

# Theoretical study about the gain in indirect bandgap semiconductor optical cavities

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**Abstract:** Indirect bandgap semiconductors such as silicon are not efficient light emitters because a phonon with a high momentum is required to transfer an electron from the conduction to the valence band. In a recent study [M. J. Chen et al., Japanese Journal of Applied Physics 45, 6576–6588 (2006)] an analytical expression of the optical gain in bulk indirect bandgap semiconductors was obtained. The main conclusion was that the free-carrier absorption was much higher than the optical gain at ambient temperature, which prevents lasing. In this work, we consider the case in which the semiconductor material is engineered to form an optical cavity characterized by a certain Purcell factor. We obtain that although the optical gain is increased, losses due to free carriers increase in the same way so lasing is also prevented even when creating a high-Q optical cavity.

## I. Introduction

Silicon photonics has boomed in the last few years as a promising way to create low-cost, high-speed optical interconnects that replace copper wires in future computers [1-3]. The main advantage of using silicon as a photonic material is that it can be processed in microelectronics foundries with high yield and low cost. However, silicon has a main drawback: it is an indirect bandgap semiconductor in which radiative transitions are unlikely and, as so, a very inefficient light emitter. A silicon laser would allow monolithic integration of photonics and electronics on a same chip [2]. Despite of huge research efforts by many groups around the world, an electrically-pumped room-temperature silicon laser - perhaps the most pursued challenge within photonics - remains elusive.

Bulk crystalline silicon has an indirect energy bandgap so emission of light requires the participation of phonons with the right momentum in order to satisfy the momentum conservation. The low probability of the phonon-mediated radiative recombination process makes silicon a highly inefficient light source. In fact, there exists the general belief that optical gain and thus laser operation in indirect bandgap semiconductors is not possible because the small optical gain- which could be achieved in principle via band-band transitions mediated by phonons- will always be overcompensated by free carrier absorption, regardless of the excitation conditions [4]. This statement, together with the fact that no silicon lasing at room temperature has been reported yet, explains why typically III-V semiconductors having a direct band gap has been used to implement lasers in the near -infrared regime (such as the important optical communications band at wavelength about 1550 nm).

However, some recent theoretical works analysing the possibility of achieving optical gain in indirect bandgap semiconductors at room temperature have given rise to certain controversy. For instance, Trupke and co-workers suggested that optical gain in silicon is theoretically possible and pointed out that the most suitable energy region is the sub-bandgap region (near infrared) where processes involving phonons could help in achieving gain [5]. Moreover, they obtained that indirect optical transitions can provide negative absorption, i.e., optical gain without an electronic population inversion, but with the assistance of proper phonons. These theoretical arguments were also supported in Ref. [6] where an analytical expression for optical gain via phonon-assisted optical transitions in indirect bandgap semiconductors is presented. The magnitude of optical gain in bulk crystalline silicon is calculated and shown to be smaller than the free carrier absorption at room temperature. However, it is shown, for

the first time, that the optical gain is greater than the free carrier absorption in bulk crystalline silicon at the temperature below 23 K [6].

Other some experimental works have reported an increased photoluminescence from silicon when photonic cavities with high Q-factor are created Ref.[7-15]. In this case, the generation of photons is enhanced in comparison to the case of bulk silicon [16] because of the Purcell effect [17] (or, in other works, the increase of the optical density of states inside the cavity). However, those results have been mainly attributed to an increase of the spontaneous emission rate but nor lasing neither optical gain have been directly observed. So the natural question that arises is: can optical gain at room temperature be obtained in indirect bandgap semiconductors when an optical cavity instead of a bulk material is considered? In this work we try to answer this question by starting from the analytical results obtained in Ref. [6].

## II. Rate equations

Figure 1 shows a schematic diagram that describes all possible optical transitions taking place in an indirect bandgap semiconductor such as silicon. It can be seen how three different kinds of particles are involved in this process: electrons, photons and phonons (which are not involved in the same process when taking place in direct bandgap semiconductors).

