A Model Calculation on Optical Gain and Co-Stimulated Emissions of Photons and Phonons in Silicon

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Group IV materials-based micro- and nano-photonics has gradually become a very active area for research worldwide.[1] A variety of passive and active components and devices have been explored and/or realized.[1] For the key component of silicon-based light sources, numerous approaches, mostly involving the experimental studies, have been explored with significant progresses.[2-23] On the theoretical study of the subject, optical gain in materials with indirect transitions such as bulk crystalline silicon was reassessed recently based on a simple two-level model.[24] In this paper, we present a model calculation on the optical gain at bandgap energy and the rate equations for electron, photon, and phonon in silicon which takes into account the detailed band-edge structures of the conduction and valence bands.

The theoretical analysis has arrived at an expression for optical gain $g(\hbar\omega)$ via phonon-assisted optical transitions in indirect bandgap semiconductors such as silicon as follows

$$g(\hbar\omega)=\frac{h^3c^2}{8\pi n^2(\hbar\omega)^2}R_{sp}(\hbar\omega)\cdot\left\{1-n_q\big/\left(n_q+1\right)\cdot\exp\left[\left(\hbar\omega+\hbar\Omega-\Delta F\right)/k_BT\right]\right\} \tag{1}$$

where $R_{sp}(\hbar\omega)$ is the spontaneous emission rate, n_q is the phonon occupation number, $\hbar\omega$ and $\hbar\Omega$ are the photon and phonon energies, $\hbar$ is the reduced Planck constant, c is the velocity of light in free space, n is the refractive index, ΔF is the difference of the quasi-Fermi levels for electrons and holes, k_B is the Boltzmann constant, and T is the temperature. It is seen that the sign of $g(\hbar\omega)$ is determined by ΔF and its magnitude is also proportional to $R_{sp}(\hbar\omega)$. Various carrier localization structures such as nanostructured PN junctions[12] may be utilized to enhance $R_{sp}(\hbar\omega)$ and thus $g(\hbar\omega)$. Clearly, an optical gain can take place if the quantity in braces is positive, i.e.

$$\left(n_q+1\right)\big/n_q>\exp\left[\left(\hbar\omega+\hbar\Omega-\Delta F\right)/k_BT\right] \tag{2}$$

Figure 1 shows the relationship between ΔF and n_q required for population inversion involving transverse optical (TO) phonon ($\hbar\Omega$ =57.8 meV)-assisted optical transition at photon energy $\hbar\omega$=1.07 eV in crystalline silicon at 300K. The solid curve in Fig. 1 depicts the condition and the region for population inversion. The phonon occupation number at thermodynamic equilibrium n_{q0} and the condition $\Delta F=\hbar\omega+\hbar\Omega$ are indicated in dotted lines, respectively. The region above the solid curve is the positive optical gain region $\left(g(\hbar\omega)>0\right)$, while the region below the solid curve is the absorption region $\left(g(\hbar\omega)<0\right)$.

Since a phonon is *emitted* during the stimulated emission of a photon and since a phonon is *absorbed* during the absorption of a photon, a net stimulated emission of phonons will occur when the population inversion is reached. Therefore, the condition for the net stimulated phonon emission resulting from the net stimulated emission of photons with energy $\hbar\omega$ is the same as Eq.(2). The increase in the phonon population due to the net stimulated phonon emission results in a deviation of phonon occupation number n_q from its value at thermal equilibrium. Figure 1 shows that as the phonon occupation number n_q increases from the value at thermodyamic equilibrium n_{q0}, a larger value of ΔF is required to facilitate population inversion.

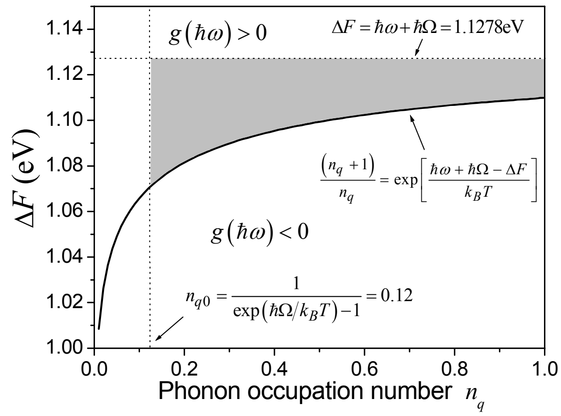

Figure 1: Relationship between ΔF and n_q required for population inversion in bulk crystalline silicon at 300K.

