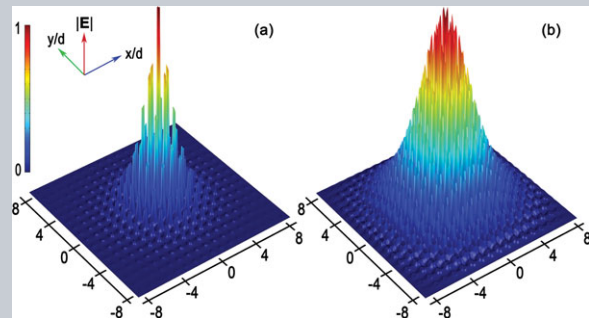


Abstract The existence and properties of plasmonic lattice solitons (PLSs) supported by periodic arrays of metallic nanowires embedded into a dielectric medium with Kerr nonlinearity are studied by solving the 3D Maxwell equations, and the conclusions are compared with the results predicted by a coupled-mode theory analysis. It is found that these two methods predict markedly different characteristics for the optical power of PLSs and its dependence on the separation distance between adjacent nanowires. In particular, the coupled-mode theory is found to be valid only when the distance between nanowires is larger than some characteristic length. The compensation of modal loss by a background optical gain is also studied and it is revealed that the gain coefficient required to balance the loss is much smaller than the



loss parameter of the metallic components of the plasmonic array.

Plasmonic lattice solitons beyond the coupled-mode theory

Ying Xue¹, Fangwei Ye^{1,*}, Dumitru Mihalache², Nicolae C. Panoiu³, and Xianfeng Chen¹

Spatial concentration and manipulation of light at subwavelength scale has become a major research area in nanophotonics, chiefly due to the technological potential of many envisioned applications as well as the theoretical and experimental challenges posed by this field of research. When the size of conventional optical circuits is decreased to nanoscale, the spatial confinement of light is inherently limited by diffraction. Because of their two-dimensional (2D) character, wave diffraction of surface plasmon polaritons (SPPs) [1–3] is markedly reduced, so that these plasma wave oscillations provide a promising solution for the control of the optical power flow at deep-subwavelength scale. Nonlinear plasmonics, which explores the nonlinear properties of SPPs, has been attracting a growing research interest [4], mostly because of the ultra-fast control of optical processes that can be achieved by employing optical nonlinearities. For example, the nonlinear Kerr effect can be used to balance the diffraction of SPPs, leading to the formation of surface beams that preserve their shape upon propagation, the so-called spatial SPP solitons [5–13]. Note that the power threshold required to generate such SPP solitons is significantly smaller than that corresponding to other species of spatial solitons, as one of the main properties of SPPs is the large field enhancement they induce.

Recently, we have proposed a plasmonic structure that makes it very convenient to investigate the properties of

a variety of subwavelength SPP solitons [8–10]. It consists of one-dimensional (1D) or 2D arrays of metallic nanowires embedded in a Kerr-type nonlinear medium, the corresponding SPP solitons being called plasmonic lattice solitons (PLSs). In such plasmonic nanostructures, tunneling of SPPs between adjacent metallic nanowires, which can be separated by just a fraction of a wavelength, is inhibited by the nonlinearity of the dielectric medium and thus deep-subwavelength PLSs can form. In this context, PLSs with various topological phase structure have been reported, including fundamental [8], vortical [9], and multipole states [10]. Such PLSs are plasmonic counterparts of the well-known discrete solitons formed in all-dielectric lattice systems, which have been actively studied in the past decades [14, 15]. However, all PLSs reported thus far have been studied using the coupled-mode theory (CMT), which assumes that the optical modes of the plasmonic nanowires or dielectric waveguides interact via their overlapping evanescent tails. As such, one expects that the CMT provides reliable predictions only when the spacing between adjacent nanowires is large enough. Therefore, a fundamental open question in this context is whether PLSs also exist in the regime where the CMT is no longer valid.