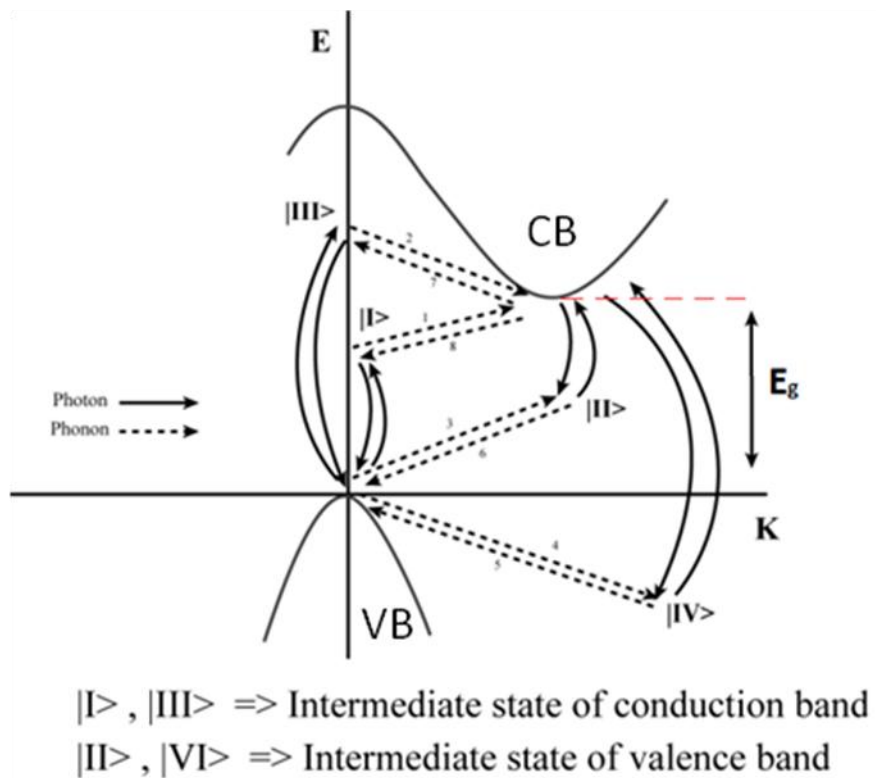


Figure1. Schematic diagram of all possible optical transitions in an indirect bandgap semiconductor

In Ref. [6], M. J. Chen and co-workers obtained a theoretical expression for the different transition rates that occur in bulk indirect bandgap semiconductors. For the sake of clarity, we represent here the expression of these rates:

$$R_{sp} = M(n_q + 1) \cdot NP \quad (1)$$

$$R_{st} = M \cdot n_p(n_q + 1) \cdot NP \quad (2)$$

$$R_{ab} = M \cdot n_p n_q \cdot NP \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \quad (3)$$

$$M = \frac{\pi}{8} B_{sp} (\hbar\omega + \hbar\Omega - E_g)^2 \exp\left(-\frac{(\hbar\omega + \hbar\Omega - E_g)}{K_B T}\right) \quad (4)$$

In Eqs. (1)-(4),  $R_{sp}$  is the spontaneous emission rate,  $R_{st}$  is the stimulated emission rate,  $R_{st}$  is the absorption rate,  $n_p$  is the photon occupation number,  $n_q$  is the phonon occupation number,  $\hbar\omega$  is the photon energy,  $\hbar\Omega$  is the phonon energy,  $\Delta F$  is the difference between the quasi-Fermi levels for electrons and holes,  $N$  is the electron concentration,  $P$  is hole concentration (in our study we consider that  $N=P$ ),  $E_g$  is the indirect bandgap energy,  $K_B$  is the Boltzman constant and  $T$  is the temperature (we assume room temperature throughout this work). In this work we consider silicon as indirect bandgap semiconductor, so the radiative transition rates can be calculated using the Eqs.(1)-(4) and the values given in the Table I in Ref.[6]. We also consider all the assumptions made in Ref. [6].

The following equations system<sup>1</sup> [6] governs the temporal variation of the photon density ( $N_p$ ), the phonon density ( $N_q$ ) and the carrier density ( $N$ ):

$$\frac{dN}{dt} = R_p - R_{st,B}(\hbar\omega) + R_{ab,B}(\hbar\omega) - R_{sp,B}(\hbar\omega) - \frac{N}{\tau_c} \quad (5a)$$

$$\frac{dN_p}{dt} = R_{st,B}(\hbar\omega) - R_{ab,B}(\hbar\omega) + \beta R_{sp,B}(\hbar\omega) - \frac{N_p}{\tau_p} \quad (5b)$$

$$\frac{dN_q}{dt} = R_{st,B}(\hbar\omega) - R_{ab,B}(\hbar\omega) + R_{sp,B}(\hbar\omega) - \frac{N_q - N_{q0}}{\tau_q} \quad (5c)$$

where  $R_p$  is the pumping rate by current injection or optical excitation,  $\beta$  is the spontaneous emission factor representing the fraction of spontaneous emission

<sup>1</sup> The subscript B stands for the different rates in bulk silicon.

entering the optical mode has been considered,  $N_{q_0}$  is the phonon density at thermodynamic equilibrium, and  $\tau_c$ ,  $\tau_p$  and  $\tau_q$  are the lifetime of carriers, photons and phonons, respectively. The losses of photons due to the effects such as optical scattering or free carrier absorption can be characterized by a photon lifetime  $\tau_p$  [6]. The loss of phonons (last term of Eq.(5c), which represent the anharmonic phonon interaction, can be characterized by a phonon lifetime  $\tau_q$ [6]. The recombination lifetime of carriers is given by  $1/\tau_C=1/\tau_{C,RAD} + 1/\tau_{C,NRAD}=1/\tau_{C,RAD} + 1/\tau_{C,SRH} + 1/\tau_{C,Auger}$ . In Ref.[6], it is assumed that the non-radiative recombination rate is determined by the non-radiative Shockley-Read-Hall (SRH) mechanism. However, in the case of a very high carrier density in silicon, the Auger recombination lifetime is the dominant recombination mechanism, so  $1/\tau_{C,SRH} \ll 1/\tau_{C,Auger}$  ,[18-20]. Considering the above and taking into account the carrier density that we consider in this work ( $\sim 10^{19} \text{cm}^{-3}$ ) then we get  $\tau_{C,RAD}=10^{-4}$  and  $\tau_{C,NRAD}=10^{-7}$  in silicon bulk.

