Resonant states induced by shallow acceptors in uniaxially strained semiconductors

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We present a detailed theoretical investigation of resonant states induced by shallow acceptors in uniaxially strained semiconductors. By applying Dirac's approach and using the Coulomb potential of an acceptor impurity, we have obtained the amplitude of resonant scattering, the probability of coherent capture and emission of holes by resonant state, and the characteristic features of the resonant state. The modified dispersion law and density-of-states of valence band by the resonant states have also been derived. The energy dependence of optical transition probability between resonant and localized impurity state have been calculated. The theoretical investigation of a new mechanism for carrier population inversion in strained semiconductors under an electric field has been presented. It has been shown that the mechanism is the result of a coherent capture-emission type inelastic scattering of holes by resonant states. The calculation based on our theory for uniaxially strained *p*-Ge explains the recently observed lasing phenomena in THz frequency region.

I. INTRODUCTION

When a semiconductor is doped with one type of shallow impurities, normally the impurity level lies in the energy-band gap with a well-defined binding energy measured from one band edge. Then the impurity states are spatially localized. As an external pressure removes the degeneracy of the valence bands, one finds an impurity level attached to each shifted valence band edges.[1] If the energy separation between two splitted valence bands becomes larger than the impurity binding energy, the impurity level attached to one valence band overlaps with another valence band. A hybridization then occurs between the overlapping localized impurity states and extended Bloch states, resulting in resonant states. Using a variational approach, the acceptor states in strained semiconductors has been calculated.[2,3] However, no resonant state has been obtained with the variational method.

Far-infrared lasing was observed from *p*-doped germanium Ge:Ga under a uniaxial stress and an electric field in the range from 10 V/cm to 3 kV/cm.[4] By analyzing the photon energy and the selection rule, it was concluded that the initial state of the optical transition is a resonant state. Two questions of fundamental importance then arise: the characteristic features of the resonant state and the mechanism of its population inversion. In our recent letter,[5] we have proved without computational details that the inversion of carrier population is due to the coherent capture-and-emission process by resonant states. Such details will be provided in the present paper.

To build up our theory unambiguously, the model Hamiltonian is introduced in Sec. II for the valence bands of cubic semiconductors under uniaxial stress. In Sec. III we use Dirac's approach to investigate the resonant state induced by the Coulomb potential of an acceptor impurity, and derive the analytical expressions of the shift and the width of the resonant state. After calculating in Sec. IV the dispersion relation and the density-of-states of the valence band modified by the resonant state, and in Sec. VI the relevant optical transition probability, the mechanism of population inversion will be studied in detail in Sec. VII.

II. VALENCE BANDS OF A STRAINED SEMICONDUCTOR

The fourfold degenerate valence-band top in germanium is at the Γ point of the Brillouin zone. The corresponding wave functions are transformed according to the Γ_8^+ representation of the double point group $\overline{O}_h$ and can be characterized by the total angular momentum $J=3/2$. Due to the spin-orbit coupling, a twofold degenerate energy level is split from the valence-band top by the spin-orbit splitting Δ. The corresponding wave functions are transformed according to the Γ_7^+ representation of the $\overline{O}_h$ group, and are characterized by $J=1/2$. Since the spin-orbit splitting in germanium is much larger than the binding energy of an acceptor, in the present paper, it is reasonable to ignore the split-off band. The effective-mass Luttinger Hamiltonian describing the Γ_8^+ valence band is a 4×4 matrix function of the operator $\hat{\mathbf{k}}=-i\nabla$. We choose the Bloch basis u_m with $m=\pm3/2$ and $\pm1/2$ for the Γ_8^+ representation, where m is the z component of the total angular momentum J of the hole at Γ point. These basis functions can be expressed explicitly as

$$u_{3/2}=-\frac{1}{\sqrt{2}}(X+iY)\uparrow,$$

$$u_{1/2}=\frac{1}{\sqrt{6}}[-(X+iY)\downarrow+2Z\uparrow],$$

$$u_{-1/2}=\frac{1}{\sqrt{6}}[(X-iY)\uparrow+2Z\downarrow],$$

$$u_{-3/2}=\frac{1}{\sqrt{2}}(X-iY)\downarrow, \tag{1}$$

where $\uparrow$ and $\downarrow$ denote the 1/2 spinor up and down. The basis states X,Y, and Z are Bloch functions, which transform like the corresponding coordinates under the symmetry operations of O_h. We set the zero reference energy at the valence-band edge, and adopt the convention that the valence-band energy is positive. In spherical approximation the Luttinger Hamiltonian is given by[6]

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

with the matrix element

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

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

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

$$\hat{c}=\sqrt{3}\gamma(\hat{k}_x-i\hat{k}_y)^2. \tag{3}$$

In the above equations, γ_1,γ_2, and γ_3 are Luttinger parameters, and $\gamma=(2\gamma_2+3\gamma_3)/5$. In our notation $\mathbf{k}$ is a vector and $\hat{\mathbf{k}}$ is an operator.

A uniaxial stress lowers the symmetry of the crystal.[1] A stress parallel to the [001] direction changes the point-group symmetry from cubic O_h to tetragonal D_{4h}. The Γ_8^+ representation is then splitted into two irreducible representations: Γ_6^+ for the Bloch wave functions $u_{\pm 3/2}$, and Γ_7^+ for the Bloch wave functions $u_{\pm 1/2}$. Consequently, the top of the valence band separates into two bands with twofold degeneracy each. The effect of this uniaxial stress along the [001] axis is to add to Eq. (2) a strain Hamiltonian[1]

$$\hat{H}_{\mathrm{str}}=\frac{\hbar^2}{2m_0}\begin{bmatrix}\zeta & 0 & 0 & 0\\ 0 & -\zeta & 0 & 0\\ 0 & 0 & -\zeta & 0\\ 0 & 0 & 0 & \zeta\end{bmatrix}. \tag{4}$$

The parameter ζ, the applied stress P and the deformation potential α are related to the split of the valence-band top E_{def} by

$$E_{\mathrm{def}}=\alpha P=2\frac{\hbar^2\zeta}{2m_0}. \tag{5}$$

For Ge with a stress along [001], $\alpha=6$ meV/kbar.

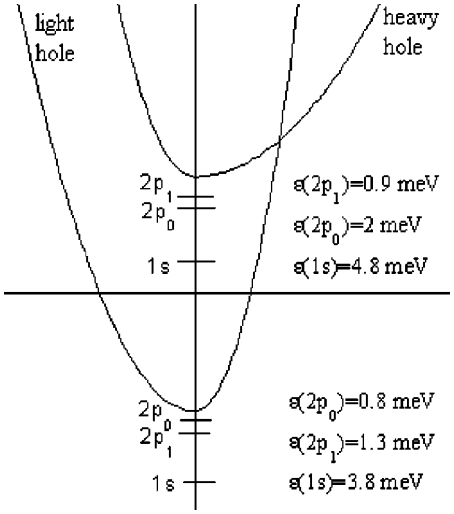

FIG. 1. Acceptor levels (measured from respective band edge) and heavy-and light-hole bands of Ge:Ga under uniaxial stress.

