Population Inversion Induced by Resonant States in Semiconductors

M. A. Odnoblyudov,[1,2] I. N. Yassievich,[1,2] M. S. Kagan,[3] Yu. M. Galperin,[2,4] and K. A. Chao[1]

[1]*Department of Theoretical Physics, Lund University, S-223 62, Lund, Sweden*

[2]*A. F. Ioffe Physico-Technical Institute RAS, 194021 St. Petersburg, Russia*

[3]*Institute for Radioengineering and Electronics RAS, 103907 Moscow, Russia*

[4]*Department of Physics, University of Oslo, P.O. Box 1048 Blindern, N 0316 Oslo, Norway*

(Received 20 November 1998)

We present a theoretical prediction of a new mechanism for carrier population inversion in semiconductors under an applied electric field with suitable field strength. 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.

PACS numbers: 78.45.+h, 42.55.Px, 72.10.–d

Unlike in an ordinary heterostructure laser where carrier population inversion is achieved by injection of electrons and holes into an active region [1], in unipolar-type lasers population inversion can be created by different mechanisms. Examples are p-Ge laser under crossing electric and magnetic fields [2] and quantum cascade laser [3], which are based on k-space population inversion between subbands. We will prove in this Letter that a novel unipolar-type population inversion can be realized when the *streaming motion* of carriers emerges in semiconductors at low temperatures where both elastic impurity scattering and acoustic phonon scattering are weak. We will demonstrate in quantitative details that our suggested mechanism is realistic. Based on a uniaxially strained p-Ge in which shallow acceptors induce resonant states [4,5], a terahertz laser has been fabricated recently [6], and the radiation emission is due to optical transitions between the resonant states and the localized acceptor (Ga) states. Up to now, the mechanism of lasing has remained a puzzle. Our theory will explain the physical origin of the population inversion which leads to the lasing. The study of lasing is a separated issue, and will be presented elsewhere.

We consider a model system of charge carriers interacting with optical phonons under an electric field $\mathcal{E}$ applied along the z axis. A carrier acquires energy from the field and *drifts* in $\mathbf{k}$ space until its energy exceeds $\hbar\omega_0$. This can happen if $\mathcal{E} \geq \hbar\omega_0/el$, where e is the carrier charge and l the carrier mean free path. When its energy becomes larger than $\hbar\omega_0$, the carrier has a finite probability to emit an optical phonon. If the field is also not so strong, there exists an energy ϵ_0 such that the number of carriers which have not emitted an optical phonon before their energies reach $\hbar\omega_0 + \epsilon_0$ is negligibly small. Although the value of ϵ_0 depends also on the mechanism of electron-optical phonon coupling, one can always tune the electric field strength to obtain an ϵ_0 much smaller than $\hbar\omega_0$. Then, all carriers in the small energy interval between $\hbar\omega_0$ and $\hbar\omega_0 + \epsilon_0$ return to the region with energy less than ϵ_0. Under these constraints, our model system includes a *drain* D at $E_\mathbf{k} = \hbar\omega_0$ and a *source* S at small k within the energy interval between zero and $\epsilon_0 \ll \hbar\omega_0$. Using this model the characteristic features of streaming motion in semiconductors have been extensively studied [2,7].

For carrier kinetic energy $E_\mathbf{k} \leq \hbar\omega_0$, the carrier distribution function $f_\mathbf{k}$ satisfies the kinetic equation

$$\partial f_\mathbf{k}/\partial t + (e\mathcal{E}/\hbar)(\partial f_\mathbf{k}/\partial k_z) = S - D\,. \qquad (1)$$

Within the region of electric field strength where the model is valid, the drain D can be well approximated by a black-wall boundary condition that $f_\mathbf{k} = 0$ for $E_\mathbf{k} \geq \hbar\omega_0$. The source S is determined by the flow of particles in $\mathbf{k}$ space across the surface defined by $E_\mathbf{k} = \hbar\omega_0$, and hence depends on the nature of electron-phonon interaction [2,7]. For covalent semiconductors, which are the materials to be studied quantitatively in this work, the source has been derived [2] as $S = S_0(t)\Theta(\epsilon_0 - E_\mathbf{k})$ where

