Mechanism of population inversion in uniaxially strained *p*-Ge continuous-wave lasers

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The recently observed continuous-wave THz lasing in a uniaxially strained *p*-Ge under weak electric-field pumping cannot be explained by the mechanism of population inversion for pulse mode lasing from the same sample but by strong electric-field pumping. With a theory including the carrier scattering by impurities, acoustic phonons, and optical phonons, our calculation shows that the specific angular dependence of the impurity scattering and the specific energy dependence of the acoustic-phonon scattering are the origin of the population inversion of the resonant states. We thus complete the theory of population inversion in an electrically pumped uniaxially strained THz *p*-Ge laser.

Terahertz (THz) physics and technology are important to radio astronomy, optical communication, medical diagnosis, nondestructive measurement of spatial distribution of mobility in doped semiconductors, and environmental related problems. Driven by the needs of new devices, the problem of both the high-speed noncoherent and the wideband coherent detection of THz radiation has been solved recently. High efficiency THz radiation sources then remain to be the central problem. Presently available sources of THz radiation include CO_2-pumped molecular or Raman gas lasers, free-electron lasers, backward-wave oscillators, *p*-Ge hot-hole lasers, Schottky diode multipliers, and various pulsed sources based on ultrafast carrier and phonon relaxation in semiconductors or superconductors under intensive femtosecond excitation, as well as utilizing similar mechanisms for nonlinear photomixing of two infrared or optical signals. Of all these sources, only photomixers produce tunable coherent-continuous-wave (cw) radiation with very limited output power.

Semiconductor THz lasers will have many advantages if they can be made. The *p*-Ge laser, which operates under crossing electric and magnetic fields, was realized earlier, but is not practical. Later, a *p*-Ge THz laser was fabricated, and under uniaxial stress it emits a THz radiation pulse if electrically pumped with a high electric field parallel to stress direction.[1] The mechanism of population inversion for such lasing, which has been shown recently,[2] is based on the *streaming motion* of carriers[3,4] and the formation of resonant states.[5] When an electric field is applied, carriers are accelerated by the field, but scattered by impurities as well as by acoustic and optical phonons. With low impurity concentration and at low temperature, if the applied field is high, carriers will have a large probability gaining enough energy to emit optical phonons. Carriers are said to be in the *streaming motion* regime. On the other hand, if the applied field is low, a carrier gains energy slowly. In this case, due to the acoustic-phonon scattering, a carrier can hardly gain enough energy to emit an optical phonon. The resulting motion of the carriers is said to be in the *diffusive regime*.

Under a sufficiently large uniaxial stress, say along the z axis, such that the split of the heavy-hole band and the light-hole band is larger than the acceptor binding energy, the energy-level structure is shown in Fig. 1. For convenience, we have inverted the valence band, and so the heavy-hole band lies above the light-hole band. The hybridization of a localized impurity orbital attached to the heavy-hole band and the Bloch states in the light-hole band results in a resonant state with energy E_0-$i\Gamma/2$. If E_0 is less than the optical-phonon energy, then in the streaming motion regime carriers can be injected into resonant states before emitting optical phonons, resulting in the required population inversion for lasing between the resonant level E_0 and the impurity levels attached to the light-hole band. The so-formulated theory[2] explains well the experimental observation.[1]