### III. Increase of the optical gain with Purcell factor.

The system of equations (5) was solved in [6] for bulk silicon. In this work we have solved the same system but considering a photonic cavity characterized by a quality factor ( $Q$ ), a modal volume ( $V_0$ ) and Purcell factor ( $F_p$ ). These three parameters are related to each other by the following equation [17]:

$$F_p = \frac{3Q(\lambda/n)^3}{4\pi^2 V_0}, \quad (6)$$

where  $\lambda$  is the resonant wavelength of the cavity and  $n$  its refractive index. It has to be mentioned that we consider that the cavity only affects the photonic density of states by means of  $F_p$  but it has no effect on the statistics of the phonons involved in the emission process. This is a good assumption taking into account that the wavelength of the phonons involved in the emission process is much smaller than the optical cavity size (which should be at least half a photon wavelength) so that phonons see a bulk material.

In the system under consideration, the spontaneous emission ( $B_{sp}$ ), stimulated emission ( $B_{st}$ ) and absorption ( $B_{ab}$ ) coefficients are given by the Fermi Golden Rule,

$W_{i \rightarrow f} = \frac{2\pi}{\hbar} |\langle f | H | i \rangle|^2 \rho$ . For instance, the spontaneous emission coefficient can be obtained as:

$$B_{sp} = \frac{2\pi}{\hbar} |\langle f | H | i \rangle|^2 \rho \quad (7)$$

The Purcell factor  $F_p$  can be obtained as the ratio between the transition rate coefficients inside the cavity ( $W_{cav}$ ) and in bulk ( $W_B$ ):

$$F_p = \frac{W_{cav}}{W_B} = \frac{B_{sp,cav}}{B_{sp,B}} = \frac{\frac{2\pi}{\hbar^2} |\langle f | H_{cav} | i \rangle|^2 \rho_{cav}}{\frac{2\pi}{\hbar^2} |\langle f | H_B | i \rangle|^2 \rho_B} \quad (9)$$

So the spontaneous emission coefficient in the cavity is obtained as:

$$B_{sp,cav} = F_p B_{sp,B} \quad (10)$$

This means that the photonic cavity increases the spontaneous emission coefficient by a  $F_p$  factor. The creation of the cavity also affects several parameters by means of  $F_p$ . For instance, the  $M$  parameter given by Eq. (4), which is proportional to  $B_{sp}$ , will be also proportional to  $F_p$ , when considering the photonic cavity:

$$M_{cav} = F_p M_B \quad (11)$$

The photon lifetime inside the cavity is given by [21]:

$$\tau_p = \frac{\lambda Q}{2\pi c} \quad (12)$$

Then, from Eq. (6) we get that the photon lifetime inside the cavity is also enhanced by  $F_p$  in comparison with the photon lifetime in bulk:

$$\tau_{p,cav} = F_p \tau_{p,B} \quad (13)$$

The density of states per energy interval for the single photon is [22]:

$$D(E) = 2Vn^2n_g \frac{(\hbar\omega)^2}{\hbar^2 c^3} \quad (14)$$

The group index  $n_g$  is proportional of a photonic cavity is proportional to the photon lifetime and therefore, to the quality factor, so we also get that the density of states per energy interval is enhanced by  $F_p$  when the photonic cavity is created:

$$D(E)_{cav} = F_p D(E)_B \quad (15)$$

This is a quite intuitive result: the density of states inside the optical cavity is increased proportional to the Purcell factor. If we consider the density of states,  $K_p$ , which can be calculated as  $K_p = \int D(E)dE$  we get that it is also proportional to  $F_p$ , as:

$$K_{p,cav} = F_p K_{p,B} \quad (16)$$

It can be seen that the main effect of the optical cavity is to enhance all these parameters ( $B_{sp}$ ,  $M$ ,  $\tau_p$ ,  $D$ ) by the Purcell factor.