$$\epsilon_0 = (2/9m_z)^{1/3}(\omega_0/\nu_A)^{2/3}(e\mathcal{E}\hbar)^{2/3}, \qquad S_0(t) = \frac{e}{\hbar}\left[\int f_\mathbf{k}(t)\,(\mathcal{E}\cdot d\mathbf{S})\right]\Big/\left[\int \Theta(\epsilon_0 - E_\mathbf{k})\,d^3k\right], \qquad (2)$$

m_z is the effective mass along the z axis, and the frequency ν_A is related to the rate $\nu_A\sqrt{(E_\mathbf{k}/\hbar\omega_0) - 1}$ of optical phonon emission by the carriers with $E_\mathbf{k} > \hbar\omega_0$. In the above expression for $S_0(t)$, the integration is performed over the surface $E_\mathbf{k} = \hbar\omega_0$ in $\mathbf{k}$ space. With the source and drain so defined, the stationary solution of Eq. (1), which corresponds to the so-called streaming motion, is that $f_\mathbf{k}$ is almost constant if $\mathbf{k}$ lies in a cylinder, and $f_\mathbf{k} = 0$ otherwise. This cylinder in $\mathbf{k}$ space is determined by $0 < k_z \leq \sqrt{2m_z\omega_0}/\hbar$ and $k_\perp \leq \sqrt{2m_\perp\epsilon_0}/\hbar$, where $m_\perp$ is the transverse component of the effective mass tensor.

Now we introduce an impurity state $\varphi(\mathbf{r})$ with energy $\varepsilon < \hbar\omega_0$, for example, the $1s$ impurity state below the

0031-9007/99/83(3)/644(4)$15.00

© 1999 The American Physical Society

upper ($m = 3/2$) subband in Fig. 1, the details of which will be explained later. This impurity state will hybridize with the extended states, which have energies $E_{\mathbf{k}} \approx \varepsilon$, and a resonant state is formed within a time interval $\hbar/\Gamma$. A resonant state thus has a complex energy $E_0 - i\Gamma/2$. Because of the streaming motion, when the energies of carriers reach E_0, they can occupy the impurity state. The carrier trapped in the impurity states can escape back into extended state, or make a radiative transition into the impurity states attached to the lower ($m = 1/2$) subband in Fig. 1. Let τ_r and $\tau_{\mathbf{k}}$ be, respectively, the lifetimes of spontaneous emission from the impurity state and the extended states. The interplay of these processes under the applied electric field drives the system to steady state within a time interval τ_ε. The *necessary* condition for lasing is that the formation time of the population inversion is shorter than the time of spontaneous emission [1,2]. For our system, this condition is $\tau_{\mathcal{E}}, \hbar/\Gamma < \tau_r, \tau_{\mathbf{k}}$. In p-Ge, τ_r is shorter than $\tau_{\mathbf{k}}$, and $\tau_r \approx 2 \times 10^{-6}$ s [5]. The value of $\hbar/\Gamma$ was obtained earlier [4,5] as $\hbar/\Gamma \approx 2 \times 10^{-13}$ s, and our numerical calculation (shown later) gives the transient time $\tau_{\mathcal{E}} \approx 10^{-11}$ s for reaching stationary nonequilibrium distribution. Thus, the necessary condition for lasing is satisfied, and we neglect the radiation transition processes in the kinetic equations for $f_{\mathbf{k}}$ and for the population of the impurity state f_r. To take into account the resonant scattering by $N_i V$ impurities in a volume V, at the right-hand side of Eq. (1), we should add the impurity collision integral I,

$$I = N_i V \sum_{\mathbf{k}'} (f_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} - f_{\mathbf{k}} W_{\mathbf{k}'\mathbf{k}}) + N_i V (W_{r\mathbf{k}} f_r - W_{\mathbf{k}r} f_{\mathbf{k}}), \qquad (3)$$