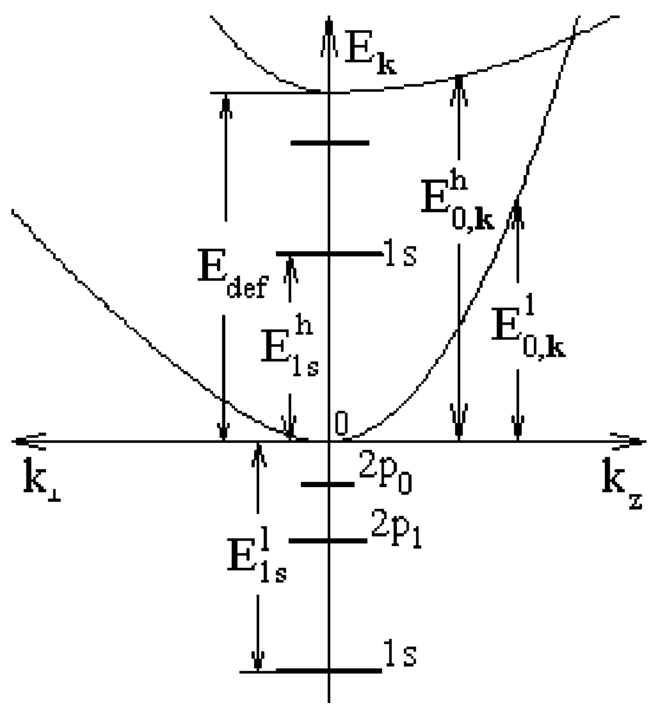

FIG. 1. Acceptor levels and heavy-hole band $E_{0,\mathbf{k}}^h$ and light-hole band $E_{0,\mathbf{k}}^l$ of Ge:Ga under uniaxial stress. The bands are inverted for convenience, and all energies are measured from the edge of the light-hole band.

However, pumping with very low electric field, cw THz lasing was observed very recently[6] from the samples used in Ref. 1, which exhibit pulse THz lasing under high electric field pumping. In this case with low-field pumping, carriers gain energy slowly and therefore the probability for a carrier to reach the energy E_0 may be expected to be very small. Furthermore, by applying a stronger stress, E_0 increases and so the laser intensity is expected to decrease. However, the experiment shows the enhancement of laser intensity with stronger stress. The fundamental problem is then the mechanism of population inversion. In this paper we will show that the formation of resonant states remains as the key factor for cw lasing. The population inversion in resonant states is due to the specific angular dependence of the scattering of an electron by an impurity ion, and due to the specific energy dependence of the electron-acoustic-phonon scattering.

The resonant state and the kinetic equation for its occupation probability were derived in details in our earlier paper.[7] Here we will only outline the key points. In terms of the Bloch basis of Γ_8^+ irreducible representation of the double point group $\overline{O}_h$, in cylindric approximation, the Luttinger Hamiltonian operator for the valence band under a uniaxial stress P along the z axis has the form

$$\hat{H}_L(\hat{\mathbf{k}},\zeta)=\frac{-\hbar^2}{2m_0}\begin{bmatrix} \hat{a}_+-\zeta & \hat{b} & \hat{c} & 0 \\ \hat{b}^* & \hat{a}_-+\zeta & 0 & \hat{c} \\ \hat{c}^* & 0 & \hat{a}_-+\zeta & -\hat{b} \\ 0 & \hat{c}^* & -\hat{b}^* & \hat{a}_+-\zeta \end{bmatrix}$$

with matrix elements

$$\hat{a}_+=-(\gamma_1-2\gamma_2)\hat{k}_z^2-(\gamma_1+\gamma_2)(\hat{k}_x^2+\hat{k}_y^2),$$

$$\hat{a}_-=-(\gamma_1+2\gamma_2)\hat{k}_z^2-(\gamma_1-\gamma_2)(\hat{k}_x^2+\hat{k}_y^2),$$

$$\hat{b}=2\sqrt{3}\gamma_3(\hat{k}_x-\mathrm{i}\hat{k}_y)\hat{k}_z,$$

$$\hat{c}=\sqrt{3}(\gamma_2+\gamma_3)(\hat{k}_x-\mathrm{i}\hat{k}_y)^2/2.$$

γ_is are Luttinger parameters, and ζ is related to the split of the valence-band top E_{def} and the deformation potential α by $E_{\mathrm{def}}=\alpha P=\hbar^2\zeta/m_0$. In our notation $\mathbf{k}$ is a vector and $\hat{\mathbf{k}}$ is an operator.

In the presence of a charged acceptor, including the Coulomb potential $-e^2/\epsilon r$, the total Hamiltonian can be expressed as

$$\hat{H}(\hat{\mathbf{k}},\zeta)=\hat{H}_L(\hat{\mathbf{k}},\zeta)-(e^2/\epsilon r)\hat{I}\equiv\hat{H}_0(\hat{\mathbf{k}},\zeta)+\hat{U}(\hat{\mathbf{k}},\zeta),$$

where $\hat{H}_0(\hat{\mathbf{k}},\zeta)$ is the diagonal part of $\hat{H}(\hat{\mathbf{k}},\zeta)$. The eigensolutions of $\hat{H}_0(\hat{\mathbf{k}},\zeta)$ are labeled by quantum number m: $m=\pm 3/2$ for heavy-hole band $E_{0,\mathbf{k}}^h$ and its associated impurity levels $E_{il_z}^h$, and $m=\pm 1/2$ for light-hole band $E_{0,\mathbf{k}}^l$ and its associated impurity levels $E_{il_z}^l$. Setting zero reference energy at the edge of the light-hole band, these energy levels are shown in Fig. 1. From now on we will drop the label ζ in the Hamiltonian operators.