In this Letter, we study the existence and properties of PLSs beyond the CMT, by solving the complete set of 3D Maxwell equations (MEs), which rigorously

¹ State Key Laboratory on Advanced Optical Communication Systems and Networks, Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

² “Horia Hulubei” National Institute for Physics and Nuclear Engineering, Department of Theoretical Physics, 407 Atomistilor, Magurele-Bucharest 077125, Romania

³ Department of Electronic and Electrical Engineering, University College London, Torrington Place, London, WC1E 7JE, UK

*Corresponding author: e-mail: fangweiye@sjtu.edu.cn

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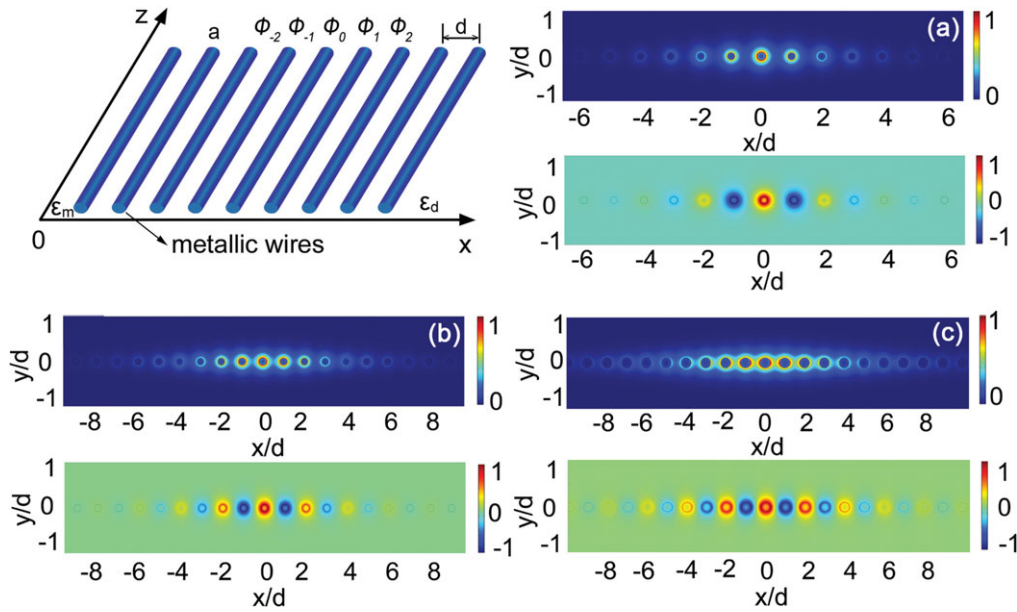


Figure 1 Schematic of an 1D array of metallic nanowire array (top left). (a), (b), and (c) show the normalized transverse profile of the amplitude (top) and the longitudinal component (bottom) of the electric field of staggered PLSs, determined for $d = 8a$, $d = 6a$, and $d = 4a$, respectively. $\delta n_{nl} = 0.045$.

incorporate the nonlinear Kerr effect. We find that, while the CMT provides a reliable description of the dynamics of the plasmonic field when the distance between nanowires is relatively large, it breaks down at short separation distance where fundamentally different physics arise. In this latter case, PLSs undergo a transition from a weak to strong coupling regime, a transformation that is correctly described only by the full set of 3D MEs. We also analyze the efficiency of the compensation of metallic losses by using the optical gain in the background material and find that, remarkably, the loss is compensated by a material gain whose coefficient is significantly smaller than the loss coefficient.

