Reversible Modulation of Spontaneous Emission by Strain in Silicon Nanowires

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Supplementary Information

In this section, we provide further details of the derivations in the manuscript that resulted in equations (4) and (5).

LA Phonons (equation 4): The quantity of $Ph_{LA}(k_f,k_i)$ in equation (4) of the manuscript is the following numerical summations over all possible transverse phonon wave vectors.

$$Ph_{LA}(k_f,k_i) = \int_0^{\tilde{q}_{t\_max}} \sqrt{\tilde{q}_t^2 + q_z^2}\, \frac{E_c(k_i) - E_v(k_f) \mp \frac{\epsilon}{a} \hbar v_s \sqrt{\tilde{q}_t^2 + q_z^2}}{\left(E_c(k_m = k_f) - E_c(k_i) \pm \frac{\epsilon}{a} \hbar v_s \sqrt{\tilde{q}_t^2 + q_z^2}\right)^2} B_{\pm}(|\tilde{\boldsymbol{q}}|) \left[\int_0^{2\pi} |S(|\tilde{\boldsymbol{q}}|)|^2 d\phi\right] \tilde{q}_t d\tilde{q}_t \quad \text{(S1)}$$

Here we provide a summary of derivation of equation (S1). Recalling that ADC transitions in Figure.4c can be ignored and inserting the matrix elements of electron-photon and electron-phonon interaction Hamiltonians in equation (2) of the manuscript, we get

$$\tau_{spon}^{-1} = \sum_{k_f} \frac{2\pi}{\hbar} \sum_{k',\sigma'} \sum_{\bar{q},l} \sum_{k_m} \frac{|P|^2 |O|^2}{(E_i - E_m)^2} \delta\left(E_f - E_i\right) F\left(k_f\right) \quad \text{(S2)}$$

where k', σ' are photon wave vector and polarization, respectively. $\bar{q}$ is phonon wave vector and l is the phonon branch index. k_f and k_m are the electron wave vectors for final and intermediate states which are within the conduction and valence band, respectively. The Dirac delta function ensures the conservation of energy. $F(k_f)$ is the Fermi factor at each valence state (k_f). $|O|^2$ and $|P|^2$ represent $|\langle m|H_{ep}|i\rangle|^2$ and $|\langle f|H_{eR}|m\rangle|^2$, respectively. E_i, E_m and E_f correspond to the energy of the mixed (Fermionic and Bosonic) initial (i), intermediate (m) and final (f) states, respectively. They are found by assuming a distribution of $n_{k,\sigma}$ photons and $n_{q,l}$ phonons before light emission occurs. For the initial and intermediate states in the conduction band, the energies can be written as

$$E_i = E_{ci} + n_{k,\sigma}\hbar\omega_{k,\sigma} + n_q\hbar\omega_q, \quad E_m = E_{cm} + n_{k,\sigma}\hbar\omega_{k,\sigma} + \left(n_q \pm_a^e 1\right)\hbar\omega_q \qquad \text{(S3)}$$

where $e(a)$ represents emission (absorption) of a phonon. Similarly the final energy in the valence band (after emission of a photon) can be written as

$$E_f = E_{vf} + \left(n_{k,\sigma} + 1\right)\hbar\omega_{k,\sigma} + \left(n_q \pm_a^e 1\right)\hbar\omega_q \qquad \text{(S4)}$$

Therefore E_i-E_m is reduced to

$$\Delta E_{im} = E_m - E_i = E_{cm} - E_{ci} \pm_a^e \hbar\omega_q \qquad \text{(S5)}$$

and the Dirac delta function is written as

$$\delta\left(E_f - E_i\right) = \delta\left(E_i - E_f\right) = \delta(E_{ci} - E_{vf} - \hbar\omega_{k,\sigma} \mp_a^e \hbar\omega_q) \qquad \text{(S6)}$$

The process of simplifying the electron-photon interaction Hamiltonian matrix element, $|O|^2$, can be found in [Anselm81] and here we show the result only

$$|O|^2 = \left(\frac{e}{m}\right)^2 \frac{\hbar\left(n_{k',\sigma'}+1\right)}{2V\epsilon\,\omega_{k',\sigma'}} \left|\left\langle a_f\middle|\hat{P}.\hat{\varepsilon}_{k',\sigma'}e^{-ik'.r}\middle|a_m\right\rangle\right|^2 \qquad \text{(S7)}$$