If the stress is along the [111] direction, to derive the strain Hamiltonian in the form of Eq. (4), we should rotate the coordinate system to bring the z axis into the [111] direction. In the similar way, for any direction of applied stress, we can always rotate the z axis into the uniaxial stress direction to obtain a diagonal form of stress Hamiltonian. Since we have used the spherical approximation for the Luttinger Hamiltonian, in the new coordinate system, it will have the same form as Eq. (2). Consequently, for any stress direction, our Hamiltonian for the hole states in a uniaxially strained semiconductor can be written in the general form

$$\hat{H}(\hat{\mathbf{k}})=\hat{H}_{\mathrm{L}}(\hat{\mathbf{k}})+\hat{H}_{\mathrm{str}}, \tag{6}$$

provided a correct value of the deformation potential is used. For example, for Ge with a stress along [111], $\alpha=4$ meV/kbar. This Hamiltonian is easily diagonalized to yield the valence-band spectra. According to our convention that hole energies are positive, the hole bands are obtained as

$$E_{\mathrm{l,h}}(\mathbf{k})=\frac{\hbar^2}{2m_0}[\gamma_1 k^2\mp\sqrt{\zeta^2-2\gamma\zeta(3k_z^2-k^2)+4\gamma^2k^4}], \tag{7}$$

where the minus sign is for the light-hole band $E_{\mathrm{l}}(\mathbf{k})$, and the plus sign for the heavy-hole band $E_{\mathrm{h}}(\mathbf{k})$. These two bands are schematically shown in Fig. 1 as solid curves.

We will study the physical properties of a resonant state, which is the hybridized product of extended states in a valence band and a localized impurity orbital in the presence of a charged acceptor. Hence, a Coulomb term should be added to Eq. (6) to give the final form of the Hamiltonian

$$\hat{\mathcal{H}}(\hat{\mathbf{k}})=\hat{H}_{\mathrm{L}}(\hat{\mathbf{k}})+\hat{H}_{\mathrm{str}}-\frac{e^2}{\epsilon r}\hat{I}, \tag{8}$$

where ϵ is the dielectric constant, e is the electron charge, and $\hat{I}$ is a 4×4 unit matrix. Since a shallow acceptor is attached to the valence-band edge, in a uniaxially strained semiconductor, both its fourfold degenerate ground state and excited states are separated into two doubly degenerate levels. The symmetry properties of localized acceptor wave

functions certainly depend on how the stress is applied to the sample,[7] and in an adopt approximation each of these functions can be characterized by the z component of its total angular momentum, which is labeled by M. Splitted acceptor states originated from the ground level are classified by $M=\pm 1/2$ and $M=\pm 3/2$.

Under a sufficiently strong stress that the valence-band splitting $E_{\rm def}$ is larger than the acceptor binding energy, two separated series of acceptor levels are formed as shown in Fig. 1. Each acceptor level attached to the heavy-hole band overlaps with the light-hole band $E_l(\mathbf{k})$, and forms a resonant state via its hybridization with the extended Bloch states. The resonant states can be classified by the same value of the z component of the total angular momentum as the classification of the original localized acceptor orbitals.

In the limit of high stress, we can expand the square root in Eq. (7) in powers of k^2/ζ and keep only the quadratic terms. This approximation is equivalent to the neglect of the off-diagonal elements in the Luttinger Hamiltonian matrix, and hence the hybridization effect is ignored. These off-diagonal terms represent the interaction between the heavy-hole band and the light-hole band. In this situation the acceptor levels near the light-hole band edge were studied earlier,[8,9] and the acceptor levels near the heavy-hole band edge were investigated recently by Odnoblyudov and Chistyakov.[10] In high stress approximation, both series of localized acceptor orbitals attached to the light-hole band and the heavy-hole band are classified by m, parity i, and the z component of the acceptor orbital angular momentum l_z. We label the localized acceptor orbitals with the conventional notations: $1s$ for $l_z=0$ and $i=+1$, $2p_{\pm 1}$ for $l_z=\pm 1$ and $i=-1$, and $2p_0$ for $l_z=0$ and $i=-1$. All acceptor levels attached to the heavy-hole subband have $m=\pm 3/2$ and all acceptor levels attached to the light-hole subband have $m=\pm 1/2$. These acceptor levels are schematically shown in Fig. 1. The z component of total angular momentum M for each level is simply $M=l_z+m$. Hence, the $1s$ orbital near the light-hole band edge has $M=\pm 1/2$, and the $1s$ orbital near the heavy-hole band edge has $M=\pm 3/2$.

III. DIRAC'S APPROACH FOR RESONANT STATES

In our earlier work[11] exact solution of resonant state was obtained if the impurity potential is zerorange. However, for a realistic Coulomb impurity potential, the problem becomes complicated. In this section we consider, in detail, the hybridization process that leads to the formation of resonant states induced by a Coulomb potential of an acceptor impurity. During the hybridization process between the localized acceptor orbital and light-hole band states, the z component of the total angular momentum is conserved, and therefore $M=l_z+m$ serves as the quantum number to label the resonant state. This process is described by the off-diagonal elements of the Luttinger Hamiltonian given by Eq. (2). Based on the full Hamiltonian $\hat{\mathcal{H}}$ in Eq. (8), which includes the Coulomb potential, we will analyze the effect of these off-diagonal terms with the Dirac's approach,[12] which is one version of the perturbation theory for continuum states. We will separate the Hamiltonian as

$$\hat{\mathcal{H}}=\hat{H}_0+\hat{U}, \tag{9}$$

where $\hat{H}_0$ is the diagonal part of $\hat{\mathcal{H}}$, and $\hat{U}$ the off-diagonal part. Since the off-diagonal terms of the Luttinger Hamiltonian couples the heavy-hole band and the light-hole band states, and this coupling decreases with increasing stress, the perturbation results are more accurate for stronger applied stress, which is the region of experimental interest.

We are interested in the eigenfunctions of $\hat{H}_0$ in the energy region around the $1s$ level attached to the heavy-hole subband. Using the basis given by Eq. (1), they can be expressed as

$$\varphi^{(+3/2)}(\mathbf{r})=\begin{bmatrix}\varphi^h_{1s}(\mathbf{r})\\0\\0\\0\end{bmatrix},\quad \psi^{(+1/2)}_{\mathbf{k}}(\mathbf{r})=\begin{bmatrix}0\\\psi^l_{\mathbf{k}}(\mathbf{r})\\0\\0\end{bmatrix},$$

$$\psi^{(-1/2)}_{\mathbf{k}}(\mathbf{r})=\begin{bmatrix}0\\0\\\psi^l_{\mathbf{k}}(\mathbf{r})\\0\end{bmatrix},\quad \varphi^{(-3/2)}(\mathbf{r})=\begin{bmatrix}0\\0\\0\\\varphi^h_{1s}(\mathbf{r})\end{bmatrix}, \tag{10}$$

where $\varphi^h_{1s}(\mathbf{r})$ is the effective-mass envelope function of the localized acceptor $1s$ orbital near the heavy-hole band edge, and $\psi^l_{\mathbf{k}}(\mathbf{r})$ is an extended state in the light-hole band.

Consider a carrier in the light-hole band Bloch state with wave vector $\mathbf{k}$. The carrier will be scattered by the impurity and therefore its wave function will be modified. We are interested in the case when the energy of the incident wave is close to the energy of the acceptor $1s$ orbital near the heavy-hole band edge. Due to the hybridization the resultant resonant state will consist of the incident wave, the scattered waves, and the localized orbital, which can be written in the general form

$$\Psi_{E_{\mathbf{k}}}(\mathbf{r})=\sum_{m=\pm 3/2} a^{(m)}_{\mathbf{k}}\varphi^{(m)}(\mathbf{r})+\sum_{\mathbf{k}',m=\pm 1/2} b^{(m)}_{\mathbf{k}\mathbf{k}'}\psi^{(m)}_{\mathbf{k}'}(\mathbf{r}). \tag{11}$$

By proper choice of the coefficients of linear combination, the resonant state wave function satisfies the Schrödinger equation

$$\hat{\mathcal{H}}\Psi_{E_{\mathbf{k}}}(\mathbf{r})=E_{\mathbf{k}}\Psi_{E_{\mathbf{k}}}(\mathbf{r}). \tag{12}$$