Beside, we have to consider that  $\tau_{C,RAD}=1/W_{RAD}$ , where  $W_{RAD}$  is the radiative transition coefficient that is proportional to Purcell Factor. Some experimental values of the Purcell factor in light-emitting silicon optical cavities tuned close to the emission wavelength can be seen in Table I of Ref. [13]. Values between 160-1000 are reported depending strongly on the considered cavity mode. However, researchers have designed cavities with quality factors of the order of  $10^6$  and modal volumes of the order  $\sim 0.1(\lambda/n)^3$  at wavelengths around 1000nm, which would enable Purcell factor values greater than  $10^5$  [23,25]. If we consider this value of the Purcell factor we can consider, as a first approximation, that  $1/\tau_{C,RAD} \gg 1/\tau_{C,NRAD}$  and then  $\tau_C \approx \tau_{C,RAD}$  can be considered a good approximation because the optical cavity will enhance the radiative transition in comparison with non-radiative transition. So we get:

$$\tau_{C,cav} = \frac{\tau_{C,B}}{F_P} \quad (17)$$

Therefore, in contrast to the previously addressed parameters, now we obtain that the total lifetime of carriers is inversely proportional to the Purcell factor when the optical cavity is created. Substituting the expressions (11), (13),(15) and (16) in our system of coupled equations (5) we get:

$$\frac{dN}{dt} = R_p - F_P M_B n_p \left[ (n_q + 1) - n_q \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \right] N^2 + F_P M_B (n_q + 1) N^2 - F_P \frac{N}{\tau_{c,B}} \quad (18a)$$

$$\frac{dn_p}{dt} = \frac{M_B}{K_{p,B}} n_p \left[ (n_q + 1) - n_q \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \right] N^2 + \frac{M_B}{K_{p,B}} (n_q + 1) N^2 - \frac{n_p}{F_P \tau_{p,B}} \quad (18b)$$

$$\frac{dn_q}{dt} = F_P \frac{M_B}{K_q} n_p \left[ (n_q + 1) - n_q \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \right] N^2 + F_P \frac{M_B}{K_q} (n_q + 1) N^2 - \left( \frac{n_q - n_{q0}}{\tau_q} \right) \quad (18c)$$

In the steady-state regime all the time derivatives are zero so from Eq. (18b) we obtain:

$$n_p = \frac{\frac{M_B}{K_{p,B}} (n_q + 1) N^2}{\frac{1}{F_P \tau_{p,B}} - \frac{M_B}{K_{p,B}} \left[ (n_q + 1) - n_q \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \right] N^2} \quad (19)$$

and

$$\frac{K_{p,B}}{\tau_{p,B}} = F_P M_B \left[ (n_q + 1) - n_q \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \right] N^2 \quad (20)$$

Eq. (20) stands for the threshold condition. Our results show that inside the optical cavity the threshold condition for laser oscillation is not so restrictive as in bulk and the photon loss of the resonant cavity is quickly compensated. We can also obtain the following expression for the optical gain in the cavity:

$$g_{cav}(\hbar\omega) = \frac{\hbar^3 c^2}{8\pi n^2(\hbar\omega)^2} R_{sp,cav}(\hbar\omega) \cdot \left[ 1 - \frac{n_q}{n_q + 1} \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \right] \quad (21)$$

which is the same as in Ref. [6] but with the addition of the Purcell factor when considering the spontaneous emission rate:

$$R_{sp,cav}(\hbar\omega) = F_P R_{sp,B}(\hbar\omega) \quad (22)$$

We can see that the optical gain increases in proportion to the Purcell factor, as it could be expected:

$$g_{cav}(\hbar\omega) = F_P g_B(\hbar\omega) \quad (23)$$

where  $g_B$  is the optical gain in bulk and  $g_{cav}$  is the optical gain inside the cavity.

#### IV. Variation of the optical gain, photon density, phonon density, carrier density, oscillation laser threshold and threshold pumping

As in Ref. [6], we will discuss the steady-state solutions in two different situations: below and above threshold, but now, in the case where we have a silicon cavity.

- a) Below threshold, the photon density is low, so the net stimulated emission rate can be neglected and:

$$F_P R_{st,B}(\hbar\omega) - F_P R_{ab,B}(\hbar\omega) = F_P [R_{st,B}(\hbar\omega) - R_{ab,B}(\hbar\omega)] \approx 0 \quad (24)$$

Then, the rate equations become:

$$R_p - F_P M_B (n_q + 1) N^2 - F_P \frac{N}{\tau_{c,B}} = 0 \quad (25a)$$

$$\frac{M_B}{K_{p,B}} (n_q + 1) N^2 - \frac{n_p}{F_P \tau_{p,B}} = 0 \quad (25b)$$

$$F_P \frac{M_B}{K_q} (n_q + 1) N^2 - \left( \frac{n_q - n_{q0}}{\tau_q} \right) = 0 \quad (25c)$$



$$N_p = K_p n_p \quad ; \quad N_q = K_q n_q \quad (25d)$$

Using the values shown in Table I of Ref. [6], which can be considered as typical values in silicon, we get that the first term in the left side of Eq. (25c) is approximately equal to  $F_p(n_q+1) \times 10^{-4}$  whilst the second term is approximately equal to  $(n_q - n_{q0}) \times 10^{12}$ . Therefore, we can neglect the first term and then approximate  $n_q \approx n_{q0}$  at room temperature, which is a good assumption provided that  $F_p \leq 10^{14}$ . Then we obtain:

$$N_q \approx N_{q0} \quad (26)$$

From Eq. (32a) we get that the carrier concentration is:

$$N = \frac{-\frac{F_p}{\tau_{c,B}} + \frac{F_p}{\tau_{c,B}} \sqrt{1 + 4M_B \frac{\tau_{c,B}^2}{F_p} (n_{q0} + 1) R_p}}{2M_B F_p (n_{q0} + 1)} \quad (27)$$