where the population number of photons is considered to be $n_{k',\sigma'} = 0$ for spontaneous emission. a_f and a_m is the mixed electronic and photonic state corresponding to final and intermediate states. Also $\omega_{k'}$ is the frequency of photon field, $\widehat{\boldsymbol{p}}$ is the momentum operator, $\hat{\varepsilon}_{k',\sigma'}$ is the unit vector pointing in polarization direction (σ'). ϵ, V and $\hbar$ are dielectric permittivity of medium, volume of photon field quantization and reduced Planck's constant (1.054×10^{-34} J.s), respectively. e is the magnitude of electronic charge (1.602×10^{-19} C) and m is the free electron mass (9.109×10^{-31} kg). The electron-LA phonon Hamiltonian matrix element, $|P|^2$, is found using the procedure which is shown in equations (10-12) of [Buin08]. Inserting these matrix elements into equation (S2) yields

$$\tau_i^{-1} = \frac{2\pi}{\hbar}\left(\frac{e}{m}\right)^2 \frac{\hbar}{2V\epsilon}\frac{D^2\hbar}{2\rho V}\sum_{k_f}\sum_{k',\sigma'}\sum_{\tilde{q},l}\frac{1}{\omega_{k',\sigma'}}\left|\left\langle\psi_f\middle|\hat{P}.\hat{\varepsilon}_{k',\sigma'}\middle|\psi_m\right\rangle\right|^2\frac{|\tilde{q}|^2}{\omega_q}\frac{|S(|\tilde{q}|)|^2B_{\pm}(|\tilde{q}|)}{\left(E_{cm}-E_{ci}\pm_a^e\hbar\omega_q\right)^2}\delta\left(E_{ci}-E_{vf}-\hbar\omega_{k',\sigma'}\mp_a^e\hbar\omega_q\right).F\left(k_f\right)$$

(S8)

Where $S(|\tilde{\boldsymbol{q}}|)$ is the overlap factor or matrix element of $e^{i\boldsymbol{q}.\boldsymbol{r}}$ terms which is defined in equation (13) of [Buin08]. After performing summation over photon (radiation) wave vectors and polarizations we have

$$\tau_{spon}^{-1} = \frac{2\pi}{\hbar}\left(\frac{e}{m}\right)^2\frac{\hbar}{2V\epsilon}\frac{D^2\hbar}{2\rho V}\frac{V}{3\pi^2}\frac{1}{vv_s}\sum_{k_f}\sum_{\tilde{q},l}\left|\left\langle\psi_f\middle|\hat{P}\middle|\psi_m\right\rangle\right|^2|\tilde{q}|\frac{|S(|\tilde{q}|)|^2B_{\pm}(|\tilde{q}|)}{\left(E_{cm}-E_{ci}\pm_a^e\hbar\omega_q\right)^2}.F\left(k_f\right)\int k'dk'\ \delta\left(E_{ci}-E_{vf}-\hbar\omega_{k'}\mp_a^e\hbar\omega_q\right)$$

(S9)

Using sifting properties of Dirac delta function, $\omega_{k'} = vk'$ (v is velocity of light in Si and it is $v = c/n_r$) and converting the momentum matrix element to position representation, we get

$$\tau_{spon}^{-1} = \frac{2\pi}{\hbar}\frac{\hbar}{2V\epsilon}\frac{e^2D^2\hbar}{2\rho}\frac{1}{3\pi^2}\frac{n_r^3}{\hbar^2c^3v_s}\sum_{k_f}\omega_{fm}^2\left|\left\langle\psi_f\middle|\hat{r}\middle|\psi_m\right\rangle\right|^2F\left(k_f\right).\sum_{\tilde{q}}|\tilde{\boldsymbol{q}}|\,|S(|\tilde{\boldsymbol{q}}|)|^2B_{\pm}(|\tilde{\boldsymbol{q}}|)\frac{E_c(k_i)-E_v(k_f)\mp_a^e\hbar\omega_q}{\left(E_c(k_m)-E_c(k_i)\pm_a^e\hbar\omega_q\right)^2}$$

(S10)

E_{cm}, E_{ci} and E_{vf} have been replaced by $E_c(k_m)$, $E_c(k_i)$ and $E_v(k_f)$, respectively to recall that they are conduction and valence state energies at the corresponding k values along the BZ. To perform summation over all phonon wave vectors, we use the linearity of phonon dispersion i.e. $\omega_q = v_s|\tilde{\boldsymbol{q}}| = v_s\sqrt{q_t^2 + q_z^2}$ (velocity of sound in Silicon is given by υ_s=9.01×10^5 cm/s). At each final state (k_f), the longitudinal component of phonon momentum is given by $q_z = k_m - k_i$ .Corresponding to this q_z, the maximum allowable transversal component of phonon momentum, $\tilde{q}_{t\_max}$, is found using

$$\tilde{q}_{t\_max} = \sqrt{\left|\frac{E_{debye}}{\hbar v_s}\right|^2 - q_z^2} \qquad \text{(S11)}$$

where E_{debye} is Debye energy of phonons in Silicon which is 55meV. Therefore there are many phonon wave vectors which have a common longitudinal component (q_z) and their transversal (radial) component starts from $\tilde{q}_{t\_min} = 0$ to $\tilde{q}_{t\_max}$ as shown in Fig. 1. If $\left|\frac{E_{debye}}{\hbar v_s}\right| > q_z$, then a phonon is available otherwise its contribution to equation (S10) is zero.

