Doped silicon quantum dots as sources of coherent surface plasmons

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Abstract
In the present work, we propose using a doped silicon quantum dot (Si-QD) as a source of coherent surface plasmons (SPASER). The possibility of spasing in single Si-QD is investigated theoretically utilizing full quantum mechanical treatment. We show that spasing can take place in doped Si-QDs whenever the quality factor of a plasmon mode exceeds some minimum value. The minimum value depends on the size and doping concentration of Si-QDs. It can be used to design an optimum structure as SPASER in silicon technologies. The condition on the quality factor is translated to a condition for radius and it is shown that for a given localized surface plasmon (LSP) mode, the radius should be less than the critical value. This value only depends on the mode index. The required relations for design purposes are derived and, as an example of feasibility of the approach, a SPASER is designed for mid infrared. Moreover, we propose a more applicable device by arranging an array of doped Si-QDs on top of a graphene layer. Interaction between the surface plasmon polariton (SPP) modes of graphene and LSP modes of Si-QDs causes outcoupling of an intense ultra narrow beam of coherent SPPs to be used in real probable applications.

Keywords: plasmonics, graphene, SPASER

(Some figures may appear in colour only in the online journal)

1. Introduction
Coherent surface plasmon generation has been a topic of interest in plasmonics field since the introduction of surface plasmon amplification by stimulated emission of radiation (SPASER) in 2003 by Bergman and Stockman [1]. The inventors showed that in some correctly tailored plasmonic structures, stimulated surface plasmons can be generated. SPASER can break the well known diffraction limit of light, which is a bottleneck in laser technology. Since the introduction of SPASER, a number of researchers around the world have been focusing on its experimental and theoretical investigation. The first claimed experimental realization of SPASER dates back to 2009 in a paper reported by Noginov et al [2]. The authors experimentally showed that an aqueous solution of gold nanoparticles surrounded by dye-doped silica shells can behave like a SPASER.

In 2010, Stockman treated the SPASER with a two level model and claimed that spasing action has only a quantum mechanical description [3]. In 2013, Zhong et al proposed a semiclassical approach for describing SPASER [4]. In the same year, Dorfman et al introduced a more controllable SPASER by its three level modeling [5]. Many other works are found in the literature that concern different aspects of SPASER [6–16].

In some ways, the SPASER acts like a laser. A device could be a SPASER if it consists of at least two main parts, a medium that supports plasmonic modes and an active medium. Carrier down transition or LSP radiation in an initially pumped active medium is stimulated by an inherently large positive feedback mechanism, which is a consequence of LSP’s intense near field. Exterior energy supplies could be optical, electrical, chemical, or any other typical pumping systems that are used in lasers too.

Optical researchers are interested in generating light from silicon. The indirect bandgap of silicon makes this material impossible to interact with photons directly. It has been shown that doped silicon quantum dots (Si-QDs) have LSP modes [17–19]. In the present paper, we claim that under some conditions a single doped Si-QD could be a SPASER alone. Our assertion is based on the fact that a doped Si-QD...
Figure 1. The structure used in this paper. Si-QDs and graphene are sketched in gold and black, respectively. The graph is not shown in scale. All the structure is embodied in a SiO$_2$ matrix.

can take both the role of an active medium and an LSP supporter. The realized Si-QD SPASER will have the advantage of its compatibility with silicon industries and capability of integration with silicon-based platforms.

In this paper, we also use graphene as a media for propagating SPP modes. Graphene is a recently invented 2D material which is synthesized by a 2D arrangement of carbon atoms in a honeycomb lattice [20, 21]. This material has excellent properties in multiple fields among which is plasmonics. Graphene has got a propagation length, lateral mode excitations, and lifetime, an order of magnitude larger than metals which are the most common materials in the plasmonics area. In our work, graphene will be used to extract the energy of spasing LSP modes for external applications. Our proposed structure is shown in figure 1. The structure consists of an array of doped Si-QDs on top of a graphene sheet which is embodied in a silica (SiO$_2$) matrix. The graphene sheet is used for outcoupling of the energy of coherent plasmons for real applications.