We will use the Dirac's approach to determine the coefficients.[12,13] Substituting this wave function into Eq. (12), we obtain the coupled linear equations for the coefficients $a^{(m)}_{\mathbf{k}}$ and $b^{(m)}_{\mathbf{k}\mathbf{k}'}$:

$$a^{(3/2)}_{\mathbf{k}}(E_{\mathbf{k}}-E_{\rm def}+\varepsilon_{1s})=\sum_{\mathbf{k}'}\left[b^{(1/2)}_{\mathbf{k}\mathbf{k}'}V_{\mathbf{k}'}+b^{(-1/2)}_{\mathbf{k}\mathbf{k}'}W_{\mathbf{k}'}\right]$$

$$a^{(-3/2)}_{\mathbf{k}}(E_{\mathbf{k}}-E_{\rm def}+\varepsilon_{1s})=\sum_{\mathbf{k}'}\left[b^{(1/2)}_{\mathbf{k}\mathbf{k}'}W^*_{\mathbf{k}'}-b^{(-1/2)}_{\mathbf{k}\mathbf{k}'}V^*_{\mathbf{k}'}\right],$$

$$b^{(1/2)}_{\mathbf{k}\mathbf{k}'}[E_{\mathbf{k}}-\varepsilon_l(\mathbf{k}')]=[a^{(3/2)}_{\mathbf{k}}V^*_{\mathbf{k}'}+a^{(-3/2)}_{\mathbf{k}}W_{\mathbf{k}'}],$$

$$b_{\mathbf{k}\mathbf{k}'}^{(-1/2)}[E_{\mathbf{k}}-\varepsilon_l(\mathbf{k}')]=[a_{\mathbf{k}}^{(3/2)}W_{\mathbf{k}'}^{*}-a_{\mathbf{k}}^{(-3/2)}V_{\mathbf{k}'}]. \quad (13)$$

In the above equations, ε_{1s} is the energy of the state with wave function $\varphi^{(\pm 3/2)}(\mathbf{r})$ measured from the heavy-hole band edge, $\varepsilon_l(\mathbf{k})$ is the light-hole band energy for $\psi_{\mathbf{k}}^{l}(\mathbf{r})$, measured from the light-hole band edge, and $E_{\mathbf{k}}$ is the resonant state energy measured also from the edge of the light-hole band. The matrix elements $V_{\mathbf{k}}$ and $W_{\mathbf{k}}$ are calculated from the off-diagonal operators of the Luttinger Hamiltonian

$$V_{\mathbf{k}}=-\langle\varphi_{1s}^{h}(\mathbf{r})|\frac{\hbar^2}{2m_0}\hat{b}(\mathbf{k})|\psi_{\mathbf{k}}^{l}(\mathbf{r})\rangle,$$

$$W_{\mathbf{k}}=-\langle\varphi_{1s}^{h}(\mathbf{r})|\frac{\hbar^2}{2m_0}\hat{c}(\mathbf{k})|\psi_{\mathbf{k}}^{l}(\mathbf{r})\rangle. \quad (14)$$

Equation (13) can be solved in the same way as for scattering problems.[12,13] For an incident wave with z component of angular momentum m, the solutions are labeled as $a_{\mathbf{k}}^{(m,m')}$ and $b_{\mathbf{k}\mathbf{k}'}^{(m,m')}$. If $m=1/2$, we have

$$a_{\mathbf{k}}^{(1/2,3/2)}=V_{\mathbf{k}}R_1,$$

$$a_{\mathbf{k}}^{(1/2,-3/2)}=W_{\mathbf{k}}^{*}R_1,$$

$$b_{\mathbf{k}\mathbf{k}'}^{(1/2,1/2)}=\delta_{\mathbf{k}\mathbf{k}'}+R_1R_2(V_{\mathbf{k}}V_{\mathbf{k}'}^{*}+W_{\mathbf{k}}^{*}W_{\mathbf{k}'}),$$

$$b_{\mathbf{k}\mathbf{k}'}^{(1/2,-1/2)}=R_1R_2(V_{\mathbf{k}}W_{\mathbf{k}'}^{*}-W_{\mathbf{k}}^{*}V_{\mathbf{k}'}), \quad (15)$$

and if $m=-1/2$, the solutions are

$$a_{\mathbf{k}}^{(-1/2,3/2)}=W_{\mathbf{k}}R_1,$$

$$a_{\mathbf{k}}^{(-1/2,-3/2)}=-V_{\mathbf{k}}^{*}R_1,$$

$$b_{\mathbf{k}\mathbf{k}'}^{(-1/2,1/2)}=R_1R_2(W_{\mathbf{k}}V_{\mathbf{k}'}^{*}-V_{\mathbf{k}}^{*}W_{\mathbf{k}'}),$$

$$b_{\mathbf{k}\mathbf{k}'}^{(-1/2,-1/2)}=\delta_{\mathbf{k}\mathbf{k}'}+R_1R_1(W_{\mathbf{k}}W_{\mathbf{k}'}^{*}+V_{\mathbf{k}}^{*}V_{\mathbf{k}'}). \quad (16)$$

In the above equations, R_1 and R_2 are defined as

$$R_1=\frac{1}{E_{\mathbf{k}}-E_{\mathrm{def}}+\varepsilon_{1s}-\Delta E_{\mathbf{k}}+i\Gamma_{\mathbf{k}}/2}, \quad (17)$$

$$R_2=\frac{1}{E_{\mathbf{k}}-\varepsilon_l(\mathbf{k}')+i\eta};\quad \eta\to 0,$$

with

$$\Delta E_{\mathbf{k}}=P\frac{V}{(2\pi)^3}\int d^3k'\frac{|W_{\mathbf{k}'}|^2+|V_{\mathbf{k}'}|^2}{E_{\mathbf{k}}-\varepsilon_l(\mathbf{k}')}, \quad (18)$$

$$\frac{\Gamma_{\mathbf{k}}}{2}=\pi\frac{V}{(2\pi)^3}\int d^3k'(|W_{\mathbf{k}'}|^2+|V_{\mathbf{k}'}|^2)\delta[E_{\mathbf{k}}-\varepsilon_l(\mathbf{k}')]. \quad (19)$$

From the expressions $a_{\mathbf{k}}^{(\pm 1/2,\pm 3/2)}$ in Eqs. (15) and (16), as well as the expression of R_1 in Eq. (17), we see that the coupling between the heavy-hole band and the light-hole band shifts the energy ε_{1s} of the localized orbital to the resonance level by an amount $\Delta E_{\mathbf{k}}<0$, and broadens the level with an width $\Gamma_{\mathbf{k}}$. We notice from Eq. (18) that the shift depends on $E_{\mathbf{k}}$, namely, $\Delta E_{\mathbf{k}}(E_{\mathbf{k}})$. Measured from the light-hole band edge, the resonant level E_0 is determined by the equation

$$E_0=E_{\mathrm{def}}-\varepsilon_{1s}+\Delta E_{\mathbf{k}}(E_0). \quad (20)$$

Using the so obtained value of E_0, the width $\Gamma_{\mathbf{k}}$ is then calculated from Eq. (19).