We start our study by considering 1D plasmonic lattices, as per Fig. 1, which consist of arrays of metallic nanowires embedded in a Kerr-type nonlinear medium. The intensity-dependent refractive index of the background is $n_d = \sqrt{\varepsilon_d} = 3.34 + n_2 I$, where $n_2 = 6.34 \times 10^{-20} \text{ m}^2/\text{W}$ is the Kerr coefficient and I is the light intensity. These values are similar to those of silicon. The permittivity of the metal is described by the Drude model, $\varepsilon_m = 1 - \omega_p^2 / [\omega(\omega + i\nu)]$. We assume that the plasmonic nanowires are made of silver, with the plasma and damping frequencies being $\omega_p = 13.7 \times 10^{15} \text{ rad} \cdot \text{s}^{-1}$ and $\nu = 2.7 \times 10^{14} \text{ rad} \cdot \text{s}^{-1}$, respectively [16]. The radius of the nanowires is fixed to $a = 40 \text{ nm}$, so that at telecom and in the visible spectrum the nanowires support only the fundamental SPP mode. Under these conditions, PLSs are essentially the nonlinear supermodes of the underlying guiding nanostructure.

In order to rigorously determine these nonlinear modes, one has to solve the full set of 3D MEs, which include the nonlinear Kerr effect. We thus express the electromagnetic field of PLSs as $(\mathbf{E}, \mathbf{H}) = [\mathbf{E}_0(x, y), \mathbf{H}_0(x, y)]e^{i[k_0\beta(P)z - \omega t]}$, where \mathbf{E}_0 and \mathbf{H}_0 are the transverse electric and magnetic

fields, respectively, and $\beta = \beta_r + i\beta_i$ is the complex effective index of the PLS. The mode power, P , is defined as $P = \frac{1}{4} \int_S [\mathbf{E}_0 \times \mathbf{H}_0^* + \mathbf{E}_0^* \times \mathbf{H}_0] \cdot \hat{z} dS$ and $k_0 = 2\pi/\lambda$ is the wave number in vacuum. The nonlinear supermodes of the array are then found self-consistently as follows [17]: we first assume that the permittivity of the dielectric host surrounding a certain metallic nanowire is slightly larger than in the other regions, which allows us to find a defect (localized) mode. For this we used a finite-element mode solver available in the COMSOL Multiphysics suit [18]. The electromagnetic field of the computed defect mode is then normalized such that it induces through optical Kerr effect a predefined maximum change of the refractive index, δn_{nl} . This scaled defect mode is then used to compute the nonlinear change of the refractive index, $\delta n_{nl}(x, y) = n_2 |\mathbf{E}(x, y)|^2$. This nonlinear index is fed back into the mode solver and the defect mode is computed again. These steps are repeated until a convergence is reached, namely, until the variation of the effective mode index, $\beta(P)$, between consecutive iterations becomes smaller than 10^{-6} .

Generic PLSs found by using this approach are shown in Fig. 1. As the dielectric host (silicon in our case) has self-focusing nonlinearity, only *staggered* PLSs exist. This situation is just the opposite to case of usual dielectric lattice systems due to the inversion of the spatial dispersion relation in plasmonic crystals [8]. In this context staggered PLSs means that the E_z field component in adjacent nanowires points in opposite directions [8]. Figures 1(a) through 1(c) show three different types of PLSs, which exist in what we call the plasmon regime, the intermediate regime, and the gap plasmon regime, respectively. Plasmon regime refers to the case when the distance between