If carriers can survive the acoustic scattering and occupy the resonant states under weak electric-field pumping, the energy of the relevant localized impurity orbital must be E_{1s}^h, and the relevant Bloch states in the light-hole band have energy $E_{0,\mathbf{k}}^l$ around E_{1s}^h. Let $\varphi_{1s}^h(\mathbf{r})$ be the effective-mass envelope function of the corresponding localized acceptor $1s$ orbital, and $\psi_{\mathbf{k}}^l(\mathbf{r})$ the corresponding Bloch state in the light-hole band. We construct four vector wave functions $\varphi^{(\pm 3/2)}(\mathbf{r})$ and $\psi_{\mathbf{k}}^{(\pm 1/2)}(\mathbf{r})$, each of which has four components but only one component is not zero. These nonzero components are $\varphi_{1s}^h(\mathbf{r})$ for the first component of $\varphi^{(+3/2)}(\mathbf{r})$ and the fourth component of $\varphi^{(-3/2)}(\mathbf{r})$, and $\psi_{\mathbf{k}}^l(\mathbf{r})$ for the second component of $\psi_{\mathbf{k}}^{(+1/2)}(\mathbf{r})$ and the third component of $\psi_{\mathbf{k}}^{(-1/2)}(\mathbf{r})$. The resonant state can then be written as

$$\Psi_{\mathbf{k}}^{\pm 1/2}(\mathbf{r},t)=\sum_{m=\pm 3/2} a_{\mathbf{k}}^{(\pm 1/2,m)}(t)\exp\left(-i\frac{E_{1s}^h}{\hbar}t\right)\varphi^{(m)}(\mathbf{r}) + \sum_{\mathbf{k}',m=\pm 1/2} b_{\mathbf{kk}'}^{(\pm 1/2,m)}(t) \times\exp\left(-i\frac{E_{0,\mathbf{k}'}^l}{\hbar}t\right)\psi_{\mathbf{k}'}^{(m)}(\mathbf{r}), \quad (1)$$

which satisfies the time-dependent Schrödinger equation

$$[\hat{H}_0(\hat{\mathbf{k}})+\hat{U}(\hat{\mathbf{k}})]\Psi_{\mathbf{k}}^{\pm 1/2}(\mathbf{r},t)=\mathrm{i}\hbar\,\partial\Psi_{\mathbf{k}}^{\pm 1/2}(\mathbf{r},t)/\partial t \quad (2)$$

with the initial conditions $b_{\mathbf{kk}'}^{(\pm 1/2,\pm 1/2)}(0)=\delta_{1/2,\pm 1/2}\delta_{\mathbf{k},\mathbf{k}'}$ and $a_{\mathbf{k}}^{(\pm 1/2,\pm 3/2)}(0)=0$. Since the two orthogonal resonant states $\Psi_{\mathbf{k}}^{+1/2}(\mathbf{r},t)$ and $\Psi_{\mathbf{k}}^{-1/2}(\mathbf{r},t)$ are degenerate, we need to study only one of them. In the following we will drop the superscript $\pm$.

The resonant states are formed from the resonant scattering of the Bloch states by the charge impurities. To investigate the population inversion, we need to know the occupation probability f_r of the localized impurity orbitals

$$f_r=\sum_{\mathbf{k}}(|a_{\mathbf{k}}^{(+1/2,+3/2)}|^2+|a_{\mathbf{k}}^{(+1/2,-3/2)}|^2)f_{\mathbf{k}}^l, \quad (3)$$

where $f_{\mathbf{k}}^l$ is the occupation probability of the $\mathbf{k}$ Bloch state in the light-hole band. In the absence of electron-phonon scattering, the static state distribution $f_{\mathbf{k}}^l$ satisfies the kinetic equation