For the case of the Coulomb potential of an acceptor impurity, we will adopt the most commonly used variational function

$$\varphi_{1s}^{h}(\mathbf{r})\equiv\varphi_{1s}^{h}(\rho,z)=\frac{1}{\sqrt{\pi a^2 b}}\exp\left[-\sqrt{\frac{\rho^2}{a^2}+\frac{z^2}{b^2}}\right]. \quad (21)$$

For the extended Bloch states in light-hole band, we use normalized plane waves $\psi_{\mathbf{k}}^{l}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$. Substituting these functions into Eq. (14), we readily obtain

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

$$W_{\mathbf{k}}=-\frac{\sqrt{3}\hbar^2\gamma}{2m_0}(k_x-ik_y)^2 I(\mathbf{k}), \quad (22)$$

where $I(\mathbf{k})=8\sqrt{\pi a^2 b/V}[1+k_z^2a^2+(k_x^2+k_y^2)b^2]^{-2}$ is the overlap integral between the envelope functions of the localized acceptor orbital and the Bloch states. Using these explicit expressions to calculate all relevant quantities in Eq. (20), it reduces to the final form for numerical solution

$$E_0=E_{\mathrm{def}}-\varepsilon_{1s}+\frac{\hbar^4}{4m_0^2}\gamma^2\frac{b}{a^5}\frac{1}{E_0}F_R(E_0). \quad (23)$$

The dimensionless function $F_R(E_{\mathbf{k}})$ depends weakly on the energy $E_{\mathbf{k}}$, and can be well approximated as a constant $F_R=-41.76$ in the limit of high stress. For p-Ge doped with Ga, the parameter values are $a=114$ Å and $b=51$ Å,[10] the numerical solution of the resonant level energy E_0 as a function of compressive stress along the [111] direction is shown in Fig. 2 by the solid curve. The edges of the heavy- and the

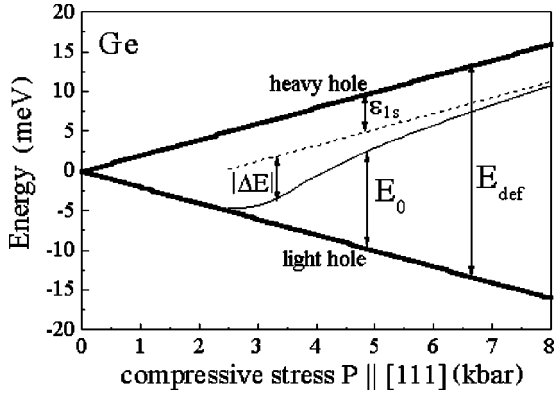

FIG. 2. Stress dependences of the resonant energy level E_0 (solid curve), the impurity level $\varepsilon_{1s}=4.78$ meV (dot line), the energy shift ΔE, and the valence-band split E_{def} in p-Ge. The edges of heavy- and light- hole bands are indicated by thick solid lines.

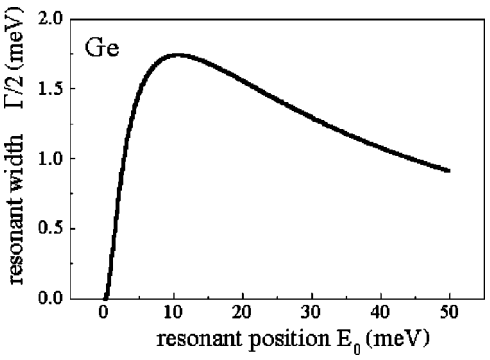

FIG. 3. Resonant level width as a function of resonant energy level in *p*-Ge.

light-hole bands (thick solid lines), as well as the energy level ε_{1s} (dotted line) are also plotted, together with the valence-band split $E_{\rm def}$ and the energy shift ΔE.

The width of the resonant state $\Gamma/2$ is then readily derived from Eq. (19) as

$$\frac{\Gamma}{2}=48\left(\frac{\hbar^2}{2m_0}\right)^{5/2}\gamma^2\frac{b}{a^6}E_0^{-3/2}F_I(E_0), \tag{24}$$

where the function $F_I(E_0)$ depends also weakly on E_0 in the region $E_0 \gg \varepsilon_{1s}$. At the other limit $E_0 \to 0, F_I(E_0)$ is proportional to E_0^4. In Fig. 3 we plot $\Gamma/2$ as a function of E_0. Γ is found to be proportional to $E_0^{5/2}$ in the region $E_0 \ll E_{\rm def}$, but proportional to $E_0^{-3/2}$ in the region $E_0 \simeq E_{\rm def} \gg \varepsilon_{1s}$.

To clarify the role of scattering in the formation of resonant state, we will substitute the solutions Eqs. (15) and (16) into Eq. (11) to obtain the proper forms of the two specific wave functions for $m=1/2$ and $m=-1/2$. By introducing two scattering amplitudes $t_{\mathbf{k}\mathbf{k}'}^{(m,m')}$ and $t_{\mathbf{k}l}^{(m,m')}$, we arrive at the explicit expressions

$$\Psi_{\mathbf{k}}^{(m)}(\mathbf{r})=\psi_{\mathbf{k}}^{(m)}(\mathbf{r})+\sum_{\mathbf{k}',m'=\pm 1/2}\frac{t_{\mathbf{k}\mathbf{k}'}^{(m,m')}}{E_{\mathbf{k}}-\varepsilon_l(\mathbf{k}')+i\eta}\psi_{\mathbf{k}'}^{m'}(\mathbf{r})$$
$$+\sum_{m'=\pm 3/2}\frac{t_{\mathbf{k}l}^{(m,m')}}{E_{\mathbf{k}}-E_0+i\Gamma/2}\varphi^{(m')}(\mathbf{r}). \tag{25}$$

In the above equation, at the right-hand side, the first term is the incident wave of a hole in the light-hole band. When this hole is scattered by the impurity potential into the light-hole band again, such elastic resonant process is represented by the second term. The corresponding scattering probability per unit time is[13]

$$W_{\mathbf{k},\mathbf{k}'}^{(m)}=\frac{2}{\hbar}|t_{\mathbf{k},\mathbf{k}'}^{(m)}|^2\lim_{\eta\to 0}\frac{\eta}{(E_{\mathbf{k}}-E_{\mathbf{k}'})^2+\eta^2}$$
$$=\frac{2\pi}{\hbar}|t_{\mathbf{k},\mathbf{k}'}^{(m)}|^2\delta(E_{\mathbf{k}}-E_{\mathbf{k}'}), \tag{26}$$

where $|t_{\mathbf{k}\mathbf{k}'}^{(m)}|^2=|t_{\mathbf{k}\mathbf{k}'}^{(m,1/2)}|^2+|t_{\mathbf{k}\mathbf{k}'}^{(m,-1/2)}|^2$. The last term at the right-hand side of Eq. (25) represents the capture of a hole, initially in the light-hole band, by the localized acceptor orbital $\varphi^{(\pm 3/2)}(\mathbf{r})$, and the subsequent coherent re-emission of the hole back into the light-hole band. A carrier in the light-hole band has a finite probability to be captured in the localized acceptor orbital $\varphi^{(\pm 3/2)}(\mathbf{r})$ if the energy of the hole lies in the region $E_0-\Gamma/2<E_{\mathbf{k}}<E_0+\Gamma/2$. As derived rigorously in Appendix A, the total probability of transition from the state $\psi_{\mathbf{k}}^l(\mathbf{r})$ in the light-hole band to the localized acceptor orbital $\varphi^{(\pm 3/2)}(\mathbf{r})$ is

$$W_{\mathbf{k}r}^{(m)}=\frac{2}{\hbar}(|V_{\mathbf{k}}|^2+|W_{\mathbf{k}}|^2)\frac{\Gamma/2}{(E_{\mathbf{k}}-E_0)^2+\Gamma^2/4}. \tag{27}$$