The paper is organized as follows. We first investigate the possibility of spasing in a single separated doped Si-QD in the next three sections. So, in sections 2–4, the system means a single doped Si-QD. Section 2 is about the subject of quantizing the LSP Hamiltonian of the system. In section 3, the required quantities in active medium are derived, and section 4 concludes the possibility of spasing in single doped Si-QD. Finally, in section 5, the whole structure is discussed and simulated numerically.

2. LSP Hamiltonian

This section includes three parts. In the first part, the permittivity model of silicon is described. The second part is about the derivation of LSP modes of a single doped Si-QD, and the third part is devoted to calculating the quantized Hamiltonian of LSP field.

2.1. Permittivity model

The dielectric constant of doped silicon can be described by a Drude model but with special attention paid to choosing effective masses (it is worth mentioning that, along the paper, the physicist’s convention $\exp(-i\omega t)$ is used for all time dependencies) [17, 19, 22–24],

$$\epsilon_r(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i\Gamma)},$$

where $\omega_p$, $\epsilon_\infty$, and $\Gamma$ are silicon’s bulk plasma frequency and dielectric constant, and carrier’s relaxation rate, respectively. We have $\omega_p^2 = \frac{N\epsilon_0 e^4}{m_e^*}$, where $N$, $\epsilon$, $\epsilon_0$, and $m_e^*$ are the doping concentration, elementary charge, vacuum permittivity, and carrier’s effective mass (which can be $m_e^*$ for n-type and $m_h^*$ for p-type), respectively. Care should be taken when we are talking about silicon’s effective masses. Having considered n-type silicon, the permittivity is mostly due to electrons in the conduction band. Silicon has an indirect band gap whose six conduction band minima are not placed around the $\Gamma$ point but along the $\langle 100 \rangle$ directions. The constant energy surfaces around the band minima are ellipsoids which are characterized by two effective masses, $m_{1s}^*$ and $m_{3s}^*$, which are called longitudinal and transverse effective masses, respectively. The best method for considering this inconvenience is to use the average effective mass derived by the following formula [19, 22],

$$\frac{1}{m_e^*} = \frac{1}{3} \left( \frac{1}{m_{1s}^*} + \frac{2}{m_{3s}^*} \right).$$

Describing the hole effective mass for p-type silicon is quite different. Although the valence band minimum is at the $\Gamma$ point, a problem arises when we notice the near degeneracy of heavy, light, and spin orbit split off (soso) hole bands with three different effective masses, $m_{1h}^*$, $m_{2h}^*$, and $m_{3h}^*$, respectively. For permittivity calculations by using Drude model, the following average effective mass should be used [19, 22],

$$m_h^* = m_{1h}^{3/2} + m_{2h}^{3/2} + m_{3h}^{3/2}.$$  

In the above relation, the soso band has been ignored. This is an acceptable approximation because, even at room temperature, only a few percent of the overall hole concentration lies in the soso band. For the rest of the paper, p-type silicon is considered for continuing the analysis.

2.2. LSP modes of a single doped Si-QD

LSP modes of a single doped Si-QD with radius $r_0$ can be derived with good accuracy by considering it as a quasi-electrostatic problem, because the discussed wavelengths are much larger than the maximum feature size of the system in hand. In the quasi-electrostatic limit, LSP modes are independent solutions of the Laplace equation, $\nabla^2 \Phi_{lm}(r, \theta, \phi) = 0$, where $l$ and $m$ are mode indices. Utilizing the spherical symmetry of the problem, LSP modes could be written in the following form,

$$\Phi_{lm}(r, \theta, \phi) = \begin{cases} \left( \frac{r}{r_0} \right)^l Y_{l1}^m(\theta, \phi) & r \leq r_0, \\ \left( \frac{r}{r_0} \right)^{l+1} Y_{l+1}^m(\theta, \phi) & r > r_0, \end{cases}$$