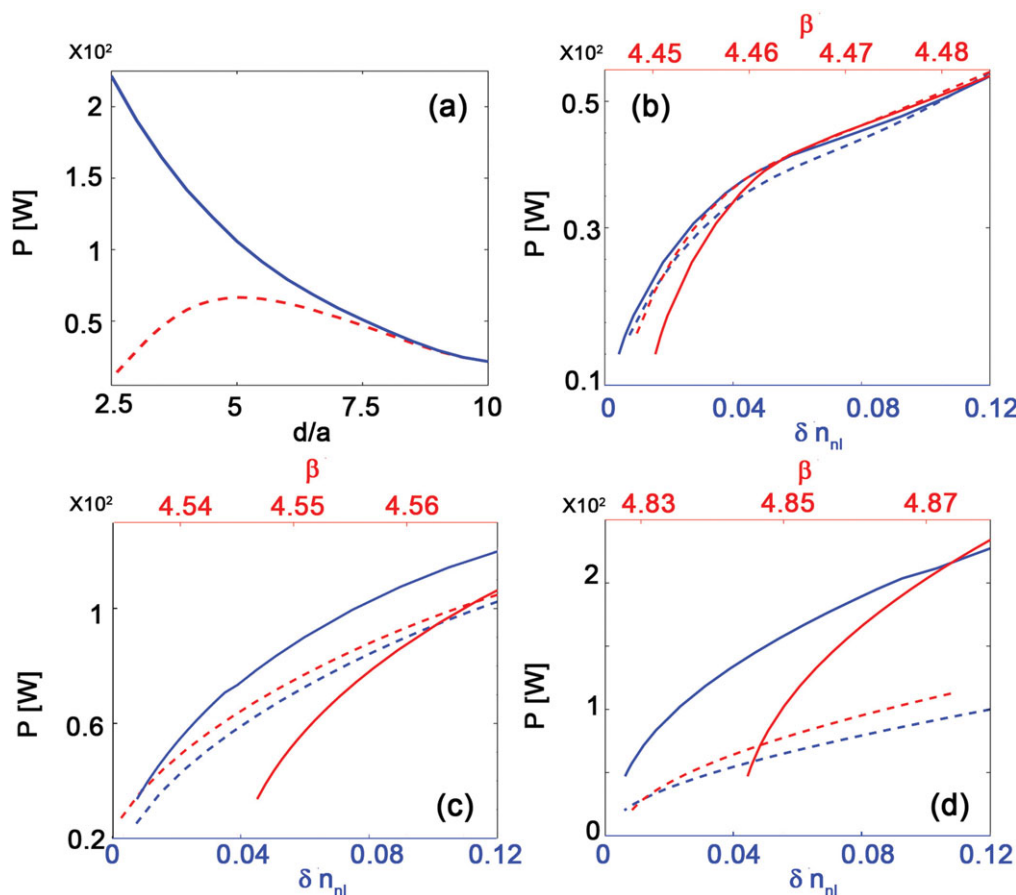


Figure 2 Comparison between the predictions of the CMT (solid lines) and MEs (dashed lines). (a) The soliton power vs. separation distance, for $\delta n_{nl} = 0.045$. (b), (c), and (d) show the soliton power vs. δn_{nl} (blue lines) and β (red lines), for $d = 8a$, $d = 6a$, and $d = 4a$, respectively.

nanowires is relatively large. In this regime, the interaction between nanowires is determined by the evanescent coupling between the corresponding plasmon modes. As a result, PLSs can be viewed as a superposition of plasmon modes of isolated metallic cylinders [see Fig. 1(a)] and therefore one expects that this regime can reliably be described by the CMT. By contrast, when the spacing between nanowires is small, the nanowires interaction increases significantly, so that most of the optical field is confined in the gaps separating the nanowires [see Fig. 1(c)]; we therefore call this case the gap plasmon regime [19, 20]. In particular, in this regime PLSs can be viewed as a superposition of gap plasmonic modes of nanowire pairs. Importantly, this regime cannot be described by the CMT as the interaction between the nanowires is no longer weak. Finally, in the intermediate regime, the optical field is distributed neither close to the nanowires nor in the gaps between them but rather uniform through the plasmonic array [see Fig. 1(b)]. Therefore, by continuously varying d , one can smoothly switched the PLSs among these three regimes.

