Population Inversion Induced by Resonant States in Semiconductors

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We present a theoretical prediction of a new mechanism for carrier population inversion in semiconductors under an applied electric field. The mechanism is originated from a coherent capture-emission type inelastic scattering of resonant states. We support our theory with concrete calculations for shallow acceptor resonant states in strained p-Ge where a lasing in THz frequency region has been recently observed.

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Besides elastic scattering, resonant states also cause a specifically strong inelastic scattering because electrons can have a finite lifetime in the resonant state. Consequently, the electron energy is not conserved, and it can be re-emitted with the energy different from the initial value. We will prove in this Letter that due to such an effect a novel population inversion of carrier distribution can be realized in non-equilibrium semiconductors in the so-called streamer regime. The streamer regime emerges in a relatively pure semiconductors at low temperatures where both impurity scattering and acoustic phonon scattering are weak. Under an applied electric field a carrier drifts in the momentum space almost scatter free until its energy reaches the optical phonon energy $\hbar \omega_0$. Then the carrier emits an optical phonon and return to the low-energy region. If there exist a resonant state with energy $E_0 < \hbar \omega_0$, it acts as a carrier trap with a finite lifetime which is field-independent. In the energy space one then finds carriers accumulation in the vicinity of the resonant energy $E_0$.

We will use a general model to analyze this novel mechanism for population inversion. While our theory applies to a variety of resonant states, in this Letter we will also demonstrate in quantitative details that our theory is realistic. For this purpose we will investigate the population inversion in uniaxially strained p-Ge where shallow acceptors induce resonant states. It is important to notice that based on such a p-Ge system, a laser operating in terahertz frequency region has been fabricated recently. By studying the emission lines positions as functions of applied stress, it was confirmed that the radiation emission is due to optical transitions between the resonant states and the localized acceptor (Ga) states. However, the mechanism of lasing has remained a puzzle. Our theory will explain the physical origin of the population inversion which leads to the lasing.

We consider a model system of charge carriers interacting with optical phonons of energy $\hbar \omega_0$ under a strong external electric field $E$ along the $z$ axis. In this case an electron acquire energy from the electric field and drift in the $k$-space until its energy reaches $\hbar \omega_0$. Then the electron emits an optical phonon and returns to the region $k \approx 0$. Thus, our model includes a drain $D$ at $E_k = \hbar \omega_0$ and a source $S$ at small $k$. In the absence of resonant scattering by impurities, for carrier kinetic energy $E_k < \hbar \omega_0$, the carrier distribution function $f_k$ can be obtained from the kinetic equation

$$\frac{\partial f_k}{\partial t} + \frac{eE}{\hbar} \frac{\partial f_k}{\partial k_z} = S - D. \tag{1}$$

For our problem we can well approximate the drain $D$ by a black-wall boundary condition that $f_k = 0$ for $E_k > \hbar \omega_0$. The source intensity $S$ is determined by the $k$-space particle flow with energy $E_k = \hbar \omega_0$. In the following we use the expression for $S$ as

$$S = S_0(t) \Theta(\epsilon_0 - E_k). \tag{2}$$

Here

$$\epsilon_0 = \left( \frac{2}{9} \right)^{1/3} \left( \frac{\omega_0}{\nu_A} \right)^{2/3} \left( \frac{eE_\perp}{m_z} \right)^{1/3}, \tag{3}$$

with $m_z$ being the effective mass along $z$-axis. The frequency $\nu_A$ is related to the rate $\nu_A \sqrt{(E_k/\hbar \omega_0) - 1}$ of optical phonon emission by the carriers with $E_k > \hbar \omega_0$. The source amplitude $S_0(t)$ is determined from the condition of particle flow conservation in the $k$-space, namely the flow out of the surface $E_k = \hbar \omega_0$ at time $t$ returns evenly back into the region $E_k < \epsilon_0$,

$$S_0(t) = \frac{e}{\hbar} \int \frac{(\mathbf{E} \cdot d\mathbf{S}) f_k(t)}{\int d^3 k \Theta(\epsilon_0 - E_k)}. \tag{4}$$

The integration is performed over the surface defined by the equation $E_k = \hbar \omega_0$.