The same expression takes place for the probability of the reverse process. Therefore, the captured hole will stay in $\varphi^{(\pm 3/2)}(\mathbf{r})$ for a time interval about

$$\sum_{\mathbf{k}'}W_{r\mathbf{k}'}^{(m)}=\frac{\Gamma}{\hbar}. \tag{28}$$

IV. DISPERSION LAW AND DENSITY-OF-STATES

Since the light-hole band state $\psi_{\mathbf{k}}^{(m)}(\mathbf{r})$ is modified into the resonant state $\Psi_{\mathbf{k}}^{(m)}(\mathbf{r})$ as shown by Eq. (25), the dispersion relation $\varepsilon_l(\mathbf{k})$ and the corresponding density-of-states $\rho_l(\varepsilon_l)$ will also change accordingly. Using the wave function given by Eq. (25), from Eq. (12) we can easily derive the self-consistent equation for $E_{\mathbf{k}}$ at the presence of a single acceptor, which includes the modification of energy spectrum $\varepsilon_l(\mathbf{k})$ of light-hole subband by the resonant state. However, there are many acceptors in a sample. We are interested in samples with low-acceptor concentration N_A/V such that each acceptor can be treated as isolated from the others. Hence, the effects of N_A acceptors are additive, and the self-consistent equation becomes

$$E_{\mathbf{k}}=\varepsilon_l(\mathbf{k})-\frac{N_A}{V}\frac{E_{\mathbf{k}}-E_0}{(E_{\mathbf{k}}-E_0)^2+\Gamma^2/4}(|V_{\mathbf{k}}|^2+|W_{\mathbf{k}}|^2). \tag{29}$$

From Eqs. (3) and (14), it is obvious that both $V_{\mathbf{k}}$ and $W_{\mathbf{k}}$ vanish if $\mathbf{k}$ is along the stress direction z axis. In this situation, there is no mixing between the light-hole subband and the heavy-hole subband.

Using the material parameters of *p*-Ge, the calculated normalized $E_{\mathbf{k}}/E_0$ as a function of normalized $\varepsilon_l(\mathbf{k})/E_0$ is shown in Fig. 4, for $\mathbf{k}$ perpendicular to z axis and for various acceptor impurity concentrations. As the concentration increases from $5\times10^{16}\,\mathrm{cm}^{-3}$ (curve 3) to $1\times10^{17}\,\mathrm{cm}^{-3}$ (curve 2) and to $2\times10^{17}\,\mathrm{cm}^{-3}$ (curve 1), the ''effective mass'' of a lighthole is dramatically enhanced. The physical origin of this enhancement is that a hole is captured in the acceptor state $\varphi_{1s}^{(\pm 3/2)}(\mathbf{r})$ for a finite amount of time $\Gamma/\hbar$.

Knowing the functional dependence of $E_{\mathbf{k}}$ on $\varepsilon_l(\mathbf{k})$, we can calculate the partial density-of-states $\rho(E_{\mathbf{k}})$ which corresponds to the spectrum $E_{\mathbf{k}}$ along any direction in $\mathbf{k}$ space. The result is shown in Fig. 5 for $\mathbf{k}$ perpendicular to the stress direction z axis, with various values of acceptor impurity concentration: curve 1 for $2\times10^{17}\,\mathrm{cm}^{-3}$, curve 2 for $1\times10^{17}\,\mathrm{cm}^{-3}$, curve 3 for $5\times10^{16}\,\mathrm{cm}^{-3}$, and curve 4 for $1\times10^{16}\,\mathrm{cm}^{-3}$. The density-of-states of N_A noninteracting acceptors is a δ function. The hybridization between the local-

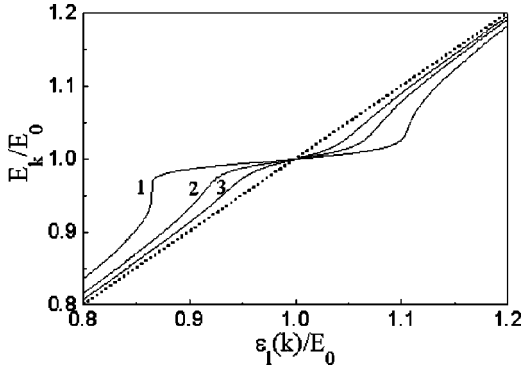

FIG. 4. Normalized resonant state energy as a function of normalized light-hole band energy in a *p*-Ge under uniaxial stress with **k** perpendicular to the stress direction *z* axis. The value of acceptor concentration is zero (dotted line), $2\times10^{17}\,\mathrm{cm}^{-3}$ (curve 1), $1\times10^{17}\,\mathrm{cm}^{-3}$ (curve 2), and $5\times10^{16}\,\mathrm{cm}^{-3}$ (curve 3).

ized orbitals of N_A acceptors and the Bloch states in the light-hole subband broadens the δ function into an asymmetric peak in the resulting density-of-states $\rho(E_{\mathbf{k}})$.

V. OPTICAL TRANSITIONS

The resonant state $\Psi_{\mathbf{k}}^{(m)}(\mathbf{r})$ given by Eq. (25) consists of two parts: an incident plane wave $\psi_{\mathbf{k}}^{(m)}(\mathbf{r})$ and a scattered part, which we label as $\Phi_{\mathbf{k}}^{(m)}(\mathbf{r})$. When a carrier in the resonant state makes the optical transition to a localized impurity orbital $\phi(\mathbf{r})$, the interference of optical matrix elements originated from $\psi_{\mathbf{k}}^{(m)}(\mathbf{r})$ and $\Phi_{\mathbf{k}}^{(m)}(\mathbf{r})$ produces an asymmetric energy dependence of the optical transition probability. This is so-called Fano resonance.[14] The asymmetry of the line shape is measured by the shape parameter or the Fano parameter q:

$$\frac{1}{2}\pi q^2=\frac{|\langle\Phi_{\mathbf{k}}^{(m)}|\hat{T}|\phi\rangle|^2}{|\langle\Psi_{\mathbf{k}}^{(m)}|\hat{T}|\phi\rangle|^2}, \tag{30}$$

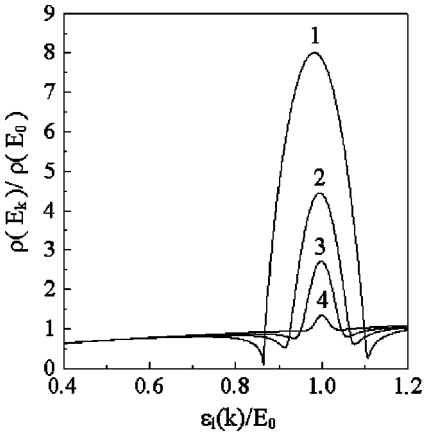

FIG. 5. The partial density-of-states for the resonant level $E_{\mathbf{k}}$ in a *p*-Ge under a uniaxially stress, with **k** perpendicular to the stress direction. The values of acceptor concentration are $2\times10^{17}\,\mathrm{cm}^{-3}$ (curve 1), $1\times10^{17}\,\mathrm{cm}^{-3}$ (curve 2), $5\times10^{16}\,\mathrm{cm}^{-3}$ (curve 3), and $1\times10^{16}\,\mathrm{cm}^{-3}$ (curve 4).

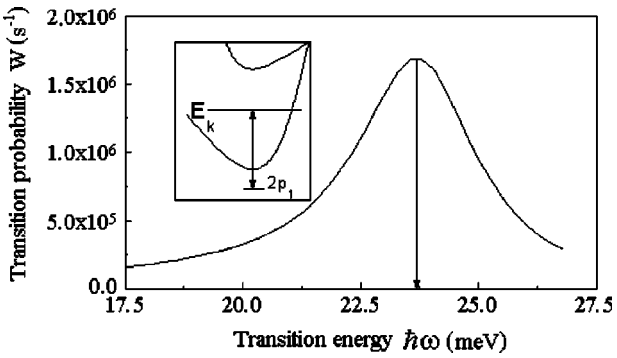

FIG. 6. Energy dependence of optical transition probability from around the lowest resonant state to impurity $2p_{\pm1}$ states. The transition process is illustrated by the inset.

where $\hat{T}$ is the operator of optical transition. For the transition in the valence band, $\hat{T}$ has the form

$$\hat{T}=\frac{e}{c}(\mathbf{A}\cdot\nabla_{\mathbf{p}}\hat{\mathcal{H}}), \tag{31}$$

where c is the speed of light and **A** is the vector potential of the electromagnetic field. With increasing value of q, the luminescence line approaches the Lorence shape.