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where $Y_l^m$'s are spherical harmonics. Applying a perpendicular electric displacement continuity condition at $r = r_0$ yields the following relation,

$$S(\omega_{lm} - i\gamma_{lm}^l = 0,$$  \hspace{1cm} (5)$$

where $\omega_{lm}$ and $\gamma_{lm}$ are the $l$th mode eigen-frequency and damping rate, respectively, and

$$S(x) = l\epsilon_s(x) + (l + 1)\epsilon_a(x).$$  \hspace{1cm} (6)$$

$\epsilon_a$ stands for ambient (which in our case is SiO$_2$) dielectric constant. In the low damping regime, $\gamma_{lm}^l \ll \omega_{lm}$, the solutions of the complex equation (5) are best approximated by the following two relations,

$$\omega_{lm} \approx \sqrt{g_l(N) - \Gamma^2} \approx \sqrt{g_l(N)},$$  \hspace{1cm} (7)$$

$$\gamma_{lm}^l \approx \frac{g_l(N)\Gamma}{2(g_l(N) - \Gamma^2)} \approx \frac{\Gamma}{2},$$  \hspace{1cm} (8)$$

where

$$g_l(N) = \frac{L^2}{\epsilon(x) + (l + 1)\epsilon_a}.$$  \hspace{1cm} (9)$$

The quality factor of modes is defined as $Q_{lm} = \omega_{lm}/\gamma_{lm}$, and a simple substitution leads to

$$Q_{lm} \approx \frac{\sqrt{g_l(N)}}{\Gamma(N, r_0)}.$$  \hspace{1cm} (10)$$

In the above relation, we emphasize the doping and size dependency of the carrier damping rate by explicitly writing it, but, for simplicity, it is treated as a constant during this paper. Solutions of equation (5) and consequently equations (7) and (8) apparently do not depend on the choice of mode index, $m$. Therefore, for a fixed value of $l$, there exist $2l + 1$ degenerate LSP modes. So, for simplicity, throughout the paper, sometimes index $m$ is omitted from the related quantities, without adding ambiguity.

For the case of doped Si-QD, using the parameter values listed in Table 1, the following approximate relations could be utilized for design purposes,

$$\omega_{lm} = 5.641 \times 10^4 \sqrt{\frac{N[\text{cm}^{-3}]/m^3[m_0]}{16 + 4.5/l}},$$  \hspace{1cm} (11)$$

$$\lambda_{lm}[\mu\text{m}] = 3.338 \times 10^{10} \sqrt{\frac{16 + 4.5/l}{N[\text{cm}^{-3}]/m^3[m_0]}},$$  \hspace{1cm} (12)$$

where $\lambda$ and $m_0$ are the LSP wavelength and electron mass, respectively. Throughout the paper, all the quantities are assumed to be measured in a SI unit system unless the unit is emphasized in a bracket next to the related quantity.

### Table 1. Physical parameters which are used in this paper. In this table, $m_0$ stands for electron mass.

| Quantity | Value  | Unit  |
|----------|--------|-------|
| $\epsilon_\infty$ | 11.5  | —     |
| $\epsilon_a$     | 4.5   | —     |
| $m_1^m$          | 0.98  | $m_0$ |
| $m_2^m$          | 0.19  | $m_0$ |
| $m_3^m$          | 0.49  | $m_0$ |
| $m_4^m$          | 0.16  | $m_0$ |
| $m_5^m$          | 0.26  | $m_0$ |
| $m_6^m$          | 0.37  | $m_0$ |
| $\Gamma$        | $4.5 \times 10^{11}$—$10^{13}$ | rad/s |
| $\Gamma_{pq}$   | 16    | meV   |
| $\Delta E_c$    | 3.4   | eV    |
| $\Delta E_v$    | 4.4   | eV    |
2.3. Quantization of LSP Hamiltonian