Using again the values of the Table I in Ref. [6] and performing some approximations we get:

$$N = \frac{-\frac{F_p}{\tau_{c,B}} + \frac{F_p}{\tau_{c,B}} \sqrt{1 + 4M_B \frac{\tau_{c,B}^2}{F_p} (n_{q0} + 1) R_p}}{2M_B F_p (n_{q0} + 1)} \approx \quad (28)$$

$$\frac{-\frac{F_p}{\tau_{c,B}} + \frac{F_p}{\tau_{c,B}} \left( 1 + 2M_B \frac{\tau_{c,B}^2}{F_p} (n_{q0} + 1) R_p \right)}{2M_B F_p (n_{q0} + 1)} = \frac{\tau_{c,B}}{F_p} R_p$$

The higher the Purcell factor (or the Q-factor of the photonic cavity), the better the approximation in Eq. (28) will be. Finally, by substituting Eqs. (26) and (28) into Eq. (25b), the photon density in the cavity is obtained as:

$$N_p \approx M_B \tau_{c,B}^2 \tau_{p,B} (n_{q0} + 1) R_p^2 \quad (29)$$

b) Above threshold, it occurs that  $\Delta F \gg \hbar\omega + \hbar\Omega$ , so finally the threshold condition for laser oscillation is:

$$\frac{K_{p,B}}{\tau_{p,B}} = F_{p,B} M_B (n_q + 1) N^2 \quad (30)$$

and the system of coupled equations in the steady-state is now:

$$R_p - F_p M_B n_p (n_q + 1) N^2 - F_p M_B (n_q + 1) N^2 - F_p \frac{N}{\tau_{c,B}} = 0 \quad (31a)$$

$$\frac{M_B}{K_{p,B}} n_p (n_q + 1) N^2 + \frac{M_B}{K_{p,B}} (n_q + 1) N^2 - \frac{n_p}{F_p \tau_{p,B}} = 0 \quad (31b)$$

$$F_p \frac{M_B}{K_q} n_p (n_q + 1) N^2 + F_p \frac{M_B}{K_q} (n_q + 1) N^2 - \left( \frac{n_q - n_{q0}}{\tau_q} \right) = 0 \quad (31c)$$

Substituting the threshold condition given by Eq. (30) into Eqs. (31a) and (31c) the following equation is obtained

$$n_q^3 + (1 - 2A_1)n_q^2 + (A_1^2 - 2A_1)n_q + (A_1^2 - A_2) = 0, \quad (32)$$

where

$$A_1 = n_{q0} + \frac{\tau_q R_p}{K_q}, \quad A_2 = \frac{K_{p,cav} \tau_q^2}{\tau_{p,cav} M_{cav} \tau_{c,cav}^2 K_q^2}$$

Using the values in Ref. [6] again, we get:

$$A_2 = \frac{K_p \tau_q^2}{\tau_p M \tau_c^2 K_q^2} = \frac{F_p K_{p,B} \tau_q^2}{F_p \tau_{p,B} F_p M_B \frac{\tau_{c,B}^2}{F_p^2} K_q^2} = \frac{F_p}{10^{19}} \quad (33)$$

If  $F_p \ll 10^{14}$  the term  $A_1^2$  is found to be much greater than  $A_2$ , so  $A_2$  can be neglected and the approximate solution to Eq. (32) is:

$$n_q \approx A_1 = n_{q0} + \frac{\tau_q R_p}{K_q} \quad (34)$$

And therefore:

$$N_q \approx N_{q0} + \tau_q R_p \quad (35)$$

Substituting Eq. (35) into Eq. (30) we get the following approximation for the threshold of the carrier density:

$$N = \sqrt{\frac{K_{p,B}}{\tau_{p,B} F_{p,B} M_B (n_{q0} + 1 + \frac{\tau_q R_p}{K_q})}} \equiv N_{th} \quad (36)$$

We can see that  $F_p$  decreases the carrier density threshold to get the laser oscillation. Substituting Eqs. (36) and (30) into Eq. (31a) and using the approximation  $n_q \approx n_{q0}$ , we get:

$$R_p - n_p \frac{K_{p,B}}{\tau_{p,B}} - F_p M_B (n_q + 1) N^2 - F_p \frac{N}{\tau_{c,B}} = 0 \quad (37a)$$

and

$$N_p = F_p \tau_{p,B} \left( R_p - F_p M_B (n_q + 1) N_{th}^2 - F_p \frac{N_{th}}{\tau_{c,B}} \right) = F_p \tau_{p,B} (R_p - R_{th}) \quad (37b)$$

$$R_{th} = F_p M_B (n_q + 1) N_{th}^2 + F_p \frac{N_{th}}{\tau_{c,B}} \quad (37c)$$

Where we must take into account that  $n_p K_{p,B}$  is the photon density in bulk but  $F_p n_p K_{p,B}$  is the photon density inside the photonic cavity, and  $R_{th}$  is the pumping rate at threshold. The final expressions we get for the carrier, photon and phonon densities are summarized in Table I.