Before we compare the results predicted by the CMT with those calculated by using the MEs, we briefly describe the CMT. Thus, a rigorous analysis based on the Lorentz reciprocity theorem [8, 21] shows that the amplitudes of the

plasmon modes of the nanowires are governed by a system of coupled discrete nonlinear Schrödinger equations,

$$i \frac{\partial \Phi_n}{\partial z} + \kappa(\Phi_{n-1} + \Phi_{n+1}) + \gamma |\Phi_n|^2 \Phi_n = 0, \quad (1)$$

where Φ_n is the normalized mode amplitude associated with the n th nanowire. The nonvanishing field components of this mode, e_r , e_z , and h_ϕ , depend only on the radial coordinate, r_\perp . Note that this model can be relevant to gap polariton solitons as well [22]. In Eq. (1), κ is the coupling coefficient between nanowires, which can be calculated using the $\mathbf{e}(r_\perp)$ and $\mathbf{h}(r_\perp)$ fields of the corresponding plasmon mode and the distribution of the dielectric constant, $\varepsilon(r_\perp)$ [8]. The modal fields in the n th nanowire are $\mathbf{E}(\mathbf{r}) = \mathbf{e}_n(r_\perp) e^{i(\beta_0 k_0 z - \omega t)}$ and $\mathbf{H}(\mathbf{r}) = \mathbf{h}_n(r_\perp) e^{i(\beta_0 k_0 z - \omega t)}$, where β_0 is the effective refractive index of the plasmon mode. The parameter γ is the effective nonlinear coefficient of the plasmon mode, with $\gamma > 0$ for a medium with self-focusing Kerr response.

The comparison of the results predicted by the CMT and the MEs are summarized in Fig. 2. Thus, Fig. 2(a) shows the dependence of the soliton power, P , on the nanowire spacing, d , for a fixed value of the maximum variation of the nonlinear refractive index, $\delta n_{nl} = 0.045$. As the plots

illustrate, when the distance between nanowires is larger than some characteristic value, $d \gtrsim 8a$, the CMT and MEs agree very well. In this plasmon regime, the soliton power decreases with the increase of d . This is because the coupling between nanowires becomes weaker with the increase of d , and thus the power required to balance the coupling-induced diffraction decreases. Note, however, that while the CMT predicts a monotonous variation of the soliton power with d , an analysis based on the MEs shows that the soliton power does not increase beyond a maximum value, which in our case is reached when $d \simeq 5a$. More specifically, when $d \lesssim 5a$, namely in the gap plasmon regime, the soliton power increases with d until it reaches its maximum and then decreases monotonously with d . The decrease of P with decreasing d in the gap plasmon regime can be explained by the field profiles shown in Fig. 1(c). Thus, in this regime, as d decreases the optical field becomes confined primarily in the gaps between nanowires and consequently the field enhancement at the surface of the nanowires decreases. This decrease in the field enhancement results in a reduced nonlinear optical response and thus smaller P . We note that, although Eq. (1) only retains the nearest-neighbor nanowire coupling, adding next-nearest-neighbor coupling will not improve the predictions of the CMT. The reason for this is that in the intermediate and gap plasmon regimes the discrepancy between CMT and MEs stems from the strong mode reshaping rather than from neglecting the long-range coupling [23].

The dependence of the soliton power on δn_{nl} and soliton wave number, β , determined in the three different regimes, is presented in Figs. 2(b)–2(d). One can see that, as expected, in the plasmon regime the predictions based on the CMT agree very well with those derived from the MEs. However, the differences between the results predicted by the two methods increase as the separation distance decreases and become significant at small d 's.

In what follows we study the influence of metallic losses on PLSs and the degree to which these losses can be compensated by optical gain. Figure 3(a) displays the dependence on d of the imaginary part of the effective mode index of PLSs, β_i . It can be seen that when d is large, the mode loss is essentially independent on d . This is because for large values of d the optical coupling between nanowires is

weak and therefore the optical loss of PLSs is essentially equal to the loss of the plasmon mode of an isolated metallic nanowire. However, the optical loss of PLSs increases rapidly as d decreases, which suggests that a larger fraction of the optical field penetrates into the metallic components of the plasmonic array.