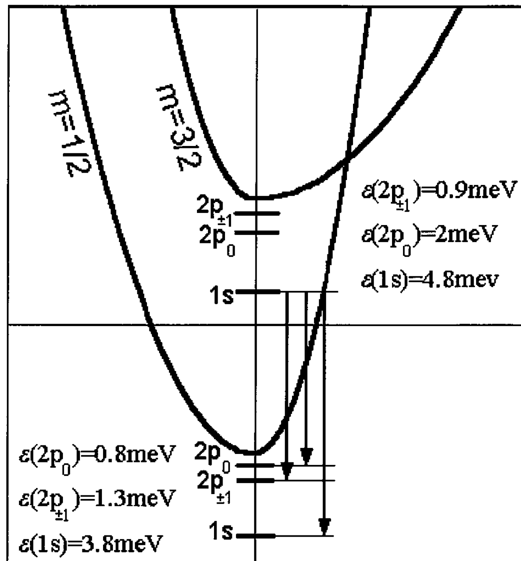

FIG. 1. The acceptor levels for [111]-uniaxially strained Ge in high stress limit. Arrows indicate the optical transitions in lasing [6].

where f_r satisfies the kinetic equation

$$\partial f_r / \partial t = \sum_{\mathbf{k}'} (W_{\mathbf{k}'r} f_{\mathbf{k}'} - W_{r\mathbf{k}'} f_r). \qquad (4)$$

The resulting equations yield a maximum of the nonequilibrium distribution function around the energy E_0. This is just the population inversion.

The transition probabilities $W_{\mathbf{k}\mathbf{k}'}$ for elastic scattering, and $W_{\mathbf{k}r}$ for the coherent capture and reemission by a resonant state, are expressed in terms of scattering amplitude $t_{\mathbf{k}\mathbf{k}'}$ and transition amplitude $t_{\mathbf{k}r}$ as

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

$$W_{\mathbf{k}r} = \frac{\Gamma |t_{\mathbf{k}r}|^2/\hbar}{(E_{\mathbf{k}} - E_0)^2 + \Gamma^2/4}.$$

$t_{\mathbf{k}\mathbf{k}'}$ and $t_{\mathbf{k}r}$ can be calculated using the Dirac approach [8] to the scattering problem at a resonant state. According to this approach, via hybridization with extended states, $\varphi(\mathbf{r})$ develops into the resonant state wave function

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}} + \sum_{\mathbf{k}'} \frac{t_{\mathbf{k}\mathbf{k}'}}{E_{\mathbf{k}} - E_{\mathbf{k}'} + i\gamma} \frac{1}{\sqrt{V}} e^{i\mathbf{k}'\mathbf{r}} + \frac{t_{\mathbf{k}r}}{E_{\mathbf{k}} - E_0 + i\Gamma/2} \varphi(\mathbf{r}), \qquad \gamma \to +0. \qquad (5)$$

We will solve all of the above equations self-consistently within the normalization condition $\sum_{\mathbf{k}} f_{\mathbf{k}} + N_i V f_r = nV$, where n is the total electron density.

Our theory can be applied to systems other than p-Ge. To demonstrate explicitly the population inversion predicted by our theory, we will investigate quantitatively the resonant states induced by shallow acceptors in [111]-uniaxially strained p-Ge.

In cubic semiconductors with symmetry group O_h the shallow acceptor wave functions $\phi^{(M)}(\mathbf{r})$ are 4-fold degenerate with the total angular momentum projections $M = \pm 1/2$ and $\pm 3/2$. A [111]-uniaxial strain splits the valence band top into two doubly degenerate energy levels. 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 $M = \pm 3/2$) along the stress direction. In our calculations, we will use the spherical approximation for the Luttinger Hamiltonian (LH) [9]. 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 quasidiagonal approximation, and is represented by two 2×2 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* and orbital momentum (l_z) on the stress axis [10]. In each of the doubly degenerate subbands, we then obtain both extended states and the localized Coulomb states below the subband. For a large strain, the energy levels are shown in Fig. 1.

It has been demonstrated in Refs. [4,5] that the lasing in uniaxially strained Ge:Ga is connected to the transitions shown by arrows in Fig. 1. The selection rules as determined by the cylindrical symmetry are (1) $\Delta M = 0, \pm 1$, and (2) the initial and final states should have opposite parities with respect to the reflection $z \rightarrow -z$. The wave function for resonant state Eq. (5) contains a plane-wave and a non-plane-wave part. The transition from the non-plane-wave part to $2p$ states are allowed, but to $1s$ state is forbidden. However, the transition from the plane wave to both $2p$ and $1s$ states are allowed. This is the reason why the "$1s$ to $1s$" transition appears in the laser spectrum. Because of the accumulation of carriers in **k** space with energy around E_0, the observed $1s$ to $1s$ laser line is sharp with linewidth $\hbar/\Gamma$.

