Inverted distributions of holes in size-quantized semiconductor films

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Theoretical investigations are reported of the energy spectrum of holes in a thin semiconductor film with a complex valence band of the type found in Ge and GaAs, and of the electrical conductivity of such a film in strong electric fields. It is shown that the presence of a cone of negative transverse heavy-hole masses results in crossing of the first two hole size-quantization subbands, which provides an opportunity for a population inversion of these subbands in strong electric fields and, consequently, a negative hf conductivity may be established in the film. In contrast to a bulk oscillator utilizing negative effective masses, this negative conductivity does not require the application of a magnetic field.

INTRODUCTION

The energy spectrum of holes in a film of a semiconductor with a diamond structure is calculated. It is shown that the presence of cones of negative transverse masses of heavy holes results in repeated crossing of the first two size-quantization subbands in the momentum space. The energy spectrum obtained in this case is shown qualitatively in Fig. 1, where $\hbar\omega_f$ is the energy of an optical phonon. The energy spectrum of holes in a film had been calculated earlier.[1,2] Crossing of the first two subbands was not predicted by these calculations, because the treatment in Ref. 1 ignored the corrugation of the constant-energy surfaces of the holes and the calculations reported in Ref. 2 were limited to small momenta.

Such crossing or intersection of the valence subbands occurs also in other cases, for example when a semiconductor is subjected to a quantizing magnetic field[3] or to uniaxial deformation.[4]

The application of a strong static electric field to a system with such a spectrum may invert the hole distribution. The physics of the process resulting in inversion is as follows. In the case of pure samples at low lattice temperatures the main mechanism of the scattering of "hot" holes (with the kinetic energy considerably higher than the lattice temperature) is spontaneous emission of optical phonons by these holes. Therefore, in the presence of an electric field the holes from both subbands acquire the optical-phonon energy, emit this phonon, and drop down to the minimum of the first subband. If there is no tunneling between the subbands, the second subband is always empty and in the range $k_0 < k < k_1$ (Fig. 1) there is no population inversion. For example, calculations showed that in the case of GaAs films of $\sim 10^{-6}$ cm thickness in fields of $\sim 10^3$ V/cm the probability of hole tunneling between the subbands during the time that a hole acquires an energy $\hbar\omega_f$ is less than 0.2 and the energy acquired by a hole exceeds the optical-phonon energy by less than $0.1\hbar\omega_f$. Therefore, these two factors have little influence on the distribution of the holes between the subbands and the population inversion is preserved.

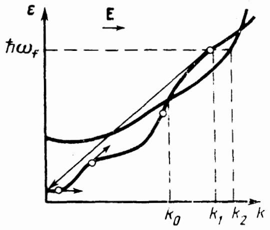

FIG. 1. Appearance of a population inversion of holes in a system with crossing valence subbands ($\hbar\omega_f$ is the energy of an optical phonon).

We shall use the approximation of an absolutely rigid "phonon lid" (implying instantaneous emission of an optical phonon by a hole whose energy reaches $\hbar\omega_f$) to calculate the small-signal conductivity of a film. We shall find the ranges of frequencies where a population inversion results in a negative conductivity.

This population inversion mechanism may apply also to other systems in which crossing of the energy terms is observed. An important example of a system which may exhibit a negative conductivity of this kind is a three-layer structure with variable thicknesses of the layers. A section through one variant of such a structure (GaAs–GaAlAs–GaAs) is shown in Fig. 2. We shall consider the specific case when size quantization occurs in the films, but this is not an essential condition. When electrons tunnel weakly in the transition region and when they flow from region B to a region A, a population inversion of the energy levels appears in the latter region. As in the preceding case, this may give rise to a negative conductivity of the structure.