The net generation rates for photon and phonon are derived as follows

$$R_{st}(\hbar\omega)-R_{ab}(\hbar\omega)+R_{sp}(\hbar\omega)$$
$$=M\cdot\left[\left(n_p+1\right)\left(n_q+1\right)-n_pn_q\exp\left(\frac{\hbar\omega+\hbar\Omega-\Delta F}{k_BT}\right)\right]\cdot NP \tag{3}$$

where $R_{st}(\hbar\omega)$, $R_{sp}(\hbar\omega)$ and $R_{ab}(\hbar\omega)$ are, respectively, the rates of stimulated emission, spontaneous emission and absorption; n_p is the photon occupation number; *M* is a constant related to radiative recombination; and *N* and *P* are the electron and hole concentrations. Note that in Eq.(3), the term $\left(n_p+1\right)\left(n_q+1\right)$ corresponds to the stimulated and spontaneous emission rates of photon and phonon, while the term $n_pn_q\exp\left[\left(\hbar\omega+\hbar\Omega-\Delta F\right)/k_BT\right]$ represents the absorption rate of photon and phonon.

The rate equations for electron, photon and phonon involved are given by

$$\frac{dN}{dt}=R_p-Mn_p\left[\left(n_q+1\right)-n_q\exp\left(\frac{\hbar\omega+\hbar\Omega-\Delta F}{k_BT}\right)\right]N^2-M\left(n_q+1\right)N^2-\frac{N}{\tau_c} \tag{4a}$$

$$\frac{dn_p}{dt}=\frac{M}{K_p}n_p\left[\left(n_q+1\right)-n_q\exp\left(\frac{\hbar\omega+\hbar\Omega-\Delta F}{k_BT}\right)\right]N^2+\beta\frac{M}{K_p}\left(n_q+1\right)N^2-\frac{n_p}{\tau_p} \tag{4b}$$

$$\frac{dn_q}{dt}=\frac{M}{K_q}n_p\left[\left(n_q+1\right)-n_q\exp\left(\frac{\hbar\omega+\hbar\Omega-\Delta F}{k_BT}\right)\right]N^2+\frac{M}{K_q}\left(n_q+1\right)N^2-\frac{n_q-n_{q0}}{\tau_q} \tag{4c}$$

where R_p is the pumping rate either by current injection or optical excitation; β is a factor which represents the fraction of spontaneous emission entering the optical mode; τ_c , τ_p and τ_q are the lifetimes of carrier, photon and phonon, respectively; and K_p and K_q are the density of states for photon and phonon, respectively.

We set $d/dt=0$ in Eqs.(4a)~(4c) and solve for the steady state solution of the rate equations. The threshold condition for laser oscillation is then obtained as follows

$$M\left[\left(n_q+1\right)-n_q\exp\left(\frac{\hbar\omega+\hbar\Omega-\Delta F}{k_BT}\right)\right]N^2=\frac{K_p}{\tau_p} \tag{5}$$

Eq.(5) shows that the photon loss of the resonant cavity must be compensated by the optical gain for the on-set of laser oscillation. The steady state solutions for electrons, photons, and phonons above the threshold are

$$N \approx \sqrt{\frac{K_p/\tau_p}{M\left\{n_{q0}\left[1-\exp\left(\frac{\hbar\omega+\hbar\Omega-\Delta F}{k_B T}\right)\right]+1\right\}}} \equiv N_{th} \tag{6a}$$

$$N_q \approx N_{q0} + \tau_q R_p \tag{6b}$$

$$N_p \approx \tau_p \left(R_p - R_{pth}\right) \tag{6c}$$

where $N_p = K_p n_q$ and $N_q = K_q n_q$ are, respectively, the photon density and the phonon density, $N_{q0} = K_q n_{q0}$ is the phonon density at thermodynamic equilibrium, and R_{pth} is the pumping rate at threshold. Below the threshold, the photon density N_p increases rather slowly. However, once the threshold is reached, the photon density N_p increases rapidly and linearly with the pumping rate R_p. As to the phonon, its density N_q remains practically constant before threshold, but increases linearly with the pumping rate R_p once the threshold is reached. Both the photon and the phonon densities grow rapidly after the threshold is reached, which indicates the co-stimulated emission of photons and phonons. On the other hand, the carrier concentration N increases linearly with the pumping rate R_p before the threshold is reached, but clamps at its threshold value N_{th} after the threshold is reached.

In summary, the approach and findings of a model calculation on the optical gain at bandgap energy and the solution of the rate equations for electron, photon and phonon in indirect bandgap semiconductors such as silicon are presented.

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