A remarkable property of PLSs, which can have important experimental implications, is that their optical loss can be compensated by a surprisingly weak optical gain. In order to illustrate this salient feature of PLSs, we assume that the nonlinear dielectric host contains optical gain that is provided, for example, via pumped quantum dots or quantum wells [24]. Thus, the refractive index of the background gain medium is considered to be $n_d = \sqrt{\varepsilon_d + \alpha i} + n_2 I$, where α is the gain coefficient. We perform our analysis for two wavelengths, $\lambda = 1550$ nm and $\lambda = 632.8$ nm, in both cases varying the gain coefficient from $\alpha = 0$ to $\alpha = 0.15$. The results are summarized in Fig. 3(b), where the dependence of β_i on α is presented.

The plots in Fig. 3(b) reveal two significant features of PLSs. First, the dependence $\beta_i(\alpha)$ is almost linear. The reason for this is that the loss/gain part of the permittivity of the metal and the gain medium is much smaller than the corresponding real part (this is particularly true in the case of metals). As a result, the field profile of PLSs remains almost unchanged as one varies α . As the effective loss of the mode is given by a certain spatially weighted average of the imaginary part of the permittivity over a nearly unchanged modal field profile, it can be seen that indeed the overall modal loss coefficient must depend on the gain/loss parameters almost linearly. Second, the gain coefficient for which the loss is compensated differs significantly from the loss coefficient of the metal, and, it is found to be much smaller than the latter one. More specifically, our simulations show that $\beta_i = 0$ is achieved at $\alpha_{\text{cr}} = 0.1 \ll 2.8426$ for $\lambda = 1550$ nm and $\alpha_{\text{cr}} = 0.087 \ll 0.1935$ for $\lambda = 632.8$ nm. In other words, at both wavelengths, the critical value of the gain coefficient, α_{cr} , at which the optical gain exactly balances the metal loss, is more than 20 times smaller than the loss coefficient. This important result is explained by the fact that PLSs do not distribute their energy evenly between the metallic and gain regions; instead, the amount of energy confined inside the nanowires is more than 20 times smaller than that flowing in the dielectric region.

Finally, we consider PLSs formed in 2D arrays of metallic nanowires. Since the general characteristics of these solitons are similar to those of their 1D counterparts, we only briefly discuss them here. Figures 4(a) and 4(b) display the spatial profile of the normalized electric field amplitude corresponding to $d = 8a$ and $d = 3a$, respectively. Similarly to the case of 1D PLSs, there are also two distinct types of 2D PLSs: plasmon solitons whose total field can be represented as the superposition of plasmon modes of individual metallic nanowires [Fig. 4(a)] and gap plasmon solitons whose total field consists of a superposition of gap plasmon modes of pairs of metallic nanowires [Fig. 4(b)]. In the plasmon regime the soliton properties can accurately be described by both the MEs and the CMT [Fig. 4(c)], whereas in the gap plasmon regime there are significant discrepancies

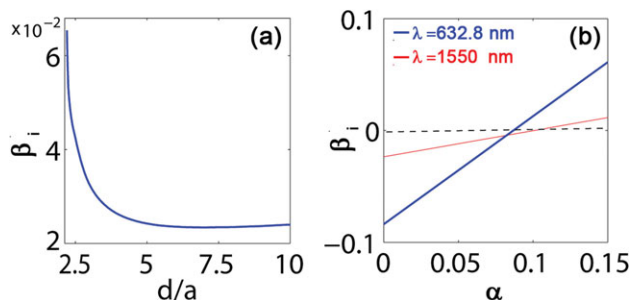


Figure 3 (a) Imaginary part of the mode index vs. d , determined for $\lambda = 1550$ nm and (b) vs. the gain coefficient α , determined for $\lambda = 1550$ nm and $\lambda = 632.8$ nm. In both cases, $\delta n_{\text{nl}} = 0.045$.