The stationary solution of Eq. (1) (the so-called streamer) is that $f_k$ is almost constant if $k$ lies in a cylinder, and $f_k = 0$ otherwise. This cylinder in $k$-space is determined by

$$0 < k_z \leq \sqrt{2m_z \omega_0/\hbar^2}, \quad k_\perp \leq \sqrt{2m_\perp \epsilon_0/\hbar^2}.$$
where $m_\perp$ is the transverse component of the effective mass tensor.

When impurities induce resonant states with complex energy $E_0 + i\Gamma/2$, charge carriers may be trapped at energy $E_0 < \hbar\omega_0$ for a time interval $\sim \hbar/\Gamma$. As a result, a maximum of the non-equilibrium distribution function is formed around the energy $E_0$. This is just the population inversion. To take into account the resonant scattering by impurities of concentration $N_i$, at the right hand side of Eq. (4), we should add the impurity collision integral $I$

$$I = N_i V \sum_{k'} [f_{k'} W_{kk'} - f_k W_{k'k}] + N_i V (W_{r,k} f_r - W_{kr} f_k), \quad (5)$$

where $V$ is a normalization volume, and $f_r$ is the resonant state population which satisfies the kinetic equation

$$\frac{\partial f_r}{\partial t} = \sum_{k'} [W_{k'k} f_k - W_{rr} f_r]. \quad (6)$$

The first term in Eq. (5) represents the elastic scattering, while the second one describes the coherent capture and re-emission by the resonant state. The sum $\sum_{k'} W_{k'k}$ is the total escape rate from the resonant state, and is equal to $\Gamma/\hbar$.

The transition probabilities $W_{kk'}$ and $W_{kr}$ can be expressed through the respective scattering amplitude $t_{kk'}$ and transition amplitude $t_{kr}$, as

$$W_{kk'} = \frac{2\pi}{\hbar} |t_{kk'}|^2 \delta(E_k - E_{k'}), \quad (7)$$

$$W_{kr} = \frac{2}{\hbar} |t_{kr}|^2 \frac{\Gamma}{(E_k - E_0)^2 + \Gamma^2/4}. \quad (8)$$

$t_{kk'}$ and $t_{kr}$ can be calculated using the Dirac approach to the scattering problem at a resonant state. According to this approach, via hybridization with extended states, the wave function $\varphi(r)$ of the bare localized impurity state develops into the resonant state. The general form of the scattering state is

$$\Psi_k(r) = \frac{1}{\sqrt{V}} e^{ikr} + \frac{t_{kr}}{E_k - E_0 + i\Gamma/2} \varphi(r) + \sum_{k'} \frac{t_{kk'}}{E_k - E_{k'} + i\Gamma} e^{ik'r}, \quad \gamma \rightarrow +0. \quad (9)$$

Finally, we will add the normalization condition

$$\sum_k f_k + N_i V f_r = nV \quad (10)$$

where $n$ is the total electron concentration, and solve all these equations selfconsistently.

The above theory is general for different types of resonant states. To demonstrate explicitly the population inversion predicted by our theory, we will investigate quantitatively the resonant states induced by shallow acceptors in uniaxially strained p-Ge.

In cubic semiconductors with symmetry group $O_h$ the shallow acceptor wave functions $\psi^{(M)}(r)$ are 4-fold degenerate with the total angular momentum projections $M = \pm 1/2$ and $\pm 3/2$. The ground state has $\Gamma^+_8$ symmetry. Under a uniaxial strain the valence band top splits into two doubly degenerate energy levels. The corresponding two sets of wave functions transform according to $\Gamma^+_8$ and $\Gamma^+_2$ representations if the stress is along the [001] direction, and according to $\Gamma^+_8$ and $\Gamma^+_2$ representations if the stress is along the [111] direction. The ground state acceptor wave functions split in the same way and can be classified by the total angular moment projections $(M = \pm 1/2$ or $\pm 3/2)$ along the stress direction. In our calculations, we will use the spherical approximation for the Luttinger Hamiltonian (LH) [2]. In the limit of large strain such that the splitting $E_d$ at the top of subband exceeds the Coulomb energy, the LH can be treated with a quasi-diagonal approximation, and is represented by two $2 \times 2$ blocks. The states in each subband can now be classified by the projections $(m = \pm 1/2$ or $\pm 3/2)$ of the hole spin on the stress axis [3].