A general solution for electrostatic potential can be written as a linear combination of all LSP modes,

$$\Phi(r, \theta, \phi) = \sum_{lm} C_{lm} \Phi_{lm}(r, \theta, \phi) \exp(-i\omega_{lm} t) + c.c., \quad (13)$$

where $C_{lm}$s are combination constants and c.c. stands for the complex conjugate of previous terms. Electric field can also be written in the same way,

$$E(r, \theta, \phi) = \sum_{lm} C_{lm} E_{lm}(r, \theta, \phi) \exp(-i\omega_{lm} t) + c.c., \quad (14)$$

where $E_{lm} = -\nabla \Phi_{lm}$.

For quantizing the LSP field, electrostatic energy has to be derived [25],

$$\mathcal{E}_e = \frac{1}{2} \int \frac{\partial (\omega_e)}{\partial \omega} E \cdot E \, d^3r. \quad (15)$$

If equation (14) is substituted in equation (15), the following result is obtained,

$$\mathcal{E}_e = \sum_{lm/l'm'} C_{lm} C_{l'm'} e^{-i(\omega_{lm} - \omega_{l'm'}) t} I_1$$

$$+ C_{lm} C_{l'm'} e^{-(\omega_{lm} - \omega_{l'm'}) t} I_2$$

$$+ C_{lm} C_{l'm'} e^{i(\omega_{lm} - \omega_{l'm'}) t} I_3$$

$$+ C_{lm} C_{l'm'} e^{i(\omega_{lm} + \omega_{l'm'}) t} I_4,$$  

where

$$I_1 = \frac{1}{2} \int \frac{\partial (\omega_e)}{\partial \omega} E_{lm} \cdot E_{l'm'} \, d^3r,$$

$$I_2 = \frac{1}{2} \int \frac{\partial (\omega_e)}{\partial \omega} E_{lm}^* \cdot E_{l'm'} \, d^3r,$$

$$I_3 = \frac{1}{2} \int \frac{\partial (\omega_e)}{\partial \omega} E_{lm}^* \cdot E_{l'm'} \, d^3r,$$

$$I_4 = \frac{1}{2} \int \frac{\partial (\omega_e)}{\partial \omega} E_{lm} \cdot E_{l'm'}^* \, d^3r.$$

Tedious manipulations lead to the following results,

$$I_1 = I_4 = \frac{r_0}{2} (-1)^m \delta_{ll'} \delta_{m,-m'} A(\omega_{lm}), \quad (24)$$

$$I_2 = I_3 = \frac{r_0}{2} \delta_{ll'} \delta_{mm'} A(\omega_{lm}). \quad (25)$$

where

$$A(\omega_{lm}) = \frac{\partial}{\partial \omega} \{ S(\omega) \}_{\omega=\omega_{lm}}. \quad (26)$$

Substitution of equations (24) and (25) into equation (15) and averaging over time lead to

$$\mathcal{E}_e = \sum_{lm} \frac{r_0}{2} A(\omega_{lm}) (C_{lm}^\dagger C_{lm} + C_{lm} C_{lm}^\dagger). \quad (27)$$

The total energy is twice the average electrostatic energy so

$$\mathcal{E} = \sum_{lm} r_0 A(\omega_{lm}) (C_{lm}^\dagger C_{lm} + C_{lm} C_{lm}^\dagger). \quad (28)$$