The selection rules in a uniaxially strained Ge, as determined by the cylindrical symmetry, are (1) $\Delta M=0,\pm1$, and (2) the initial and final states should have opposite parities with respect to the reflection $z\rightarrow-z$. In the resonant state given by Eq. (25), the transitions from the nonplane wave part to impurity $2p$ states are allowed, but to the impurity $1s$ 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 may appear in the optical spectrum, but its intensity will be weaker than the intensity of $1s$-to-$2p_{\pm1}$ transition.

We have mentioned earlier that the main peak in the observed far-infrared lasing spectrum of strained Ge:Ga corresponds to the $1s$-to-$2p_{\pm1}$ transition, which is illustrated by the inset in Fig. 6.[15] Now we will calculate the optical transition probabilities between these degenerate localized impurity orbitals and the resonant states with energies close to E_0. Let $\varepsilon_{2p_{\pm1}}$ be the energy level of impurity $2p$ states. For the impurity orbitals we will use the variational function[10]

$$\varphi_{2p_{\pm1}}^{l}(\mathbf{r})=\frac{1}{\sqrt{\pi c^4 d}}\rho e^{\pm i\varphi}e^{-\sqrt{\rho^2/c^2+z^2/d^2}}, \tag{32}$$

where $\mathbf{r}=(\rho,z,\varphi)$. For an acceptor in Ge, $c=157$ Å and $d=230$ Å.

The energy dependence of optical transition probability $W_{E_{\mathbf{k}}}$ can be expressed as

$$W_{E_{\mathbf{k}}}=R_{E_{\mathbf{k}}}/n_h, \tag{33}$$

where n_h is the free-hole concentration. $R_{E_{\mathbf{k}}}$ is the radiative recombination rate of holes[16]

$$R_{E_{\mathbf{k}}}=\frac{4\pi e}{\hbar cV}\sum_{\mathbf{k}',\mathbf{Q},\mathbf{R},\alpha}\sum_{m=\pm 1/2}\delta(E_{\mathbf{k}'}-\varepsilon_{2p_{\pm 1}}+\hbar cQ/\sqrt{\epsilon})$$
$$\times f_{\mathbf{k}'}|\langle\Psi^{(m)}_{\mathbf{k}'}|\mathbf{A}_\alpha\cdot\nabla_{\mathbf{p}}\hat{\mathcal{H}}|\varphi^{l}_{2p_{\pm 1}}(\mathbf{r}-\mathbf{R})\rangle|^2. \quad (34)$$

Here $\mathbf{R}$ is the impurity position, and $\mathbf{A}_\alpha$ is the vector potential of photon with polarization α and wave vector $\mathbf{Q}$. The normalized carrier distribution function

$$f_{\mathbf{k}'}=n_h V\delta(E_{\mathbf{k}'}-E_{\mathbf{k}})/\sum_{\mathbf{k}}\delta(E_{\mathbf{k}'}-E_{\mathbf{k}}) \quad (35)$$

represents a uniform occupation of states with energy $E_{\mathbf{k}}$.

The shape parameter for the impurity $2p_{\pm 1}$ states in a uniaxially stressed Ge doped with Ga can now be readily calculated from Eq. (30) as

$$\frac{1}{2}\pi q^2=36\frac{\gamma^4}{(\gamma_1+2\gamma)^2}\frac{c^8}{a^8}\frac{E_0}{\Gamma}C, \quad (36)$$

where C is the angular average of the matrix element part in Eq. (34). C has a weak energy dependence and its value is approximately 0.1. The spectrum of stimulated emission was measured at $E_{\mathrm{def}}=27.4$ meV, corresponding to a resonant energy $E_0=22.4$ meV and $\Gamma=3$ meV. Hence, the Fano parameter is $q\simeq 45$. Under this situation, the effect of interference is negligible and the broadening of the luminescence line should be Lorence type without detectable asymmetry. Our calculated transition probability is shown in Fig. 6.

VI. KINETICS OF RESONANT STATES

The formation of resonant states is accompanied by the coherent capture and emission of carriers by localized impurity orbitals. Since a carrier can be trapped in a localized impurity orbital for a time interval $\hbar/\Gamma$, such process has profound influence on the non-equilibrium distribution function in a relatively pure semiconductor at low temperatures. In this situation the only significant scattering is due to optical phonons with energy $\hbar\omega_0$. Under an applied electric field $\mathcal{E}$ (assuming along z axis), a carrier drifts in the momentum space almost scatter free, and its energy can exceed $\hbar\omega_0$ if $\mathcal{E}\geqslant\hbar\omega_0/el$, where e is the carrier charge and l its mean free path. The carrier thus has a finite probability to return to the low-energy region by emitting an optical phonon. Such phenomenon, the so-called *streaming motion*, has been extensively studied.[17,18]

However, if a resonant state exists with energy less than $\hbar\omega_0$, then under an applied electric field a carrier will charge the resonant state before its energy reaches $\hbar\omega_0$. In our earlier letter[5] we have proved that such process provides a new mechanism of carrier population inversion, which explains the origin of far-infrared lasing from strained p-Ge.[4] The detailed analysis, which was not given in Ref. 5, will be presented in this section.

We will first outline briefly the model studied in Ref. 5. It includes a *drain D* at $E_{\mathbf{k}}=\hbar\omega_0$, which describes the process of removal of holes in the energy region $E_{\mathbf{k}}\geqslant\hbar\omega_0$ due to emission of optical phonons, and a *source S* at small k within the energy interval between zero and $\epsilon_0\ll\hbar\omega_0$, which presents the generation of holes removed by *drain*. Let $f_{\mathbf{k}}$ be the carrier distribution function. As justified in Ref. 5, the drain D can be well approximated by $f_{\mathbf{k}}=0$ for $E_{\mathbf{k}}\geqslant\hbar\omega_0$, and the source intensity S was derived[18] as

$$S=S_0(t)\Theta(\epsilon_0-E_{\mathbf{k}}) \quad (37)$$

with

$$\epsilon_0=\left(\frac{2}{9}\right)^{1/3}\left(\frac{\omega_0}{\nu_A}\right)^{2/3}\frac{(e\mathcal{E}\hbar)^{2/3}}{m_z^{1/3}} \quad (38)$$

and

$$S_0(t)=\frac{e}{\hbar}\frac{\int(\mathcal{E}\cdot d\mathbf{S})f_{\mathbf{k}}(t)}{\int d^3k\Theta(\epsilon_0-E_{\mathbf{k}})}, \quad (39)$$

where m_z is the effective mass along the z axis, and the characteristic frequency ν_A is related to the optical phonon emission rate $\nu_A\sqrt{(E_{\mathbf{k}}/\hbar\omega_0)-1}$ for the carriers with $E_{\mathbf{k}}>\hbar\omega_0$. In Eq. (39) the integration is performed over the surface defined by the equation $E_{\mathbf{k}}=\hbar\omega_0$.

In the absence of resonant impurity scattering, for carrier kinetic energy $E_{\mathbf{k}}\leqslant\hbar\omega_0$, $f_{\mathbf{k}}$ can be obtained from the kinetic equation[18,19]

$$\frac{\partial f_{\mathbf{k}}}{\partial t}+\frac{e\mathcal{E}}{\hbar}\frac{\partial f_{\mathbf{k}}}{\partial \mathrm{k}_z}=S-D. \quad (40)$$

The stationary solution of Eq. (40) is an almost constant $f_{\mathbf{k}}$ if $\mathbf{k}\equiv(k_z,k_\perp)$ lies in a cylinder in $\mathbf{k}$ space, and $f_{\mathbf{k}}=0$ otherwise. This cylinder is confined by

$$0<k_z\leqslant\sqrt{2m_z\omega_0/\hbar^2},\quad k_\perp\leqslant\sqrt{2m_\perp\epsilon_0/\hbar^2},$$

where $m_\perp$ is the transverse component of the effective-mass tensor.