SPECTRUM OF HOLES IN A FILM

The valence band of a semiconductor with the diamond structure (Ge, Si) is quadruply degenerate at the point in a momentum space characterized by $p = 0$. The behavior of holes near this point is described by the Luttinger Hamiltonian for a particle with spin 3/2 (Ref. 5), which can be represented in the form

$$H_L = \frac{1}{2m_0}\left\{\left[\gamma_1 + 2\gamma_2\left(2\delta + \frac{1}{2\delta}\right)\right]\mathbf{p}^2 - \frac{2\gamma_2 S^2 \mathbf{p}^2}{\delta}\right\}, \quad (1)$$

here m_0 is the mass of a free electron; $\mathbf{p}$ and $p_{x,y,z}$ are the

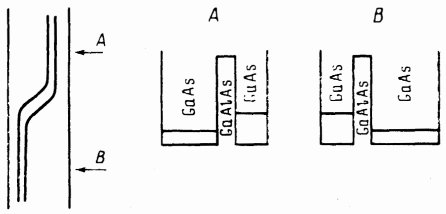

FIG. 2. Three-layer GaAs-GaAlAs-GaAs system.

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momentum operator and its projections along the principal axes of a crystal, selected as the Cartesian coordinate axes; **J** and $J_{x,y,z}$ are the operator of spin 3/2 and its projections along the same axes; $\gamma_{1,2,3}$ are dimensionless parameters which govern the dispersion laws of light (ε_l) and heavy (ε_h) holes in an unbounded crystal:

$$\varepsilon_{l,h}=(\hbar^2/2m_0)\{\gamma_1\mathbf{k}^2\pm2[\gamma_2^2\mathbf{k}^4+3(\gamma_3^2-\gamma_2^2)(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)]^{1/2}\}, \qquad (2)$$

$\mathbf{p}=\hbar\mathbf{k}$; $\delta=/\gamma_3/\gamma_2$; S is a quasihelicity operator which in the momentum space has the form

$$S={}^1/_6(13\delta-7)\varkappa\mathbf{J}+{}^2/_3(1-\delta)(\varkappa_xJ_x^3+\varkappa_yJ_y^3+\varkappa_zJ_z^3),\quad \varkappa=\mathbf{k}/k, \qquad (3)$$

i.e., S depends only on the direction of the momentum and is independent of its value. In the case of an isotropic model ($\delta=1$) the operator S represents the projection of the spin along the momentum, i.e., it represents the helicity. The operator S commutes with H_L. Therefore, in the case of an unbounded crystal the quasihelicity is conserved and the state of a hole is defined uniquely by the eigenvalues of **p** and S. Light holes have smaller absolute eigenvalues of S (in the isotropic model we have $S_l=\pm1/2$), whereas heavy holes have larger values (in the same isotropic model we find that $S_h=13/2$). When the direction of the three-dimensional momentum is altered (or reversed), the states of heavy and light holes become mixed. In particular, such a situation occurs in a film because holes are reflected from its boundaries. Therefore, the eigenstate of a hole in a film is generally a super-position of states of heavy and light holes.

We shall consider a homogeneous film of thickness d. We shall assume that it is cut at right-angles to the principal crystallographic axis z of a crystal and the coordinates of the boundaries are $z=\pm d/2$. The energy spectrum of holes in such a film is described by the Schrödinger equation with zero boundary conditions[6]:

$$H_L\psi_\nu=\varepsilon_\nu\psi_\nu,\qquad \psi_\nu(x,y,d/2)=\psi_\nu(x,y,-d/2)=0. \qquad (4)$$

In accordance with the symmetry of the system, the state of a hole in a film will be described by the following integrals of motion: the number of the size-quantization subband, the two-dimensional wave vector $\mathbf{k}_s$ (k_x, k_y) lying in the plane of the film, and the parity reflection by the $z=0$ plane. Using the momentum representation and the $|J,m_j\rangle$ basis (m_j is the projection of the spin along the z axis), we find that the Hamiltonian and the reflection operator in question are described by

$$H_L=\frac{\hbar^2}{2m_0}\begin{vmatrix} P & k_zL & M & 0\\ k_zL^* & R & 0 & M\\ M^* & 0 & R & -k_zL\\ 0 & M^* & -k_zL^* & P\end{vmatrix},$$

$$T_z=i\begin{vmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{vmatrix}O(z), \qquad (5)$$

where

$$P=\gamma_1\mathbf{k}^2+\gamma_2(\mathbf{k}_s^2-2k_z^2),\qquad R=\gamma_1\mathbf{k}^2-\gamma_2(\mathbf{k}_s^2-2k_z^2),$$

$$L=-2\sqrt{3}\gamma_3(k_y+ik_x),\qquad M=\sqrt{3}[\gamma_2(k_x^2-k_y^2)-2i\gamma_3k_xk_y]. \qquad (6)$$