LSP field quantization is obtained by replacing coefficients with ladder operators using the following rule,

$$C_{lm} \rightarrow \gamma_{lm} \hat{a}_{lm},$$

$$C_{lm}^\dagger \rightarrow \gamma_{lm}^\dagger \hat{a}_{lm}^\dagger, \quad (29)$$

where $\hat{a}_{lm}$ and $\hat{a}_{lm}^\dagger$ are the annihilation and creation operators of the $lm$th mode, which follow bosonic algebra, and the following definition has been made,

$$\gamma_{lm}^2 = \frac{\hbar \omega_{lm}}{2 r_0 A(\omega_{lm})}. \quad (31)$$

The resulting quantized Hamiltonian is in the form of a harmonic oscillator,

$$\hat{H}_{LSP} = \sum_{lm} \frac{\hbar \omega_{lm}}{2} (\hat{a}_{lm}^\dagger \hat{a}_{lm} + \hat{a}_{lm} \hat{a}_{lm}^\dagger). \quad (32)$$

The operators of electrostatic potential and electric field also can be obtained by simply inserting equations (29) and (30) into equations (13) and (14),

Figure 4. Electric field magnitude distribution on graphene for (a) the first and (b) the second resonance occurring in figure 3. Apparently, in the case of (a), the energy of LSP mode has outcoupled from Si-QDs and starts to propagate along graphene. For visual convenience, outlines of Si-QDs have been sketched in red.
where $H_c$ means hermitian conjugate of previous terms. Until now, the results have been general and did not depend on what model we used for describing permittivity of doped silicon, but if the specific form of $\varepsilon_c(\omega)$, from equation (1), is substituted in $\gamma_{lm}$, the following result is obtained,

$$\phi(r, \theta, \phi; t) = \sum_{lm} \gamma_{lm} \Phi_{lm} \exp(-i\omega_{lm}t) \hat{a}_{lm} + H.c.,$$  

$$\tilde{E}(r, \theta, \phi; t) = \sum_{lm} \gamma_{lm} E_{lm} \exp(-i\omega_{lm}t) \hat{a}_{lm} + H.c.,$$

where $H_c$ means hermitian conjugate of previous terms. Until now, the results have been general and did not depend on what model we used for describing permittivity of doped silicon, but if the specific form of $\varepsilon_c(\omega)$, from equation (1), is substituted in $\gamma_{lm}$, the following result is obtained,

$$\gamma_{lm}^2 = \frac{\hbar}{4\epsilon_0 \omega_p} \frac{\omega_0^3}{r_0^4}.$$  

3. SiQD as an active medium

According to table 1, the barrier height in the valence band of Si-QD is large enough to approximate it as an infinite well spherical QD.

The actual wave functions are approximately the slowly varying envelope functions over QD times the periodic parts of Bloch functions with the periodicity of crystal lattice, i.e. $\Xi(r) = \psi(r) \omega_{nk}(r)$, where $\omega_{nk}(r)$ is the periodic part around $k = k_0$ and $\psi(r)$ is the envelope function, which should fulfill the effective mass equation [26, 27].

Because of the degeneracy of three or at least two (ignoring the soso band) hole bands, the effective mass methodology leads to the Luttinger-Kohn (LK) Hamiltonian equation [26, 27]. Depending on whether three or two hole bands are selected, LK Hamiltonian is a $6 \times 6$ or $4 \times 4$ matrix of PDEs. Also, the carrier modulation due to doping of QD leads to the band bending. Considering band bending, the Poisson equation should be solved simultaneously with the wave function solution. Having considered these complexities, deriving analytic results becomes so much more complicated and almost impossible. Because, the aim of this paper is to rigorously assess and design the system and to leave the more accurate calculations to the optimization processes, some simplifying, and of course not weak, assumptions are used. First, it is assumed that using a single band effective mass equation with the hole effective mass defined in equation (3) obtains sufficiently good results, and second, that the band bending due to doping and carrier modulation has little effect on the energy differences between energy levels, and its only effect is to modify Fermi level of QD. This latter assumption is reasonable due to the high level of doping. By using these assumptions, it is sufficient to solve the following equation for envelope functions inside QD,

$$-\frac{\hbar^2}{2m^*} \nabla^2 \psi(r, \theta, \phi) = E \psi(r, \theta, \phi).$$