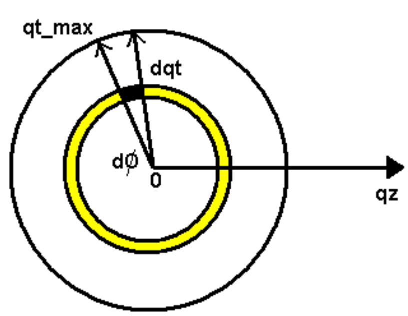

FIG. 1 Available LA phonons with a common q_z and transversal vectors which span $\tilde{q}_{t\_min} = 0$ to $\tilde{q}_{t\_max}$.

Therefore the summation over phonon wave vectors reduces to integration over area of the circle shown in Fig. 7. Since the element of area is $\tilde{q}_t d\tilde{q}_t d\phi$,

$$\sum_{\tilde{q}}[\ldots] = \frac{A}{4\pi^2}\int[\ldots]\,.\,\Delta q_{Area\,element} = \frac{A}{4\pi^2}\int_0^{2\pi}[\ldots]\,.\,d\phi\int_0^{\tilde{q}_{t\_max}}\ldots\,\tilde{q}_t d\tilde{q}_t \qquad \text{(S12)}$$

$S(|\bar{q}|)$ is the only term which depends on ϕ, therefore

$$\tau_{spon}^{-1} = \frac{2\pi}{\hbar}\frac{\hbar}{2V\epsilon}\frac{e^2D^2\hbar}{2\rho}\frac{1}{3\pi^2}\frac{n_r^3}{\hbar^2c^3v_s}\sum_{k_f}\omega_{fm}^2\left|\langle\psi_f|\hat{r}|\psi_m\rangle\right|^2F(k_f)\times \frac{A}{4\pi^2}\int_0^{\tilde{q}_{t\_max}}\sqrt{\tilde{q}_t^2+q_z^2}\frac{E_c(k_i)-E_v(k_f)\mp_a^e\hbar v_s\sqrt{\tilde{q}_t^2+q_z^2}}{\left(E_c(k_m=k_f)-E_c(k_i)\pm_a^e\hbar v_s\sqrt{\tilde{q}_t^2+q_z^2}\right)^2}B_\pm(|\tilde{\boldsymbol{q}}|)\left[\int_0^{2\pi}|S(|\tilde{\boldsymbol{q}}|)|^2d\phi\right]\tilde{q}_t d\tilde{q}_t$$

(S13)

where $\Phi(\tilde{q}_t, q_z) = \int_0^{2\pi}|S(|\tilde{\boldsymbol{q}}|)|^2d\phi$ is a dimensionless form factor. $B_\pm(|\tilde{\boldsymbol{q}}|)$ is the Bose-Einstein factor of phonons and it is $1/(e^{\frac{\hbar\omega_q}{K_BT}}-1)$ for absorption and $1+\frac{1}{(e^{\frac{\hbar\omega_q}{K_BT}}-1)}$ for emission of a phonon.

The result of integration over $\tilde{q}_t$ cannot be simplified analytically and it is shown by $Ph_{LA}(k_f, k_i)$ (see equation (S1)) and its value depends on $k_m=k_f$. Further simplification of equation (S13) results in equation (4) of the manuscript

$$\tau_{spon}^{-1} = \frac{e^2D^2n_r}{\epsilon_0\rho c^3v_s\hbar}\frac{1}{48\pi^4}\sum\omega_{fm}^2\left|\langle\psi_f|\hat{r}|\psi_m\rangle\right|^2F(k_f).Ph_{LA}(k_f,k_i)\Delta k_f \qquad \text{(S14)}$$

LO Phonons (equation 5): Derivation of spontaneous emission life time from the indirect conduction band minimum by including optical phonons proceeds with the same logic as discussed in the previous section, however some extra modifications are required due to the nature of optical phonons. First, the quantity of $|P|^2$, the electron-phonon interaction Hamiltonian matrix element, should be replaced with

$$\left|\langle i|H_{op}|f\rangle\right|^2 = \frac{|D_{op}|^2\hbar}{2\rho V\omega_0}|S(|\tilde{\boldsymbol{q}}|)|^2(N(\hbar\omega_0)+\frac{1}{2}\pm_a^e\frac{1}{2})\,\delta_{k_z',k_z\pm q_z} \qquad \text{(S15)}$$

where it is assumed that LO phonon is dispersion-less i.e. all phonons have constant energy of $E_P = \hbar\omega_0$= 63 meV regardless of their momentum (wave vector). D_{op} is the electron deformation potential for LO phonon (D_{op}=13.24×10^8 eV/cm) and ρ is the mass density of Silicon (ρ= 2329 kg/m^3). Krönecker delta imposes momentum conservation i.e. $k'_z = k_z \pm q_z$.