The labeling of the rows from top to bottom and of the columns from left to right corresponds to $m_j=+3/2$, $+1/2$, $-1/2$, and $-3/2$. The operator $O(z)$ represents the substitution $z\to-z$ as a function of the coordinate or $k_z\to-k_z$ as a function of the momentum. Since $-T_z^2$ is a unit matrix, its eigenvalue are $T_z=\pm i$. The states with $T_z=i$ will be called even ($\psi^{(S)}$) and those with $T_z=-i$ will be called odd ($\psi^{(A)}$). They are transformed into one another by the coupling operator C: $\psi^{(A,S)}=C\psi^{(S,A)}$ (C represents a product of the operator of time reversal and of inversion, and in particular C reverses the spin of a hole). This relationship follows from the commutation of C with T_z. The $\psi^{(A)}$ and $\psi^{(S)}$ states differ in respect of the signs of the average values of the odd powers of J_z, whereas the even powers of J_z are the same and the odd powers of $J_{x,y}$ vanish. The commutation of H_L with T_z leads double degeneracy of the spectrum in respect of the parity. This degeneracy is lifted in the absence of the $z=0$ symmetry plane in a film, but it is still retained at the point $k_s=0$ (see, for example, Ref. 7).

The dispersion equation and the corresponding eigenfunctions of holes in a homogeneous film deduced from Eqs. (4) and (5) are of the following form

$$\operatorname{tg}(q_1/2)\operatorname{ctg}(q_2/2)=-f\pm(f^2-1)^{1/2}, \qquad (7)$$

$$\psi^{(A)}(\mathbf{k}_s,\mathbf{r})=e^{i\mathbf{k}_s\mathbf{r}}\times A\begin{vmatrix} i\tilde{L}\left\{q_1(\tilde{\varepsilon}_\nu-\tilde{R}_2)-q_2(\tilde{\varepsilon}_\nu-\tilde{R}_1)\operatorname{tg}\frac{q_2}{2}\operatorname{ctg}\frac{q_1}{2}\right\}\left(\sin\frac{q_1z}{d}-\frac{\sin(q_1/2)}{\sin(q_2/2)}\sin\frac{q_2z}{d}\right)\\ \left\{(\tilde{\varepsilon}_\nu-\tilde{P}_1)(\tilde{\varepsilon}_\nu-\tilde{R}_2)-|\tilde{M}|^2-q_1q_2\operatorname{tg}\frac{q_2}{2}\operatorname{ctg}\frac{q_1}{2}\right\}\left(\cos\frac{q_1z}{d}-\frac{\cos(q_1/2)}{\cos(q_2/2)}\cos\frac{q_2z}{d}\right)\\ i\tilde{L}\tilde{M}^*\left(q_1-q_2\operatorname{tg}\frac{q_2}{2}\operatorname{ctg}\frac{q_1}{2}\right)\left(\sin\frac{q_1z}{d}-\frac{\sin(q_1/2)}{\sin(q_2/2)}\sin\frac{q_2z}{d}\right)\\ \tilde{M}^*(\tilde{R}_1-\tilde{R}_2)\left(\cos\frac{q_1z}{d}-\frac{\cos(q_1/2)}{\cos(q_2/2)}\cos\frac{q_2z}{d}\right)\end{vmatrix}, \qquad (8)$$

where A is a normalization constant. The quantities $P_{1,2}$ and $R_{1,2}$ are equal to P and R with $k_z=k_z^{(1,2)}$:

$$\frac{\tilde{P}}{P}=\frac{\tilde{R}}{R}=\frac{\tilde{M}}{M}=\left(\frac{\tilde{L}}{L}\right)^2=\frac{d^2}{\gamma_2}=\frac{\tilde{\varepsilon}_\nu}{\varepsilon_\nu}\frac{\hbar^2}{2m_0},$$