In the presence of N_A localized impurity orbitals attached to the heavy-hole subband, free carriers in the light-hole band can be trapped into these orbitals, and such trapped carriers can either escape back to the light-hole subband, or make radiative transitions into the impurity orbitals attached to the light-hole subband. These processes drive the system to a steady state within a time interval τ_ε. As will be shown later by our calculation, for p-Ge this transient time is $\tau_{\mathcal{E}}\simeq 5\times 10^{-12}$ s. The typical value of $\hbar/\Gamma$ calculated from Eq. (24) is $\hbar/\Gamma\simeq 2\times 10^{-13}$ s. We see that both $\tau_{\mathcal{E}}$ and $\hbar/\Gamma$ are less than $1/W$, where W is the optical transition probability calculated in Sec. V. Consequently, in the kinetic equations for $f_{\mathbf{k}}$ and for the occupation probability f_r of impurity states, the unimportant radiation transition process will be ignored.

Then, f_r satisfies the kinetic equation

$$\frac{\partial f_r}{\partial t}=\sum_{\mathbf{k}'}[W_{\mathbf{k}'r}f_{\mathbf{k}'}-W_{r\mathbf{k}'}f_r], \quad (41)$$

and the impurity collision integral

$$I=N_A\sum_{\mathbf{k}'}[f_{\mathbf{k}'}W_{\mathbf{k}\mathbf{k}'}-f_{\mathbf{k}}W_{\mathbf{k}'k}]+N_A(W_{r\mathbf{k}}f_r-W_{\mathbf{k}r}f_{\mathbf{k}}) \quad (42)$$

should be added to the right hand side of Eq. (40). The probabilities $W_{\mathbf{k}r}$ and $W_{\mathbf{k}\mathbf{k}'}$ are defined by Eqs. (26) and (27). Since the localized orbitals and the extended Bloch states are doubly degenerate, we have $f_r^{+3/2}=f_r^{-3/2}\equiv f_r$ and $f_{\mathbf{k}}^{+1/2}=f_{\mathbf{k}}^{-1/2}\equiv f_{\mathbf{k}}$. The conservation of carriers imposes the normalization condition

$$\sum_{\mathbf{k}} f_{\mathbf{k}}+N_A f_r=N_h \tag{43}$$

where N_h is the total number of holes. All above equations will be solved self-consistently.

Since in p-Ge the transient time $\tau_{\mathcal{E}}$ is much larger than the lifetime of the resonant state $\hbar/\Gamma$, we can set the left-hand side of Eq. (41) to zero. Hence, the occupation probability f_r of the quasilocal states follows adiabatically the distribution function $f_{\mathbf{k}}$ of the Bloch states. We then obtain from Eq. (41),

$$f_r(t)=\sum_{\mathbf{k}} f_{\mathbf{k}}(t)(|a_{\mathbf{k}}^{1/2,3/2}|^2+|a_{\mathbf{k}}^{1/2,-3/2}|^2). \tag{44}$$

This relation implies the following physical picture. $f_{\mathbf{k}}$ is the probability to find a hole in a plane-wave state with momentum $\mathbf{k}$ when the hole is far away from any impurity. As the hole approaches an impurity, it induces the probability $|a_{\mathbf{k}}^{1/2,3/2}|^2+|a_{\mathbf{k}}^{1/2,-3/2}|^2$ to find the hole in a resonant state. Then the total probability f_r to find a hole in a resonant state is given by Eq. (44). Substituting Eq. (44) into Eqs. (40) and (42), we obtain the kinetic equation for $f_{\mathbf{k}}$:

$$\begin{aligned}\frac{\partial f_{\mathbf{k}}}{\partial t}+\frac{e\mathcal{E}}{\hbar}\frac{\partial f_{\mathbf{k}}}{\partial k_z}=&\frac{2\pi N_A V}{\hbar}\sum_{\mathbf{k}'}|t_{\mathbf{k}\mathbf{k}'}|^2\delta(E_{\mathbf{k}}-E_{\mathbf{k}'})(f_{\mathbf{k}'}-f_{\mathbf{k}})\\&+\frac{N_A V|t_{\mathbf{k}r}|^2\Gamma}{\hbar[(E_{\mathbf{k}}-E_0)^2+\Gamma^2/4]}\\&\times\left[\sum_{\mathbf{k}'}\frac{|t_{\mathbf{k}'r}|^2 f_{\mathbf{k}'}}{(E_{\mathbf{k}'}-E_0)^2+\Gamma^2/4}-f_{\mathbf{k}}\right]\\&+S(t)\Theta(\epsilon_0-E_{\mathbf{k}}),\end{aligned} \tag{45}$$

with the boundary condition $f_{\mathbf{k}}=0$ at $E_{\mathbf{k}}=\hbar\omega_0$.

Equation (45) will be solved numerically. We start with a guessed initial distribution and follow the evolution of the distribution function until it reaches a stationary solution. The collision integral can be conveniently calculated in terms of the two independent variables $E_{\mathbf{k}}$ and ϑ instead of $\mathbf{k}$, where ϑ is the angle between $\mathbf{k}$ and the z axis. Accordingly, we transform Eq. (45) to

$$\frac{\partial f_{\mathbf{k}}}{\partial t}+a(E_{\mathbf{k}},\vartheta)\frac{\partial f_{\mathbf{k}}}{\partial E_{\mathbf{k}}}+b(E_{\mathbf{k}},\vartheta)\frac{\partial f_{\mathbf{k}}}{\partial \vartheta}=I(E_{\mathbf{k}},\vartheta)+S_0(E_{\mathbf{k}},\vartheta,t), \tag{46}$$

where

$$\begin{aligned}a(E_{\mathbf{k}},\vartheta)=&\frac{e\mathcal{E}}{\hbar}\sqrt{\frac{\hbar^2}{2m_0}}\frac{1}{k(E_{\mathbf{k}},\vartheta)}\left(\frac{\partial k(E_{\mathbf{k}},\vartheta)}{\partial E_{\mathbf{k}}}\right)^{-1}\\&\times\left[k(E_{\mathbf{k}},\vartheta)\cos\vartheta+\frac{\partial k(E_{\mathbf{k}},\vartheta)}{\partial\vartheta}\sin\vartheta\right],\end{aligned}$$

$$b(E_{\mathbf{k}},\vartheta)=-\frac{e\mathcal{E}}{\hbar}\sqrt{\frac{\hbar^2}{2m_0}}\frac{\sin\vartheta}{k(E_{\mathbf{k}},\vartheta)}.$$

The explicit expressions of $I(E_{\mathbf{k}},\vartheta)$ and $S_0(E_{\mathbf{k}},\vartheta,t)$ can be easily obtained by straightforward substitutions.

The differential parts at the left-hand side of the above equation can be further simplified by introducing the variable $\tilde{E}_{\mathbf{k}}$ through the following relation using the functional dependence of $\mathbf{k}$ on $E_{\mathbf{k}}$ and ϑ,

$$k(\tilde{E}_{\mathbf{k}},\vartheta=\pi/2)=k(E_{\mathbf{k}},\vartheta)\sin\vartheta. \tag{47}$$

In terms of the pair of independent energy variables ($E_{\mathbf{k}}$ and $\tilde{E}_{\mathbf{k}}$), Eq. (45) becomes

$$\frac{\partial f_{\mathbf{k}}}{\partial t}+a(E_{\mathbf{k}},\tilde{E}_{\mathbf{k}})\frac{\partial f_{\mathbf{k}}}{\partial E_{\mathbf{k}}}=I(E_{\mathbf{k}},\tilde{E}_{\mathbf{k}})+S(E_{\mathbf{k}},\tilde{E}_{\mathbf{k}},t). \tag{48}$$

With only one coordinate derivative operator, this time-dependent integral differential equation can be solved with routine numerical procedure.