$$\frac{\mathrm{e}\mathcal{E}}{\hbar}\frac{\partial f_{\mathbf{k}}^l}{\partial k_z}=N_i\sum_{\mathbf{k}'}W_{l\mathbf{k},l\mathbf{k}'}f_{\mathbf{k}'}^l-N_i f_{\mathbf{k}}^l\sum_{\mathbf{k}'}W_{l\mathbf{k}',l\mathbf{k}}, \quad (4)$$

where N_i the number of impurities, and $W_{\lambda\mathbf{k},\lambda'\mathbf{k}'}$ is the transition probability from the $\mathbf{k}'$ Bloch state in the λ' band to the $\mathbf{k}$ Bloch state in the λ band. Our normalization condition is set as

$$\sum_{\mathbf{k}} f_k^l+N_i f_r=N, \quad (5)$$

where N is the total number of holes.

The detail derivation can be found in our earlier work Ref. 7, and here we will summarize the final results. Using the commonly accepted variational function[8]

$$\varphi_{1s}^{h}(\mathbf{r})=\frac{1}{\sqrt{\pi a^2 b}}\exp\left[-\sqrt{\frac{x^2+y^2}{a^2}+\frac{z^2}{b^2}}\right]$$

for the localized acceptor orbital, and normalized plane waves $e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$ for the Bloch state $\psi_{\mathbf{k}}^{l}(\mathbf{r})$ in the light hole band, the transition probability is derived as

$$W_{l\mathbf{k},l\mathbf{k}'}=(|W_{\mathbf{k}}|^2+|V_{\mathbf{k}}|^2)(|W_{\mathbf{k}'}|^2+|V_{\mathbf{k}'}|^2)\times\left[\frac{2\pi}{\hbar}\frac{\delta(E_{0,\mathbf{k}'}^{l}-E_{0,\mathbf{k}}^{l})}{(E_{0,\mathbf{k}}^{l}-E_0)^2+\Gamma^2/4}\right], \tag{6}$$

where

$$V_{\mathbf{k}}=-(\sqrt{3}\hbar^2\gamma/m_0)(k_x-ik_y)k_z I(\mathbf{k}),$$

$$W_{\mathbf{k}}=-(\sqrt{3}\hbar^2\gamma/2m_0)(k_x-ik_y)^2 I(\mathbf{k}), \tag{7}$$

with $I(\mathbf{k})=8\sqrt{\pi a^2 b/V}[1+k_z^2 b^2+(k_x^2+k_y^2)a^2]^{-2}$.

As we mentioned earlier, while the applied electric field may help holes to occupy resonant states, this possibility may be suppressed by the scattering of phonons, especially by acoustic phonons when the applied electric field is weak. The relevant theory of scattering was formulated in detail by Bir and Pikus,[9] and their results will be used here. The transition probability per unit time from the $\mathbf{k}'$ Bloch state in the λ' band to the $\mathbf{k}$ Bloch state in the λ band with the emission or absorption of an acoustic phonon of frequency $\omega_{\mathbf{q},\nu}$ is given by

$$W_{\lambda\mathbf{k},\lambda'\mathbf{k}'}^{\mathrm{ac},\pm}=\frac{\pi}{\hbar}\sum_{\mathbf{q},\nu}\left(\frac{\hbar(n_{\mathbf{q},\nu}+\frac{1}{2}\pm\frac{1}{2})}{2\rho\omega_{\mathbf{q},\nu}V}\right)\times\sum_{m,m'}|H^{\mathrm{ac}}(\mathbf{q}\nu)_{\mathbf{k}m,\mathbf{k}'m'}|^2\delta_{\mathbf{q},\pm(\mathbf{k}-\mathbf{k}')}\times\delta(E_{\mathbf{k}'}^{\lambda'}-E_{\mathbf{k}}^{\lambda}\pm\hbar\omega_{\mathbf{q},\nu}), \tag{8}$$

where ρ is the mass density of the system, $\mathbf{q}$ the phonon wave vector, ν the polarization, $n_{\mathbf{q},\nu}$ the number of phonons. In the summation, $m=\pm 1/2$ for light-hole band $\lambda,\lambda'=l$, and $m=\pm 3/2$ for heavy-hole band $\lambda,\lambda'=h$. The $+$ corresponds to the emission and $-$ to the absorption of acoustic phonons. The explicit matrix form of the electron-acoustic-phonon interaction matrix element $H^{\mathrm{ac}}(\mathbf{q}\nu)_{\mathbf{k}m,\mathbf{k}'m'}$ can be found in Ref. 9.