Solving the equation leads to the following envelope functions [15],

$$\psi_{kn}(r, \theta, \phi) = \begin{cases} B_{nk} J_\ell \left( \frac{r}{r_0} \right) Y_\ell^m(\theta, \phi) & r \leq r_0, \\ 0 & r > r_0, \end{cases}$$

where $x_{nk}$ is the $k$th zero of the $n$th order spherical Bessel function of the first kind, $j_\ell$, and

$$B_{nk} = \left( \frac{2}{r_0^2} J_{\ell+1}(x_{nk})^2 \right)^{0.5}$$

is a normalization constant. Energy eigenvalues can be calculated by the following formula,

$$E_{lm} = \frac{\hbar^2 x_{nk}^2}{2m^* r_0^2}.$$  

The important quantities in the active medium, which are involved in the interaction Hamiltonian, are dipole matrix elements. By using an integral factorization rule [27], it can be shown that dipole matrix elements between two wave functions are approximately the same as ones calculated between corresponding envelope functions. It is straightforward to compute these quantities by using equation (37). Calculation leads to the following relation for the dipole matrix element $d_{pq}$ between general levels $p \equiv nk$ and $q \equiv n\ell k^\prime s^\prime$ (where $\equiv$ means equals by definition),

$$d_{pq} = -\hat{r} \delta_{m\ell} \delta_{s s^\prime} \epsilon_{0} f_{nk\ell \prime},$$

where $f$ is a dimensionless parameter which is independent of the choice of geometry and has been defined by [15],

$$f_{nk\ell \prime} = \frac{2}{J_{\ell+1}(x_{nk}) J_{\ell+1}(x_{nk})} \int_0^1 r J_{\ell}(x_{nk} r) J_{\ell}(x_{nk \ell} r) dr.$$  

For design purposes, $r_0$ should be considered such that there is a $p \leftrightarrow q$ transition that is getting close to resonance with one of LSP modes, say $l = L$. The numerical calculations in the rest of the paper are based on $|\psi_{100}\rangle \leftrightarrow |\psi_{200}\rangle$ transitions. The result of calculation of $f_{102}$ for this case becomes 0.180 128. In this case, if zero energy is chosen such that it coincides with the middle of two levels in resonance, the approximate active medium Hamiltonian in the second quantized form would be [28, 29]

$$H_l = \frac{\hbar \omega_0}{2} \hat{\gamma}_z,$$

where

$$\hat{\gamma}_z = \hat{c}_q^\dagger \hat{c}_q - \hat{c}_p^\dagger \hat{c}_p,$$

$$\omega_0 = \frac{E_q - E_p}{\hbar}.$$  

In the above relations $\hat{\gamma}_z$, $\hat{c}_q$, $\hat{c}_p$ are pseudo-spin operator, fermionic annihilation and creation operators of the $j$th level (for $j = p, q$, respectively). Furthermore, it is assumed that $E_q > E_p$, without loss of generality.

4. Spasing in a single doped SiQD

For the rest of the paper, we suppose that only those LSP modes with $l = L$ are in near resonance with $\hbar \omega_0$ transition with $d_{pq} \equiv d$ $\hat{r}$ and so the interaction Hamiltonian can be
written as [28, 29],

$$H_1 = \int_{\Omega-4\pi} d\Omega \sum_{m=-L}^{L} \hbar \Omega_{lm}(\theta, \phi) (\hat{a}_{lm}^\dagger \hat{c}_+ + \hat{c}_+ \hat{a}_{lm}), \quad (45)$$

where $\Omega_{lm} = -d_{pq} \cdot \mathbf{E}_{lm}/\hbar$ is the Rabi frequency and

$$\hat{c}_+ = \hat{c}_p^\dagger \hat{c}_q, \quad \hat{c}_- = \hat{c}_q^\dagger \hat{c}_p, \quad \hat{\sigma}_z = \hat{c}_p^\dagger \hat{c}_q - \hat{c}_q^\dagger \hat{c}_p, \quad (46, 47)$$

are ladder operators. Rabi frequency is a measure of interaction strength. Using the electric field from equation (34) in the Rabi frequency, the following result is obtained,

$$\Omega_{lm}(\theta, \phi) = \frac{d_{pq} y_{lm}}{r_0/h} (\theta, \phi). \quad (48)$$