**Table I** Summary of theoretical expression for for the carrier, photon and phonon densities

	Below threshold	Above threshold
Carrier density	$N = \frac{\tau_{c,B}}{F_p} R_p$	$N = \sqrt{\frac{K_{p,b}}{\tau_{p,B} F_p M_B (n_{q0} + 1 + \frac{\tau_q R_p}{K_q})}} \equiv N_{th}$
Photon density	$N_p \approx M_B \tau_{c,B}^2 \tau_{p,B} (n_{q0} + 1) R_p^2$	$N_p = F_p \tau_{p,B} (R_p - R_{th})$
Phonon density	$N_q \approx N_{q0}$	$N_q \approx N_{q0} + \tau_q R_p$

Table 1 Final expressions for  $N_p$ ,  $N_q$  and  $N$  in the photonic cavity.

## V. Numerical results

In all the numerical results displayed in this section we employ again the parameters summarized in Table I of Ref. [6]. To start with, in Fig. 2 we represent the pumping rate

at threshold,  $R_{p,th}$ , as a function of the cavity Purcell factor. The  $R_{th}$  dependence on  $1/\sqrt{F_p}$  is intuitive since  $F_p$  decreases the carrier lifetime, so increasing the pumping rate is necessary to get the population inversion. We should mention that we have considered that the carrier lifetime is equal to the radiative lifetime, which can be considered a good approximation in our scenario as previously discussed.

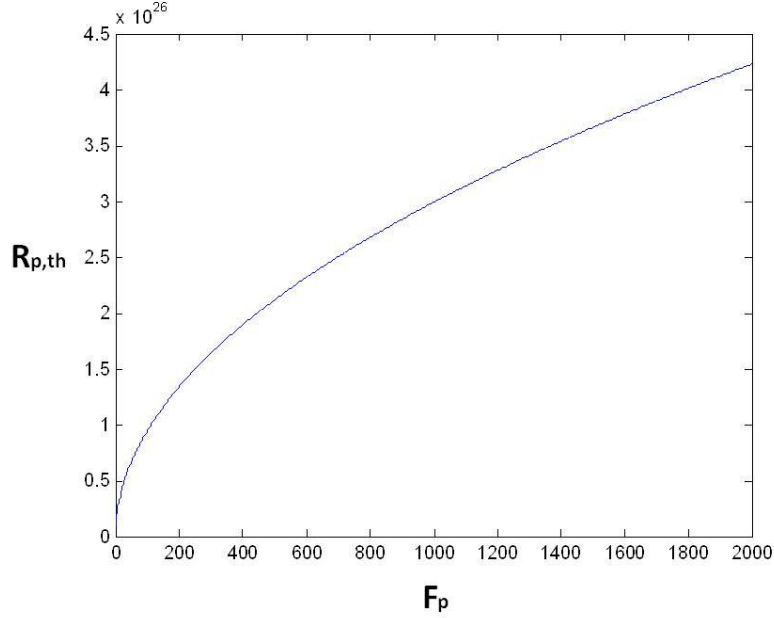
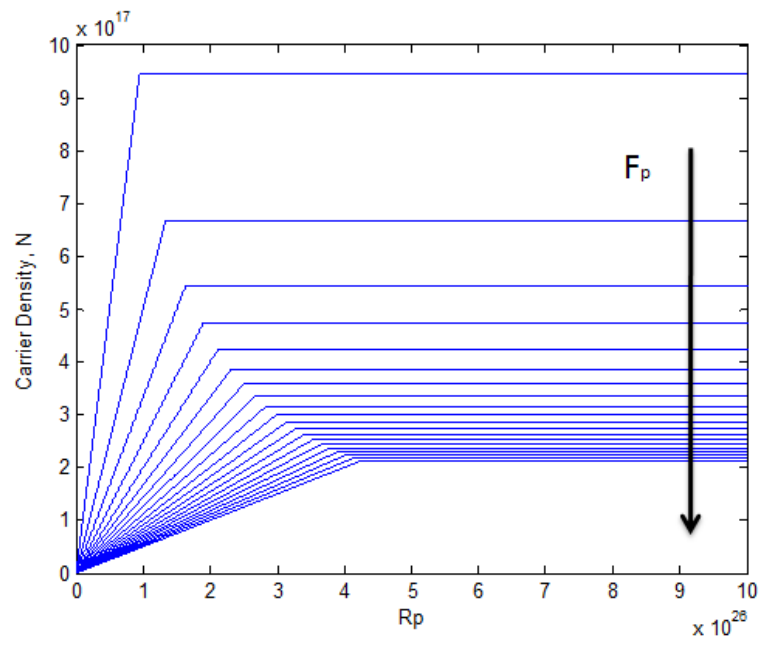
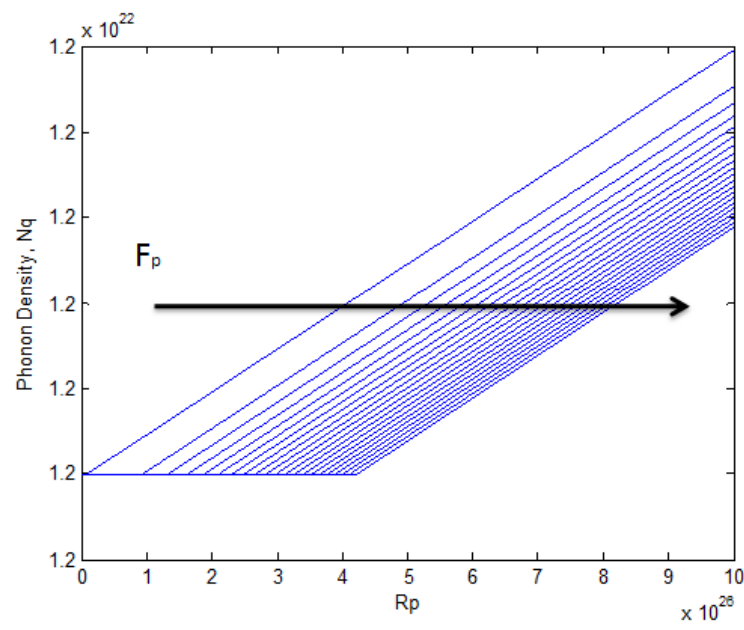