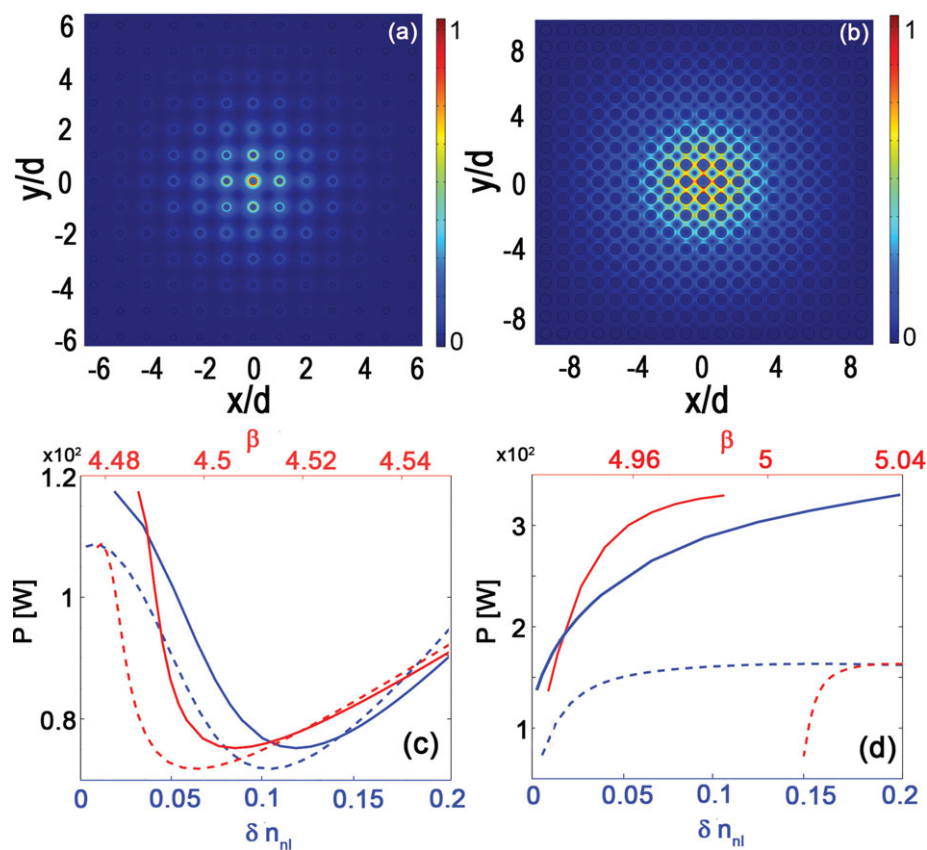


Figure 4 Normalized electric field amplitude (top panels) and the soliton power vs. δn_{nl} (blue lines) and β (red lines) (bottom panels). Left (right) panels correspond to $d = 8a$ ($d = 3a$). Dotted and solid lines correspond to calculations based on the MEs and the CMT, respectively. Calculations are performed for $\lambda = 1550$ nm, $a = 40$ nm, and $n_2 = 6.339 \times 10^{-20}$ m²/W. For (a) and (b), $\delta n_{nl} = 0.045$.

between the predictions of the CMT and MEs [Fig. 4(d)]. In particular, the large discrepancy in the dependence $\beta(P)$ suggests that the two methods would predict very different parameter domains in which 2D PLSs exist and are stable.

In conclusion, by solving the complete set of 3D Maxwell equations, we have investigated the existence and properties of plasmonic lattice solitons formed in 1D and 2D arrays of metallic nanowires embedded into a host dielectric medium with Kerr nonlinearity. Our analysis shows that the transition from a weak to strong optical coupling between plasmonic nanowires results in the formation of plasmonic lattice solitons with markedly different characteristics of their optical power and field distribution. Importantly, the coupled-mode theory that is widely used to investigate solitons formed in dielectric waveguide arrays is found to have a limited range of validity when applied to plasmonic arrays. We have also investigated the compensation of the modal optical loss by an optical gain of the background medium and revealed that the gain coefficient needed to cancel the loss is much smaller than the loss parameter of the metallic components of the plasmonic array.

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