In this way, in each of doubly-degenerate subbands, we obtain both extended states and the localized Coulomb states below the subband. The corresponding energy levels and wave functions are calculated following the variational procedure in Ref. [3]. For a large strain, the energy levels are shown in Fig. 1.

![FIG. 1. The acceptor levels diagram for uniaxially strained Ge in the large strain limit along [001]. The optical transitions observed in the lasing [6] are indicated by arrows.](image)
the characteristic frequency \( \nu \) and the transition amplitudes \( t_{kk'} \) for various values of applied electric field and impurity concentration.

We are ready to use these scattering and transition amplitudes to solve the set of kinetic equations (4) and (3), respectively. However, for p-Ge the kinetic equations can be simplified. Let \( \tau_\varepsilon \) be the transient time during which the stationary non-equilibrium distribution is established. \( \tau_\varepsilon \) depends on both the electric field \( \varepsilon \) and the impurity concentration \( N_i \). As will be shown below, for p-Ge, there exists rather large region of electric fields and impurity concentrations where \( \tau_\varepsilon \) is much larger than the lifetime of the resonant state \( \hbar/\Gamma \). In this case we can set the left hand side of Eq. (6) to zero, and so the occupation of the quasi-local states, \( f_r \), follows adiabatically the distribution function \( f_k \) of the extended states. Since the localized and the extended states are doubly degenerate, we have \( f_k^{3/2} = f_k^{1/2} = f_k \) and \( f_k^{1/2} = f_k^{1/2} = f_k \). If we define \( |t_{kr}|^2 \equiv \frac{|t_{kr}|^2 f_k}{(E_k - E_0)^2 + \Gamma^2/4} \), we obtain

\[
 f_r = \sum_k \frac{|t_{kr}|^2 f_k}{(E_k - E_0)^2 + \Gamma^2/4}. \tag{11}
\]

Substituting Eq. (11) into Eqs. (4) and (3), we arrive at the kinetic equation for \( f_k \)

\[
 \frac{\partial f_k}{\partial t} + \frac{\alpha}{\hbar} \frac{\partial f_k}{\partial \varepsilon} = 2\pi N_i V \sum_{k'} |t_{kk'}|^2 \delta(E_k - E_{k'})(f_{k'} - f_k) + \frac{N_i V |t_{kr}|^2 \Gamma}{\hbar[(E_k - E_0)^2 + \Gamma^2/4]} \sum_{k'} \frac{|t_{kr}|^2 f_{k'}}{(E_k - E_0)^2 + \Gamma^2/4} - f_k 
\]

\[
 + S_0(t) \Theta(\epsilon_0 - E_k), \tag{12}
\]

where \( |t_{kk'}|^2 \equiv \left| \frac{t_{kk'}}{w_{kk'}} \right|^2 \). The boundary condition for the above kinetic equation is \( f_k = 0 \) at \( E_k = \hbar \omega_0 \). The source \( S_0(t) \) and the energy \( \epsilon_0 \) are given by Eqs. (1) and (1), respectively.

We will solve Eq. (12) numerically as a non-stationary equation. We start from some initial distribution and then follow the evolution of the distribution function until it reaches a stationary one. In this way, the final stationary distribution and the transient time \( \tau_\varepsilon \) are obtained for various values of applied electric field and impurity concentration. In our numerical calculation, the values of material parameters for p-Ge are\ Luttinger parameters \( \gamma_1 = 13.38 \), \( \gamma_2 = 4.24 \), \( \gamma_3 = 5.69 \), \( \hbar \omega_0 = 36 \) meV, and the characteristic frequency \( \nu_A = 5 \times 10^{12} \) s\(^{-1}\).