Figure 2. Dependence of  $R_{p,th}$  on the Purcell factor.

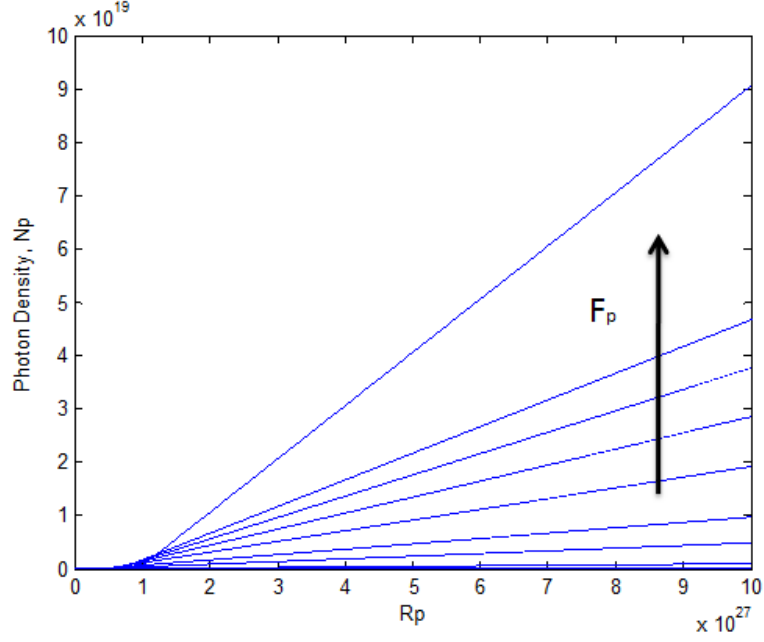
Figure 3 shows the carrier concentration, phonon density and photon density as a function of the pumping rate  $R_p$  for  $F_p$  values between 100 and 2000 (the arrow indicates the direction of increasing  $F_p$ ). In Fig. 3(a) we can see that the threshold charge concentration decreases with  $F_p$ , which means that we do not need a very high population inversion to reach the laser oscillation, and as a result, the laser oscillation condition is less restrictive. In Figs. 3(b) and (c) we can see that both the phonon and photon densities grow rapidly after the threshold, which is a clear signature of the co-stimulated emission of photons and phonons. But we can also observe that the phonon and photon densities do not grow in the same way. This can be explained by considering that the Purcell effect affects only the photons lifetime but not the phonons lifetime. This observation leaves an open door to investigate a possible Purcell effect for phonons.



(a)



(b)



(c)

Figure 3. Carrier density (a), phonon density (b) and photon density (c) as a function of the pumping rate for values of the Purcell factor between 100 and 2000.