Similarly, for scattering by optical phonons, the transition probability per unit time has the form[9]

$$W_{\lambda\mathbf{k},\lambda'\mathbf{k}'}^{\mathrm{opt}}=\frac{\pi}{\hbar}\left(\frac{\hbar}{2\rho\omega_{\mathrm{opt}}V}\right)\sum_{s,m,m'}|H^{\mathrm{opt}}(\mathbf{e}_s)_{\mathbf{k}m,\mathbf{k}'m'}|^2\times\delta(E_{\mathbf{k}'}^{\lambda'}-E_{\mathbf{k}}^{\lambda}-\hbar\omega_{\mathrm{opt}}), \tag{9}$$

where $\mathbf{e}_s$ is the polarization vector. Again, the expression of the electron-optical-phonon interaction matrix element $H^{\mathrm{opt}}(\mathbf{e}_s)_{\mathbf{k}m,\mathbf{k}'m'}$ is given in Ref. 9.

Including the scattering of both acoustic and optical phonons, the occupation probability of the $\mathbf{k}$ Bloch state in the heavy-hole band $f_{\mathbf{k}}^{h}$, in light-hole band $f_{\mathbf{k}}^{l}$, and the occupation probability f_r of the localized impurity orbitals should be solved self-consistently from the following coupled equations:

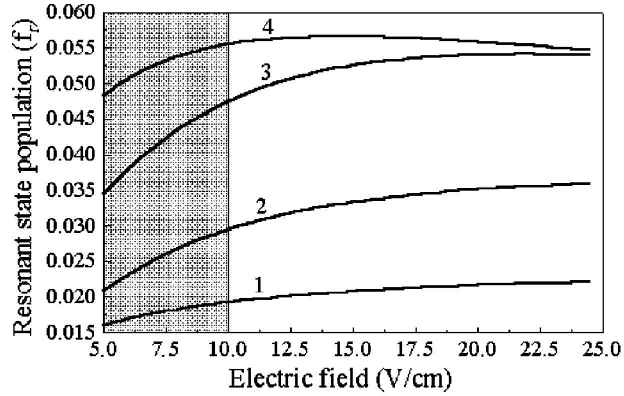

FIG. 2. Occupation probability of resonant states f_r as a function of the applied electric field for different values of stress. cw lasing has been observed in the electric-field range marked by the shaded region.

$$\frac{e\mathcal{E}}{\hbar}\frac{\partial f_{\mathbf{k}}^{l}}{\partial k_z}=N_i\sum_{\mathbf{k}'}W_{l\mathbf{k},l\mathbf{k}'}f_{\mathbf{k}'}^{l}-N_i f_{\mathbf{k}}^{l}\sum_{\mathbf{k}'}W_{l\mathbf{k}',l\mathbf{k}}+\sum_{\lambda'=l,h;\mathbf{k}'}f_{\mathbf{k}'}^{\lambda'}W_{l\mathbf{k},\lambda'\mathbf{k}'}^{\mathrm{ac},\pm}-f_{\mathbf{k}}^{l}\sum_{\lambda'=l,h;\mathbf{k}'}W_{\lambda'\mathbf{k}',l\mathbf{k}}^{\mathrm{ac},\pm}+\sum_{\lambda'=l,h;\mathbf{k}'}f_{\mathbf{k}'}^{\lambda'}W_{l\mathbf{k},\lambda'\mathbf{k}'}^{\mathrm{opt}}-f_{\mathbf{k}}^{l}\sum_{\lambda'=l,h;\mathbf{k}'}W_{\lambda'\mathbf{k}',l\mathbf{k}}^{\mathrm{opt}}, \tag{10}$$

$$\frac{e\mathcal{E}}{\hbar}\frac{\partial f_{\mathbf{k}}^{h}}{\partial k_z}=\sum_{\lambda'=l,h;\mathbf{k}'}f_{\mathbf{k}'}^{\lambda'}W_{h\mathbf{k},\lambda'\mathbf{k}'}^{\mathrm{ac},\pm}-f_{\mathbf{k}}^{h}\sum_{\lambda'=l,h;\mathbf{k}'}W_{\lambda'\mathbf{k}',h\mathbf{k}}^{\mathrm{ac},\pm}+\sum_{\lambda'=l,h;\mathbf{k}'}f_{\mathbf{k}'}^{\lambda'}W_{h\mathbf{k},\lambda'\mathbf{k}'}^{\mathrm{opt}}-f_{\mathbf{k}}^{h}\sum_{\lambda'=l,h;\mathbf{k}'}W_{\lambda'\mathbf{k}',h\mathbf{k}}^{\mathrm{opt}},f_r=\sum_{\mathbf{k}}(|a_{\mathbf{k}}^{(+1/2,+3/2)}|^2+|a_{\mathbf{k}}^{(+1/2,-3/2)}|^2)f_{\mathbf{k}}^{l},$$