The condition for spasing has been derived in [3] and for near resonance circumstances, it simplifies to the following inequality condition,

$$\sum_{m=-L}^{L} \int_{\Omega-4\pi} d\Omega |\Omega_{lm}(\theta, \phi)|^2 \geq \gamma_L^2 \Gamma_{pq}, \quad (49)$$

where $\Gamma_{pq}$ is the polarization relaxation rate of $h\omega_0$ transition. By substituting equation (48) into equation (49) and some computations the following relation is obtained [15],

$$\frac{\pi d^2 \omega_L^3}{3V_{QD} h c \omega_p^2} \geq \gamma_L^2 \Gamma_{pq} \quad (50)$$

where $V_{QD}$ is QD’s volume. This relation can be translated to the neat form, $Q_L \geq Q_{L \text{min}}$, where

$$Q_{L \text{min}} = \frac{3\hbar V_{QD} \epsilon_0 \omega_p^2 \gamma_p^2 L}{2\pi d^2 \omega_L^2 (2L + 1)}. \quad (51)$$

It is seen that $Q_{L \text{min}}$ is capable of engineering because it depends on QD size and doping concentration through $\omega_p$. This result can be compared with [15] where the SPASER is made by a spherical graphene shell and an array of QDs around it. The present SPASER has two main advantages over it, which are integration capability with silicon platforms and simplicity of fabrication [19]. Design parameters of the present work include the QD’s size and doping concentration in comparison to that work, which were QD’s size, array density and graphene sphere’s radius. For numerical purposes, it can be shown that

$$Q_{L \text{min}} = 5.451 \times 10^4 \frac{16L + 4.5}{2L + 1} r_0. \quad (52)$$

By combining equations (10), (39) and (52), and also considering that QD’s transition energy should coincide with plasmon energy at mode L, a simpler design condition, $r_0 \leq r_{0c}$ is obtained, where

$$r_{0c} = 1.465 \times 10^{-3} \left(\frac{1}{m^* [m_0]} \frac{2L + 1}{16L + 4.5}\right)^{1/3}. \quad (53)$$

So, the required relations for design have already been derived and for compactness are listed below,

$$N [\text{cm}^{-3}] = 1.114 \times 10^{21} m^*[m_0]^{16 + 4.5/L} (\lambda_L [\mu \text{m}])^2, \quad (54)$$

$$r_0 [\text{nm}] = 0.953 \sqrt{\left(\frac{\lambda_L [\mu \text{m}]}{m^*[m_0]}\right)}; \quad (55)$$

$$r_{0c} [\text{nm}] = 14.650 \left(\frac{1}{m^*[m_0]} \frac{2L + 1}{16L + 4.5}\right)^{1/3}. \quad (56)$$

For example, we could have a SPASER that radiates at $\lambda = 3 \mu \text{m}$ by $L = 1$, $N = 9.40 \times 10^{20} \text{ cm}^{-3}$, $r_0 = 2.72 \text{ nm}$, and $r_{0c} = 10.75 \text{ nm}$, which are typical values in fabrication technologies [19]. It can be shown from equation (39) that $E_{20\nu} - E_{0\nu} = hc/\lambda \approx 6.6 \times 10^{-20}$, where $h$ and $c$ are Planck’s constant and the speed of light in vacuum, respectively, which again verifies that the transition energy in QD coincides with the plasmon energy of interest.