## VI. Free-carrier absorption and optical gain

In order to achieve optical amplification, and eventually lasing, the magnitude of optical amplification has to be large enough to overcome the optical losses resulting from the silicon itself and the optical cavity. A major loss mechanism that can hinder amplification is free carrier absorption (FCA). The FCA magnitude,  $\alpha_{FC}$ , in bulk silicon at around room temperature is given by following empirical expression [25, 26],

$$\alpha_{FC} = (1.01 \cdot 10^{-20} N + 0.51 \cdot 10^{-20} P) \lambda^2 T \quad (38)$$

where  $N$  and  $P$  are, respectively, the electrons and holes densities. The expression of the optical gain inside the cavity as a function of  $N$  is:

$$g_{cav}(\hbar\omega) = F_p \frac{\hbar^3 c^2}{8\pi m^2 (\hbar\omega)^2} M_B (n_q + 1) \left[ 1 - \frac{n_q}{n_q + 1} \exp\left(\frac{(\hbar\omega + \hbar\Omega - \Delta F)}{K_B T}\right) \right] N^2 \quad (39)$$

If we compare the FCA (Eq. (38)) and the optical gain (Eq. (39)) for different values of Purcell factor we get that the optical gain exceeds the FCA for  $F_p > 30$ . However, this result is in contrast with the fact that optical gain in silicon cavities at room temperature has not been observed experimentally, which leads us to conclude that we need to consider also how the photonic cavity affects the FCA losses. In Ref. [27], T. F. Bogges and co-workers study both two photon absorption (TPA) and FCA in

crystalline silicon. They describe the propagation of a optical pulse travelling along the  $z$  direction taking into account the presence of linear absorption, TPA and FCA, using this expression:

$$\frac{dI}{dz} = -\alpha I - \beta I^2 - \sigma NI \quad (40)$$

where  $I$  is the irradiance,  $\alpha$  is the linear absorption,  $\beta$  is TPA coefficient and  $\sigma$  is the FCA cross section. The irradiance dimension is:  $[I] = Wm^2 = \frac{\Pi_p \hbar \omega}{tm^2}$ , where  $\Pi_p$  is the photon number. Since  $\Pi_p = N_p V$  Eq.(40) can be transformed into:

$$\frac{d\Pi_p}{dz} = -\alpha \Pi_p - \beta \Pi_p^2 - \sigma N \Pi_p \quad (41)$$

And finally we get

$$V \frac{dN_p}{dz} = -\alpha N_p V - \beta N_p^2 V^2 - \sigma N N_p V \quad (42)$$

The last term in the right side of Eq.(42) is the loss due to FCA,  $\alpha_{FCA} = \sigma N N_p V$ . We obtained before that the photon density is proportional to Purcell factor inside of the cavity. Therefore, it is straightforward to conclude that the FCA losses inside of the cavity are proportional to  $F_p$ :  $\alpha_{FCA,cav} \propto F_p$ . The result is that both FCA losses and optical gain scale with the Purcell factor in the same way, just as it occurs in a bulk semiconductor. In the cavity at room temperature we get the results depicted in Fig. 4 which show an identical behaviour to those presented in Ref. [6] for bulk silicon.

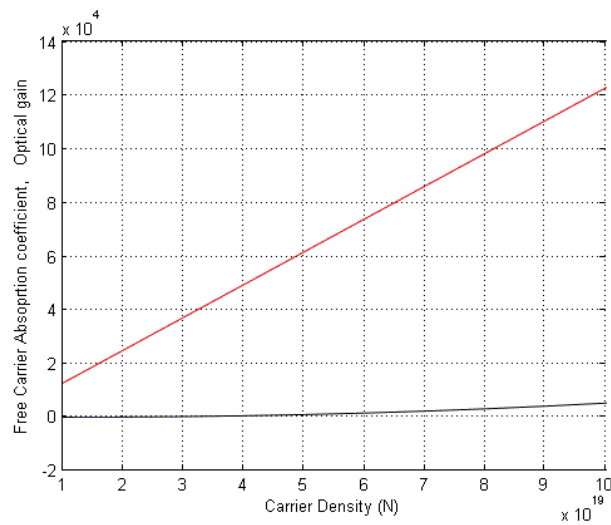


Figure 4. FCA loss (red line) and optical (black line) in an indirect bandgap semiconductor cavity at ambient temperature

By taking into account this finding, we believe that the luminescence peaks from silicon cavities reported in Refs. [7,18-20] are not due to optical gain, but to an increase of the quantum efficiency in the process of emission. The quantum efficiency in the radiative process can be defined as:

$$\eta = \frac{W_{cav}^{rad}}{W_{cav}^{rad} + W^{nrad}} \quad (43)$$

Since  $W_{cav}^{rad} \propto F_p$ , we get:

$$\eta = \frac{W_{bulk}^{rad}}{W_{bulk}^{rad} + \frac{W^{nrad}}{F_p}} \quad (44)$$

It can be seen that the quantum efficiency approaches unity for large values of the Purcell factor, which can explain the luminescence peaks, but lasing is not feasible in silicon cavities at room temperature.

## VII. Conclusion

In this work we have described theoretically the different processes related to light emission from indirect bandgap semiconductor cavities. We have obtained that net optical gain in silicon at room temperature is not feasible despite the use of a high-Q photonic cavity since the Purcell factor affects the optical gain and the free-carrier absorption losses in the same way. In this sense, it has to be mentioned that we only have considered the losses to due free carrier absorption. However, other losses mechanisms will also co-exists in the system under study, which will further hinder the possibility of lasing emission.

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