The *off-diagonal* terms of LH mix the states belonging to different subbands. We will treat these terms as perturbation in the Dirac approach [8]. Along the Dirac approach one also obtains the scattering amplitudes $t_{\mathbf{k}\mathbf{k}'}^{mm'}$ ($m, m' = \pm 1/2$) and the transition amplitudes $t_{\mathbf{k}r}^{mm'}$ ($m = \pm 3/2$ and $m' = \pm 1/2$).

We are ready to use these scattering and transition amplitudes to solve the set of kinetic equations (1)–(4). However, for p-Ge the kinetic equations can be simplified. As $\tau_{\mathcal{E}}$ depends on both the electric field $\mathcal{E}$ and the impurity concentration N_i, it will be shown below, for p-Ge, that there exists a rather large region of electric fields and impurity concentrations where $\tau_{\mathcal{E}}$ is much larger than the lifetime of the resonant state $\hbar/\Gamma$. In this case we can set the left-hand side of Eq. (4) to zero, and so the occupation of the resonant states, f_r, follows adiabatically the distribution function $f_{\mathbf{k}}$ of the extended states. Since the localized and the extended states are doubly degenerate, we have $f_r^{+3/2} = f_r^{-3/2} \equiv f_r$ and $f_{\mathbf{k}}^{+1/2} = f_{\mathbf{k}}^{-1/2} \equiv f_{\mathbf{k}}$. If we define $|t_{\mathbf{k}r}|^2 \equiv |t_{\mathbf{k}r}^{1/2,3/2}|^2 + |t_{\mathbf{k}r}^{1/2,-3/2}|^2$, we obtain

$$f_r = \sum_{\mathbf{k}} \frac{|t_{\mathbf{k}r}|^2 f_{\mathbf{k}}}{(E_{\mathbf{k}} - E_0)^2 + \Gamma^2/4}\,. \tag{6}$$

Substituting Eq. (6) into Eqs. (1) and (3), we arrive at the kinetic equation for $f_{\mathbf{k}}$

$$\partial f_{\mathbf{k}}/\partial t + (e\mathcal{E}/\hbar)(\partial f_{\mathbf{k}}/\partial \mathrm{k}_z) = S_0(t)\Theta(\epsilon_0 - E_{\mathbf{k}}) + (2\pi N_i V/\hbar)\sum_{\mathbf{k}'} |t_{\mathbf{k}\mathbf{k}'}|^2 \delta(E_{\mathbf{k}} - E_{\mathbf{k}'})(f_{\mathbf{k}'} - f_{\mathbf{k}})$$
$$+ \frac{N_i V |t_{\mathbf{k}r}|^2 \Gamma}{\hbar[(E_{\mathbf{k}} - E_0)^2 + \Gamma^2/4]}\left[\sum_{\mathbf{k}'} \frac{|t_{\mathbf{k}'r}|^2 f_{\mathbf{k}'}}{(E_{\mathbf{k}'} - E_0)^2 + \Gamma^2/4} - f_{\mathbf{k}}\right], \tag{7}$$

where $|t_{\mathbf{k}\mathbf{k}'}|^2 \equiv |t_{\mathbf{k}\mathbf{k}'}^{1/2,1/2}|^2 + |t_{\mathbf{k}\mathbf{k}'}^{1/2,-1/2}|^2$. The boundary condition for the above kinetic equation is $f_{\mathbf{k}} = 0$ at $E_{\mathbf{k}} = \hbar\omega_0$. The source $S_0(t)$ and the energy ϵ_0 are given by Eq. (2).