5. Numerical results and discussions

As mentioned in section 1, the whole structure consists of an array of doped Si-QDs on top of a sheet of graphene. Until now, the response of a single separated doped Si-QD is assessed. Arranging doped Si-QDs in an array and also coupling to the SPP modes of graphene sheet cause the LSP eigen-frequencies to be split and shifted. Furthermore, we expect a large field enhancement in the gap between Si-QDs and graphene due to the constructive interference. SPP modes have a traveling wave character. So, this specific structure helps outcoupling of the spasing mode energy for real applications, just the same as what is done in lasers by using imperfect mirrors for cavities.

Figure 2 compares the extinction cross section of a single separated doped Si-QD with $r_0 = 2.72 \text{ nm}$ and $N = 9.40 \times 10^{20} \text{ cm}^{-3}$ calculated from theory and finite difference time domain (FDTD) simulations. Theoretical extinction has been derived by the following formula [30, 31],

$$C_{\text{ext}} = C_{\text{ca}} + C_{\text{abs}}, \quad (57)$$

where scattering and absorption cross sections are calculated by

$$C_{\text{ca}} = \frac{8\pi k_L^2 L_0^6}{3} \left| \frac{\epsilon_s - \epsilon_a}{\epsilon_s + 2\epsilon_a} \right|^2, \quad (58)$$

$$C_{\text{abs}} = 4\pi k_L r_0^4 \text{Im} \left[ \frac{\epsilon_s - \epsilon_a}{\epsilon_s + 2\epsilon_a} \right], \quad (59)$$

and where $k_L$ is the ambient wavenumber of the $L$th mode. The good agreement between theory and simulation verifies the accuracy of our analysis.

The whole structure is illuminated by a normally incident plane wave. The SPP modes of graphene cannot be coupled to this wave directly. But, for the efficient coupling between SPPs and the spasing LSP, array’s period ($\Lambda$) could be chosen such that the first order diffracted wave coincides with an SPP mode in LSP wavelength, $2\pi/\Lambda = k_{\text{SPP}}(\lambda_L)$, where $k_{\text{SPP}}(\lambda_L)$
satisfies the following implicit equation \[32\],
\[
\frac{1}{k_{SPP}^2 - \varepsilon_a k_L^2} = \frac{\sigma_2D(\omega_L)}{2i\omega_L\varepsilon_a\varepsilon_0}.
\] (60)

The calculated period for \(\lambda_L = 3 \mu m\) is \(\Lambda = 18.833 nm\). The simulated absorption spectra for this choice of parameters is shown in figure 3. This figure exhibits two main peaks. The coupling of SPP and LSP is responsible for the sharper peak around 2.94 \(\mu m\). The second peak around 3.47 \(\mu m\) indicates a higher order LSP mode. It can be seen from this figure that the 3 \(\mu m\) designed wavelength for single Si-QD is slightly blue-shifted due to the coupling nature. The electric field distribution for SPP and LSP peaks are shown in figure 4(a) and (b), respectively. Apparently, LSP mode has been coupled to a SPP mode in figure 4(a) but the distribution in figure 4(b) is mostly localized.

6. Conclusion

In summary, we have claimed that correctly designed doped Si-QDs can have some spasing modes. The inspiration behind that is the existence of LSP modes in doped Si-QDs. Because a single doped Si-QD can take both the role of active medium and LSP supporter, there could be some conditions under which the system can spase. We have analyzed the structure thoroughly using full quantum mechanical treatment and derived the required conditions for spasing. We have shown that by appropriately choosing the Si-QD’s size and doping concentration, a SPASER could be designed for a given wavelength. We have also explained how to choose the array period for efficient coupling of spasing energy from Si-QDs. During the paper, a SPASER has been designed at \(\lambda = 3 \mu m\) and the results have been verified by using the FDTD simulations.

It is worth mentioning that most of the analyses throughout the paper, except those that are explicitly explained, are not restricted to the material system which is used for the fabrication of QD. We have made our best efforts to formulate the relations parametrically. So, this work, with slight modifications, can be applied to other material systems, with p-type or n-type doping, but with the same geometry.

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