$$k_z^{(1,2)}=\{-(\sigma^2-4-2\xi)\mathbf{k}_s^2+\tilde{\varepsilon}_\nu\sigma/d^2\pm2[\xi(\xi^2-\sigma^2+4)\mathbf{k}_s^4+\tilde{\varepsilon}_\nu^2d^{-4}+\xi\sigma\tilde{\varepsilon}_\nu\mathbf{k}_s^2d^{-2}+(\sigma^2-4)\xi k_x^2k_y^2]^{1/2}\}^{1/2}(\sigma^2-4)^{-1},$$

$$f=\{(\tilde{P}_2-\tilde{P}_1)(\tilde{R}_2-\tilde{R}_1)-|\tilde{L}|^2(q_1^2+q_2^2)\}/2|\tilde{L}|^2q_1^2q_2^2,$$

$$q_{1,2}=dk_z^{(1,2)},\qquad \sigma=\gamma_1/\gamma_2,\qquad \xi=3(\gamma_3^2/\gamma_2^2-1). \qquad (9)$$

Equation (7) defines an infinite set of two-dimensional subbands. It is equivalent to the expression obtained in Ref. 6 and in the isotropic case it reduces to a dispersion equation investigated in detail in Ref. 1.

The spectrum is simplest at $k_s = 0$ when, because of conservation (apart from the sign) of the direction of momentum of a hole reflected by the boundary of a film, there is no mixing of the states of heavy and light holes. We then have

$$\varepsilon^h(n_1)=\frac{1}{2m_h}\left(\frac{\hbar\pi n_1}{d}\right)^2, \quad \varepsilon^l(n_2)=\frac{1}{2m_l}\left(\frac{\hbar\pi n_2}{d}\right)^2, \quad n_1, n_2=1, 2, 3, \ldots \tag{10}$$

(m_h and m_l are the masses of heavy and light holes along the z axis). The projection of the spin along the z axis has a specific value and the coordinate and spin parts of the eigenfunctions of Eq. (8) are separable:

$$\psi^{(S,A)}(n_1^a) \sim \chi_{\pm 3/2} \cos\left(\frac{n_1^a \pi z}{d}\right), \quad \psi^{(S,A)}(n_1^s) \sim \chi_{\mp 3/2} \sin\left(\frac{n_1^s \pi z}{d}\right),$$
$$\psi^{(S,A)}(n_2^a) \sim \chi_{\mp 1/2} \cos\left(\frac{n_2^a \pi z}{d}\right), \quad \psi^{(S,A)}(n_2^s) \sim \chi_{\pm 1/2} \sin\left(\frac{n_2^s \pi z}{d}\right), \tag{11}$$

where $n_{1,2}^a$ are the odd and $n_{1,2}^s$ the even integers; χ_m is a spinor with an eigenvalue of the spin projection along the z axis amounting to m. In general ($k_s \neq 0$) the function of Eq. (8) are a mixture of the states of heavy and light holes and do not have a specific spatial parity (i.e., they are not even or odd functions of z).

Following Ref. 1, we shall denote the solutions of the dispersion equation (7) by $\varepsilon_n^{(j)}(\mathbf{k}_s)$, where the indices $j = l$, h, and $n = 1,2,\ldots$ identify the level into which a given subband transforms in the limit $k_s \to 0$. The subbands $\varepsilon_n^{(h)}(\mathbf{k}_s)$ with odd values of n and $\varepsilon_m^{(l)}(\mathbf{k}_s)$ with even values of m are described by the dispersion equation (7) with the minus sign in front of the root, whereas the subbands with even n and odd m are described by Eq. (7) with the plus sign in front of the root. The two signs in Eq. (7) correspond to two families of the dispersion surfaces $\varepsilon(\mathbf{k}_s)$. These two surfaces may intersect only if they belong to different families, i.e., intersecting surfaces should either have the same values of j and different parities of n and m, or different values of j and the same parity of n and m. Along the lines of intersection we have $k_z^{(1,2)} = \pi n_{1,2}/d$, where n_1 and n_2 are integers of the same parity. These lines (and the values of $\mathbf{k}_s$ and ε) can be found easily since they are identical with the corresponding lines of intersection of auxiliary surfaces governed by the dispersion relationships of the type (2) with $k_z = \pi n_{1/2}/d$. However, the common lines of intersection in the case of the auxiliary and dispersion surfaces does not allow us to deduce unambiguously the qualitative shape of the latter from the former, contrary to the isotropic model of Ref. 1. Breakdown of the procedure of Ref. 1 for determination of the nature of the dispersion surfaces occurs at the lines of intersection of the auxiliary heavy-hole surface with one another, which occurs because they have cones of negative transverse masses.[8] These intersections do not occur when the dispersion law is isotropic ($\delta = 1$).

