM/MDR resonance. Squares: resonance wavelength. Circles: electric-field-intensity enhancement at resonance (averaged over the horizontal monitor plane 5 nm above the top of the NPs). In these simulations, the array period is fixed at 1035 nm.](image2)
the first-order LSMs of the array overlap with the MDRs of the NPs. The dispersive properties of the resulting scattering resonances were investigated by computing the spatially-averaged electric-field-intensity enhancement spectrum under illumination with $p$-polarized light at a variable angle of incidence $\theta$ on the $x$-$z$ plane. The results are shown in the log10-scale color map of Fig. 5, where several branches associated with different orders of diffraction [(±1, 0) and (0, ±1)] can be identified. This identification is confirmed by the dashed lines in the same plot, which show the Rayleigh-Wood anomalies corresponding to the same orders of diffraction, computed as described, e.g., in Refs. 45 and 46 with the refractive index of the cap layer. Interestingly, a large anticrossing gap is also observed in the LSM/MDR dispersion curves near $\theta = 0$ (where the different Rayleigh-Wood anomalies converge towards one another), indicative of strong coupling mediated by the NP MDRs.

![Fig. 5. Spatially averaged electric-field-intensity enhancement on the horizontal monitor plane through the center of the 1035-nm-period NP array of Fig. 2(b), plotted on a log10-scale as a function of wavelength and angle of incidence. The dashed white lines show the Rayleigh-Wood anomalies of the same array corresponding to the (±1, 0) and (0, ±1) orders of diffraction. Inset: line cut of the same color map at the wavelength indicated by the horizontal arrow.](image)

The sharp dispersive features observed in this figure are favorable to promote directional light emission, as can be argued based on reciprocity. In general, an electric-dipole fluorescent source located in the near-field vicinity of a metasurface will primarily emit into the radiation modes that produce the strongest electric-field intensity at the dipole location and emission wavelength. Therefore, the radiation pattern of a dipole near the metasurface of Fig. 5 can be estimated based on the data shown in the color map. In particular, if its emission wavelength is tuned to that of maximum field intensity at normal incidence (indicated by the horizontal arrow), the dipole will primarily radiate in the direction perpendicular to the NP array. The divergence angle of the resulting radiation pattern can be evaluated from the line cut of the color map at the same wavelength (shown in the inset), and an ultrasmall value of less than 0.3° full width at half maximum is obtained. At longer or shorter wavelengths, the electric-field intensity on the monitor plane is maximum for light incident at a finite angle $\theta_{\text{max}}$, and as a result a dipole source on this plane will primarily emit along the same off-axis directions (i.e., at ±$\theta_{\text{max}}$). Within this general framework, additional near-field beam shaping functionalities (including the possibility of asymmetric off-axis unidirectional light emission) can be envisioned with similar metasurfaces by using suitably designed asymmetric unit cells [53,54].

Finally, we investigate the importance of a close refractive-index match between the substrate and cap layer for producing maximal coupling between LSMs and localized Mie resonances. Figure 6 shows the spatially-averaged electric-field-intensity enhancement spectra of the same metasurface geometry considered so far, computed for different values of the cap index $n_{\text{cap}}$
from 1.4 to 1.0 and plotted on a log10 scale. In each trace, the array period \( \Lambda \) is selected so as to maximize the field enhancement produced by the LSM/MDR resonance (the specific values of \( \Lambda \) used in the simulations are listed in the caption). The substrate material is again SiO\(_2\), with an index \( n_{\text{sub}} \) of about 1.45. As the index difference \( \Delta n = n_{\text{sub}} - n_{\text{cap}} \) increases, the LSM/MDR resonance peak in these spectra becomes progressively weaker and broader, with an order-of-magnitude degradation in both peak value and linewidth across the five traces displayed in the figure. This behavior can be ascribed to the phase mismatch of LSMs propagating in the two surrounding media, which reduces their ability to coherently couple MDRs localized on distant NPs, and therefore effectively limits the number of unit cells that can contribute to the constructive interference responsible for the enhanced field intensity. A similar behavior has been observed in diffractive arrays of plasmonic NPs [40], where novel effects related to the impact of a finite index difference \( \Delta n \) on the array transmission resonances have also been studied more recently [55].

![Fig. 6. Electric-field-intensity enhancement spectra of the metasurface geometry of Fig. 1 (averaged over the horizontal monitor plane 5 nm above the top of the NPs), for different values of the refractive index of the cap layer \( n_{\text{cap}} \). The specific values of the array period \( \Lambda \) used in these simulations are 1020, 940, 880, 845, and 825 nm for \( n_{\text{cap}} = 1.4, 1.3, 1.2, 1.1, \) and 1.0, respectively. The sharp peak in each trace is due to the coupled LSM/MDR resonance, whereas the broader feature at longer wavelength is the EDR.](image)

It should be noted that the aforementioned prior experimental reports involving diffractive Mie resonances [29,50] have employed uncapped NP arrays with \( \Delta n \approx 0.5 \) or larger. These measurements produced reflection dips with quality factors \( \sim 10 \) [50] and directional radiation patterns with divergence angles of several degrees [29], substantially smaller and larger, respectively, than the values computed above. While several other factors may have contributed to this difference, both quantities are ultimately limited by the refractive-index-mismatch behavior just described. More in general, the results presented in Fig. 6 highlight the importance of including a suitable cap layer to maximize the ability of dielectric metasurfaces to promote and enhance light-matter interactions.

4. Conclusions

In summary, we have investigated numerically the coupling of Mie scattering resonances and LSMs in periodic arrays of dielectric NPs. The resulting excitations can produce extremely large optical-field-intensity enhancements over extended surface areas in the near-field vicinity of the NPs, combined with ultranarrow spectral bandwidths and negligible absorption losses. The simulations presented above provide a detailed quantitative description of these enhancements, including their spectral properties, spatial distribution, and dependence on angle of illumination and surrounding refractive-index contrast. While these calculations have focused on square-periodic arrays of Si nanocylinders excited by near-infrared light, similar conclusions can be
expected for different materials systems, metasurface geometries, and spectral regions. In particular, Mie-resonance LSMs at visible wavelengths could be obtained in similar arrays of NPs based on larger-bandgap dielectric materials, such as TiO$_2$ or GaP [4]. These diffractive dielectric metasurfaces therefore appear to be particularly attractive for applications that require low optical losses and large field enhancements over extended regions of space (rather than at highly localized hot spots), and that can benefit from (or at least are not limited by) extreme spectral and angular selectivity. Specific examples include surface-enhanced spectroscopy, sensing, photochemistry, and nonlinear optics, as well as spontaneous light emission with extremely high temporal and spatial coherence.

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**References**