For p-Ge, the optical phonon energy is $\hbar\omega_0=36$ meV, and the characteristic frequency is $\nu_A=5\times10^{12}\,\mathrm{s}^{-1}$. In our calculation we have adopted the approximation of a single hole band, which is not unreasonable under experimental conditions. One can show that under such conditions, including the second band will only change the tail of the distribution, which is not important for the problem under consideration.

For given values of uniaxial pressure and electric-field strength, the distribution function $f_{\mathbf{k}}$ is calculated from Eq. (48). The so-derived results have been thoroughly analyzed in Ref. 5. Our theory gives the origin of population inversion that is required to explain the detected lasing from strained p-Ge.[4] To close this section, we will demonstrate the self-consistency of our calculation. If we set the pressure at 5 kbar and the electric field at $\mathcal{E}=300$ V/cm along the [111] direction, the calculated resonant level is at the energy $E_0=10$ meV and has a width $\Gamma=2$ meV. From Eq. (38) we obtain the source width $\epsilon_0=4.25$ meV, which is much less than the optical phonon energy 35 meV. Furthermore, from the numerical solution of the distribution function, we obtain the transient time about $\tau_{\mathcal{E}}\simeq5\times10^{-12}$ s, which is much longer than the lifetime $\hbar/\Gamma\simeq2\times10^{-13}$ s. Consequently, our calculation based on the condition that $\Gamma\tau_{\mathcal{E}}\gg\hbar$ is self-consistent.

VII. CONCLUSION

We have shown that acceptor impurities in uniaxially strained semiconductors can produce resonant states. There exists a threshold stress for the appearance of the lowest resonant state, and the threshold value can be calculated with high precision within the zero range potential model. In the high-stress region, via Dirac's approach and using the Coulomb potential for an acceptor impurity, we have obtained the energy and the width of a resonant state, the amplitude of resonant scattering, and the probability of coherent capture and emission of holes by resonant state.

The dispersion law and the density-of-states of the valence band are modified by the presence of resonant states. We have calculated the energy-dependent optical transition

probability between resonant states and localized impurity. We have also presented the detailed theoretical analysis of a mechanism for carrier population inversion induced by resonant states in strained semiconductors under an external electric field. This mechanism is the result of a coherent capture-emission type inelastic scattering of holes by resonant states. As a result of this population inversion, the recently observed lasing in THz frequency region from uniaxially strained *p*-Ge is finally understood.

APPENDIX A: DERIVATION OF TRANSITION PROBABILITY $W_{\mathbf{k}L}$

We consider the total Hamiltonian $\hat{\mathcal{H}}=\hat{H}_0+\hat{U}$ at the high-stress limit. Initially the eigenstate $\psi_{\mathbf{k}}^{(1/2)}(\mathbf{r})$ of the unperturbed Hamiltonian $\hat{H}_0$ is occupied by a hole. At time $t=0$ the interaction $\hat{U}$ is switched on.

The evolution of system is described by the time dependent Schrödinger equation

$$[\hat{H}_0+\hat{U}(t)]\Psi_{\mathbf{k}}(\mathbf{r},t)=i\hbar\frac{\partial\Psi_{\mathbf{k}}(\mathbf{r},t)}{\partial t}. \tag{B1}$$

The time-dependent solution of this equation

$$\Psi_{\mathbf{k}}(\mathbf{r},t)=\sum_{m'=\pm 3/2} a_{\mathbf{k}}^{(1/2,m')}(t)\varphi^{(m')}(\mathbf{r}) + \sum_{\mathbf{k}'m'=\pm 1/2} b_{\mathbf{k}'}^{(1/2,m')}(t)\psi_{\mathbf{k}\mathbf{k}'}^{(m')}(\mathbf{r}) \tag{B2}$$

is similar to Eq. (11), but with time-dependent coefficients $a_{\mathbf{k}}^{1/2,m'}(t)$ and $b_{\mathbf{k}\mathbf{k}'}^{1/2,m'}(t)$. The initial conditions are

$$a_{\mathbf{k}}^{(1/2,\pm 3/2)}=0; \quad b^{(1/2,m')}=\delta_{1/2,m'}\delta_{\mathbf{k},\mathbf{k}'} \tag{B3}$$

for $t\leqslant 0$.

The probability to find a hole in the localized impurity orbital $\varphi_{1s}^{(m')}(\mathbf{r})$ at time t is given by $|a_{\mathbf{k}}^{(1/2,m')}(t)|^2$. Substituting Eq. (B1) into Eq. (B2) and following the standard algebraic procedure, we obtain

$$|a_{\mathbf{k}}^{(1/2,3/2)}(t)|^2=\frac{|V_{\mathbf{k}}|^2}{[\varepsilon_l(\mathbf{k})-E_0]^2+\Gamma^2/4}\left[1+e^{-\Gamma t/\hbar}-2e^{-\Gamma t/2\hbar}\times\cos\left([\varepsilon_l(\mathbf{k})-E_0]\frac{t}{\hbar}\right)\right],$$

$$|a_{\mathbf{k}}^{1/2,-3/2}(t)|^2=\frac{|W_{\mathbf{k}}|^2}{(\varepsilon_l(\mathbf{k})-E_0)^2+\Gamma^2/4}\left[1+e^{-\Gamma t/\hbar}-2e^{-\Gamma t/2\hbar}\times\cos\left([\varepsilon_l(\mathbf{k})-E_0]\frac{t}{\hbar}\right)\right]. \tag{B4}$$

In the limit $t\to\infty$ these coefficients approach their stationary solutions $|a_{\mathbf{k}}^{(1/2,m)}|$ given by Eq. (15).

The total transition probability per unit time from the initial light-hole state $\psi_{\mathbf{k}}^{(1/2)}(\mathbf{r})$ to the degenerate localized impurity orbitals $(1s,m=\pm 3/2)$ is simply

$$W_{\mathbf{k}r}=\frac{\partial}{\partial t}[|a_{\mathbf{k}}^{(1/2,3/2)}(t)|^2+|a_{\mathbf{k}}^{(1/2,-3/2)}(t)|^2]. \tag{B5}$$

To study the long time ($\gg\tau=\hbar/\Gamma$) behavior of the system, we can average the transition probability over the time interval τ:

$$W_{\mathbf{k}r}=\frac{1}{\tau}\int_0^\infty dt\frac{\partial}{\partial t}[|a_{\mathbf{k}}^{(1/2,3/2)}(t)|^2+|a_{\mathbf{k}}^{(1/2,-3/2)}(t)|^2] = \frac{\Gamma}{\hbar}[|a_{\mathbf{k}}^{(1/2,3/2)}(\infty)|^2+|a_{\mathbf{k}}^{(1/2,-3/2)}(\infty)|^2-|a_{\mathbf{k}}^{(1/2,3/2)}(0)|^2 + |a_{\mathbf{k}}^{(1/2,-3/2)}(0)|^2]. \tag{B6}$$

Using the initial conditions [Eq. (B3)], we obtain Eq. (27),

$$W_{\mathbf{k}r}=\frac{\Gamma}{\hbar}[|a_{\mathbf{k}}^{(1/2,3/2)}(\infty)|^2+|a_{\mathbf{k}}^{(1/2,-3/2)}(\infty)|^2]. \tag{B7}$$

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