together with the modified normalization condition

$$\sum_{\mathbf{k}}f_k^l+\sum_{\mathbf{k}}f_k^h+N_i f_r=N. \tag{11}$$

The experimental sample in Ref. 6 has acceptor concentration about $N=1\times 10^{14}$, and at liquid-helium temperature cw THz lasing was observed under an external electric field up to 10 V/cm. For the stress values used in the experiment, from the measurement of the current-voltage curve, it has been known[10] that all impurities are ionized ($N_i=N$) by impact ionization when the electric-field strength exceeds 5 V/cm. We have used these experimental conditions to solve Eqs. (10) and (11) numerically for the occupation probability f_r of the resonant states, and the results are shown in Fig. 2 for various values E_{def} of the split of the valence-band top: $E_{\mathrm{def}}=20$ meV for curve 1, 24 meV for curve 2, 28 meV for curve 3, and 32 meV for curve 4. The corresponding resonant energy E_0 and resonant width Γ in units meV are calculated as $(E_0;\Gamma)=(3.2;2.3),(11;3.5),(18.6;3.2)$, and (24.5; 2.9) for curves 1, 2, 3, and 4, respectively. cw lasing has been observed in the electric-field range marked by the shaded region.

The few percents of occupation probability f_r shown in Fig. 2 for low electric-field pumping in the diffusive regime are the same order of magnitude as the value of f_r for the case of strong electric-field pumping in the streaming motion regime, which we found earlier.[2] Furthermore, f_r is enhanced by increasing stress, as observed in the experiment.[6] To find out the physical origin of these important results, let us write Eq. (3) as $f_r=\Sigma_{\mathbf{k}}T(r,\mathbf{k})f^l_{\mathbf{k}}$, where $T(r,\mathbf{k}) \equiv|a_{\mathbf{k}}^{(+1/2,+3/2)}|^2+|a_{\mathbf{k}}^{(+1/2,-3/2)}|^2$ is the probability that a carrier in the $(l,\mathbf{k})$ Bloch state will be trapped in a resonant state. The explicit expressions for $a_{\mathbf{k}}^{(+1/2,\pm 3/2)}$ are given in Eq. (15) of Ref. 7. We can then prove that $T(r,\mathbf{k})$ is proportional to $\sin^2\theta$, where θ is the angle between the direction of carrier momentum vector $\mathbf{k}$ and the direction of the applied electric field, which is along the z axis. When an electron moves along the z axis and is scattered by an acoustic phonon, let $\mathbf{k}$ be the momentum vector of the final electron state, which makes an angle θ to the z axis. It is obvious that the total number of final electron states having the same θ increases with θ. Therefore, under the combined effect of electric-field acceleration and the acoustic-phonon scattering, the angle θ of a carrier's momentum increases towards $\pi/2$, where $T(r,\mathbf{k})$ has its maximum value. As a result, in the diffusive regime, the occupation probability f_r of the resonant states can be large enough to achieve the required population inversion for lasing.

Besides the fact that the total number of final electron states increases with θ, for a given angle θ, it is also obvious that the number of available final electron states for the electron-acoustic-phonon scattering increases with the carrier energy $E^l_{0,\mathbf{k}}$ according to $\sqrt{E^l_{0,\mathbf{k}}}$. Since the resonant state energy E_0 increases with the applied stress, the corresponding occupation probability f_r increases with the applied stress, resulting in stronger THz radiation intensity as observed in the experiment.[6]

To close this paper, we would like to emphasize that the *necessary* condition for lasing is that the formation time of the population inversion is shorter than the time of spontaneous emission.[3,11] We have estimated these times and they satisfy the condition. Consequently, we have neglected the radiation transition processes in our kinetic equations.

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