Equation (7) has been solved numerically for p-Ge with $\gamma_1 = 13.38$, $\gamma_2 = 5.69$, $\gamma_3 = 4.24$, $\hbar\omega_0 = 36$ meV, and $\nu_A = 5 \times 10^{12}\ \mathrm{s}^{-1}$. The final stationary distribution and the transient time $\tau_{\mathcal{E}}$ are obtained for various values of applied electric field and impurity concentration. We will set the pressure at 5 kbar and the electric field at $\mathcal{E} = 100$ V/cm along [111]. In this case, the resonant level is $E_0 = 10$ 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. (2) we obtain the source width $\epsilon_0 = 4.25$ meV. If we define $\alpha = \sqrt{2m_0E_0/\gamma_1}/\hbar$ as the unit for wave vector, where m_0 is the free electron mass, our calculated normalized distribution functions $\tilde{f}_{\mathbf{k}} \equiv (\alpha/2\pi)^3 n^{-1} f_{\mathbf{k}}$ for various impurity concentrations are shown in Fig. 2 as functions of normalized k_z/α (upper panel) and of normalized $k_\perp/\alpha$ (lower panel). 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 because of 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 $\tau_{\mathcal{E}} \approx 10^{-11}$ s, which is much longer than the lifetime $\hbar/\Gamma \approx 2 \times 10^{-13}$ s. Consequently, our calculation based on the condition that $\Gamma\tau_{\mathcal{E}} \gg \hbar$ is self-consistent.

In order to demonstrate precisely which scattering process is responsible to the population inversion, we have used the same values of material parameters and the same electrical field strength to calculate the distribution functions for three cases, and the results are shown in Fig. 3. In the absence of impurity scattering, at the right-hand side of Eq. (5) we have only the plane-wave term, and the corresponding distribution function is curve (a). Outside the source region which is marked as the shaded area, the distribution function is a characteristic constant for streaming motion. When the elastic scattering due to acceptors [the second term at the right-hand side of Eq. (7)] is taken into account, the result changes into the steplike curve (b) which has a very small value in the energy region above the acceptor level. Finally, by adding the inelastic scattering process due to the coherent capture and reemission of the resonant states, a peak emerges in curve (c) and the energy at the peak position is just E_0. It is then clear that the population inversion is induced by the capture and reemission mechanism. The population accumulated in resonant states is controlled by the distribution function in the continuous spectrum, as indicated by Eq. (6). Because of the condition $\sum_{\mathbf{k}} f_{\mathbf{k}} + N_i V f_r = nV$, where n is the

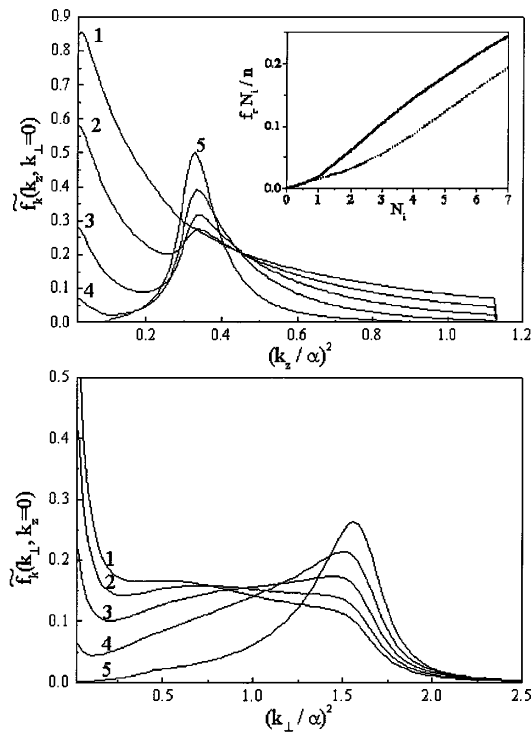

FIG. 2. $\tilde{f}_{\mathbf{k}} \equiv (\alpha/2\pi)^3 n^{-1} f_{\mathbf{k}}$ as a function of $(k_z/\alpha)^2$ (upper panel) and $(k_\perp/\alpha)^2$ (lower panel) in a [111]-uniaxially strained p-Ge under an electric field $\mathcal{E} = 100$ V/cm along the z axis, with impurity concentration $N_i = 1$, 1.2, 1.5, 2, and 4 (in units 10^{15} cm^{-3}) for curves 1, 2, 3, 4, and 5, respectively. The inset shows f_r as a function of N_i (10^{15} cm^{-3}) for $\mathcal{E} = 100$ V/cm (upper solid curve) and $\mathcal{E} = 300$ V/cm (lower dotted curve).