We will set the pressure at 5 kbar and the electric field at \( \varepsilon = 100 \) V/cm along [111]. In this case, the resonant level is at the energy \( E_0 = 10 \) meV and has a width \( \Gamma = 2 \) meV. Here we have adopted the approximation of a single hole band, and we are aware of the fact that at a pressure of 5 kbar the inter-hole-band splitting \( E_d = 20 \) meV is less than \( \hbar \omega_0 \). One can show that including the second band will only change the tail of the distribution, and such change is not important for the problem under consideration. From Eq (13) we obtain the source width \( \epsilon_0 = 4.25 \) meV. If we define \( \alpha = \sqrt{2 m_0 E_0 / \hbar^2 \gamma_1} \) as the unit for wave vector, where \( m_0 \) is the free electron mass, our calculated normalized distribution functions are shown in Fig. 2 as functions of normalized \( k_z / \alpha \) (upper panel) and \( k / \alpha \) (lower panel). The curves in Fig. 2 are for impurity concentration \( N_i = 1 \) (curve 1), 1.1 (curve 2), 1.2 (curve 3), 1.4 (curve 4), and 1.5 (curve 1), in units \( 10^{15} \) cm\(^{-3}\). While the distribution function peaks are
centered at the resonant energy $E_0$, their corresponding peak positions in the upper panel are different from those in the lower panel. This is due to the anisotropy of the effective mass: $m_z=0.04m_0$ and $m_{\perp}=0.13m_0$. For the results shown in Fig. 2, the transient time is about $\tau_{2}\approx10^{-11}$ s, which is much longer than the lifetime $\hbar/\Gamma\approx2\times10^{-13}$ s. Consequently, our calculation based on the condition that $\Gamma\tau_{2}\gg\hbar$ is selfconsistent.

![Normalized distribution function as a function of squared normalized momentum](image)

FIG. 3. Normalized distribution function as a function of squared normalized momentum $(k_z/\alpha)^2$ for impurity concentration $N_i=5\times10^{15}$ cm$^{-3}$. The curves are: (a) no resonant scattering, (b) include only elastic scattering from resonant states, and (c) include full resonant scattering.

In order to demonstrate precisely which scattering process is responsible to the population inversion, we have used the same values of material parameters and same electrical field strength to calculate the distribution functions for 3 cases, and the results are shown in Fig. 3. In the absence of resonant states, the distribution function follows curve (a). When elastic scattering due to resonant states is taken into account, the result change into the step-like curve (b). Finally, by adding the inelastic scattering process, a peak emerges in curve (c). It is then clear that the population inversion is induced by the capture-emission component. The population accumulated in resonant states is controlled by the distribution function in the continuous spectrum, as indicated by Eq. (1). At the same time, the non-equilibrium population in the localized states can be only less than that in the low-energy continuous states. Consequently, under the conditions imposed on our calculation, the intra-center population is also inverted. It has been demonstrated in Ref. [3] that the lasing in uniaxially strained Ge:Ga is connected to the transitions shown by arrows in Fig. 1. Among these transitions, besides the allowed intra-center optical transitions between the lowest resonant $s$-type state and excited localized $p$-type states, there is also transition corresponding to the forbidden $s$-type to $s$-type. The observed forbidden transition is due to the accumulation of the continuous spectrum carriers at the energy around $E_0$. These states are almost plane waves and so turn the forbidden process into an allowed one. The sharp emission line in the observed optical spectrum proves the existence of the peak in the distribution function $f_{k}$. Thus, the resonant-states-induced population inversion predicted by our theory explains the origin of lasing in terahertz frequency range observed in these strained Ge:Ga samples.

In conclusion, we have predicted that resonant states can produce a population inversion in the carrier distribution function in strained semiconductors under an external electric field. Our theoretical prediction is confirmed by concrete calculations for strained $p$-Ge, where resonant states give rise to the lasing observed in THz frequency region. We believe that the proposed mechanism for population inversion is rather general since resonant states can be created by various means.

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