Second, ΔE_{im} in equation (S5) and Dirac's delta function in equation (S6) are modified accordingly i.e.

$$\Delta E_{im} = E_{cm} - E_{ci} \pm \hbar\omega_0\,, \quad \delta\left(E_f - E_i\right) = \delta\left(E_{ci} - E_{vf} - \hbar\omega_{k',\sigma} \pm \hbar\omega_0\right) \qquad \text{(S16)}$$

Including aforementioned changes and using the electron-photon interaction Hamiltonian matrix element, $|O|^2$, as given in equation (S7), the spontaneous emission time calculation starts from equation (S2) to give

$$\tau_{spon}^{-1} = \frac{2\pi}{\hbar}\left(\frac{e}{m}\right)^2 \frac{\hbar}{2V\epsilon}\frac{\left|D_{op}\right|^2\hbar}{2\rho V\omega_0}\sum_{k_f}\sum_{k',\sigma}\sum_{\tilde{\mathbf{q}},l}\frac{1}{\omega_{k',\sigma}}\left|\langle\psi_f|\hat{p}.\hat{\varepsilon}_{k',\sigma}|\psi_m\rangle\right|^2 \frac{|S(|\tilde{\mathbf{q}}|)|^2 B_\pm(\hbar\omega_0)}{(E_{cm}-E_{ci}\pm\hbar\omega_0)^2}\delta\left(E_{ci} - E_{vf} - \hbar\omega_{k',\sigma} \pm \hbar\omega_0\right).F(k_f)$$

(S17)

The summation over photon wave vectors and polarizations can be performed as explained before. With the help of Dirac delta function it can be reduced to

$$\tau_{spon}^{-1} = \frac{2\pi}{\hbar}\frac{\hbar}{2V\epsilon}\frac{e^2\left|D_{op}\right|^2\hbar}{2\rho V\omega_0}\frac{V}{3\pi^2}\frac{n_r^3}{\hbar^2c^3}\sum_{k_f}\omega_{fm}^2\left|\langle\psi_f|\hat{r}|\psi_m\rangle\right|^2 F(k_f)\sum_{\tilde{\mathbf{q}}}|S(|\tilde{\mathbf{q}}|)|^2 B_\pm(\hbar\omega_0)\frac{E_c(k_i)-E_v(k_f)\pm\hbar\omega_0}{(E_c(k_m)-E_c(k_i)\pm\hbar\omega_0)^2}$$

(S18)

Summations over k_f and $\tilde{q}$ can be converted to integrations. Recalling that k_f and k_m step together i.e. $k_m=k_f$ and $B_\pm$ is independent of $\tilde{q}$, further simplifications result in

$$\tau_{spon}^{-1} = \frac{e^2\left|D_{op}\right|^2 n_r^3}{\epsilon\rho c^3\hbar\omega_0}.\frac{1}{48\pi^4}.B_\pm(\hbar\omega_0)\int_{k_f}\omega_{fm}^2\left|\langle\psi_f|\hat{r}|\psi_m\rangle\right|^2\left\{\int_{q_t=0}^{q_{cmax}} q_t\int_0^{2\pi}|S(q_t,q_z,\varphi)|^2 d\varphi dq_t\right\}\times \frac{E_c(k_i)-E_v(k_f)\pm\hbar\omega_0}{\left(E_c(k_f)-E_c(k_i)\pm\hbar\omega_0\right)^2}F(k_f)dk_f$$

(S19)

where {...} returns a quantity which depends on k_f since $q_z=k_f-k_i$. This quantity and Bose-Einstein factor, $B_{\pm}$, are merged together and called $Ph_{LO}(k_f)$ for the sake of brevity. The spontaneous emission life time is then given as

$$\tau_i^{-1} = \frac{e^2|D_{op}|^2 n_r^3}{\epsilon\rho c^3 \hbar\omega_0} \cdot \frac{1}{48\pi^4} \int_{k_f} dk_f\, \omega_{fm}^2 \left|\langle u_f|\hat{r}|u_m\rangle\right|^2 Ph_{LO}(k_f) \frac{E_c(k_i)-E_v(k_f)\pm\hbar\omega_0}{\left(E_c(k_f)-E_c(k_i)\pm\hbar\omega_0\right)^2} F(k_f) \qquad \text{(S20)}$$

This is equation (5) of the manuscript after the integration over k_f is converted to numerical summation.

References:

[Anselm81] Anselm, A. *Introduction to Semiconductor Theory,* (Mir Publishers, Moscow, 1981).

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