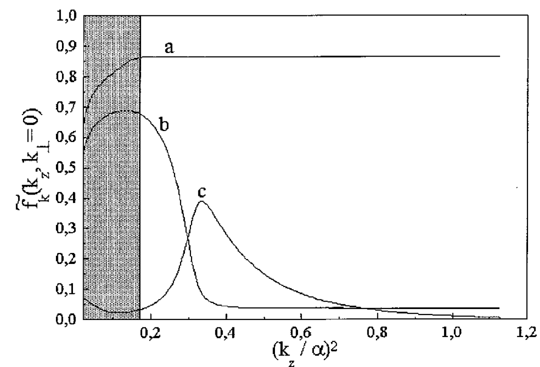

FIG. 3. Normalized distribution function as a function of the squared normalized momentum $(k_z/\alpha)^2$ for impurity concentration $N_i = 4 \times 10^{15}$ cm^{-3}. See text for details.

total electron density, $f_r N_i/n$ is the mean occupation probability in each resonant state. The behavior of $f_r N_i/n$ as a function of the impurity concentration N_i is demonstrated with the inset in the upper panel of Fig. 2 for the electric field strength $\mathcal{E} = 100$ V/cm (upper solid curve) and $\mathcal{E} = 300$ V/cm (lower dotted curve).

We mention that the nonequilibrium population of the localized states near the edge of the light-hole subband can only be less than that in the low-energy continuous states. Consequently, under the conditions imposed on our calculation, both the intracenter and intraband populations are inverted. Thus, the resonant states induced population inversion predicted by our theory explains the origin of lasing in the terahertz frequency range observed in 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. Guided by our theory, a tunable CW laser has been fabricated recently [11]. Our proposed mechanism for population inversion is valid not only for strained p-Ge, since resonant states can be created by various means. This mechanism of population inversion will be the foundation for future study on *unipolar resonant states laser.*

We thank V. I. Perel and A. A. Andronov for useful discussions. Financial support from Swedish Natural Science Research Council Grants No. Ö-AH/KG 03996-322 and No. 03996-321, by Nordic Academy for Advanced Study (NorFA) Grant No. 98.55.002-O, and by Russian Foundation for Basic Research Grants No. 98-02-18268 and No. 97-02-16820 are acknowledged.

[1] H. C. Casey and H. B. Panish, *Heterostructure Lasers* (Academic, New York, 1978).

[2] A. A. Andronov, Sov. Phys. Semicond. **21**, 701 (1987); in *Spectroscopy of Nonequilibrium Electrons and Phonons,* edited by C. V. Shank and B. P. Zakharchenya, Modern Problems in Condensed Matter Sciences Vol. 35 (North-Holland, Amsterdam, 1992).

[3] J. Faist, F. Capasso, D. L. Sivco, A. L. Hutchinson, and A. Y. Cho, Science **264**, 553 (1994); J. Faist, F. Capasso, C. Sirtori, D. L. Sivco, A. L. Hutchinson, M. S. Hybertsen, and A. Y. Cho, Phys. Rev. Lett. **76**, 411 (1996).

[4] M. A. Odnoblyudov, V. M. Chistyakov, I. N. Yassievich, and M. S. Kagan, Phys. Status Solidi (b) **210**, 873 (1998).

[5] I. V. Altukhov, E. G. Chirikova, M. S. Kagan, K. A. Korolev, V. P. Sinis, M. A. Odnoblyudov, and I. N. Yassievich, Sov. Phys. JETP **88**, 51 (1999).

[6] I. V. Altukhov, E. G. Chirikova, M. S. Kagan, K. A. Korolev, V. P. Sinis, and F. A. Smirnov, Sov. Phys. JETP **74**, 404 (1992).

[7] I. B. Levinson, Sov. Phys. Usp. **26**, 176 (1983).

[8] P. A. M. Dirac, *Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1930), p. 354.

[9] A. Baldereschi and N. O. Lipari, Phys. Rev. B **8**, 2697 (1973).

[10] G. L. Bir and G. E. Pikus *Symmetry and Strain Effects in Semiconductors* (Wiley, New York, 1974).

[11] Yu. P. Gousev, I. V. Altukhov, K. A. Korolev, V. P. Sinis, M. S. Kagan, E. E. Haller, M. A. Odnoblyudov, I. N. Yassievich, and K. A. Chao, Appl. Phys. Lett. (to be published).