Figure 3 shows the auxiliary and dispersion cures of holes in a film of germanium, plotted for the [100] and [110] directions to illustrate the above discussion. Features

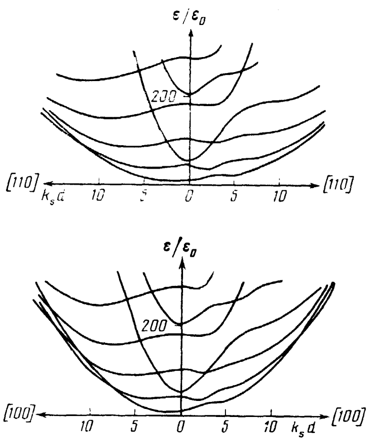

FIG. 3. Sections across auxiliary (to the left of the ordinate) and dispersion (to the right of the ordinate) surfaces of holes in a film of Ge along the [110] and [100] directions in the wave-vector space; $\varepsilon_0 = \hbar^2\gamma_2/2m_0d^2$.

which distinguish these curves from those of a bulk sample, mentioned earlier also in Refs. 1 and 2, are a strong nonparabolicity of the spectrum, appearance of additional energy extrema and of regions of negative longitudinal and transverse effective masses, and crossing of the subbands. Multiple (double in Fig. 1) crossing of the first and second size-quantization subbands, formally related to single intersection of all the auxiliary surfaces of heavy holes with one another, is a new feature most important from the point of view of realization of the inverted hole distributions. Figure 4 shows the difference $\varepsilon_2^{(h)}(\mathbf{k}_s) - \varepsilon_{-1}^{(h)}(\mathbf{k}_s = \Delta\varepsilon(\mathbf{k}_s)$ of the energies of the second and first subbands plotted as a function of k_x. We shall show later that an important feature for the realization of a negative differential conductivity (NDC) of a film is the presence of a minimum of the difference $\Delta\varepsilon(\mathbf{k}_s) = -\hbar\omega_0$ in the negative range of its values.

TUNNELING OF HOLES BETWEEN TWO-DIMENSIONAL SUBBANDS IN AN ELECTRIC FIELD

We shall now consider the behavior of a hole in a static electric field $\mathbf{E}$ directed along the film. This electric field alters the two-dimensional wave vector of a hole state and also a set of directions of three-dimensional momenta, which (because of inertia of the spin vector) generally alters the quasihelicity, i.e., it gives rise to transitions between the size-quantization subbands. The parity of the states introduced above is thereby preserved, confirming the convenience of the selected wave-function basis.

We shall find the probability of tunneling of a hole

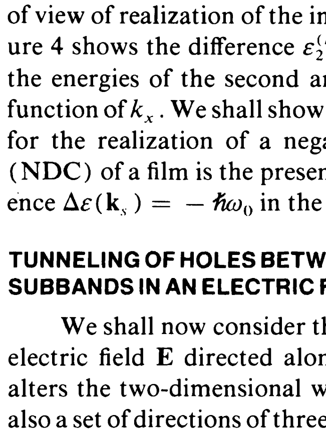

FIG. 4. Dependence of the difference between the energies of the first and second hole size-quantization subbands in a Ge film of k_x: the continuous curve corresponds to $k_y = 0$ and the dashed curve to $k_x = k_y$.

between the first and second subbands and ignore the influence of the other subbands. We shall assume that at the initial moment $t = 0$ a hole is located in the upper subband near its minimum characterized by a wave vector $\mathbf{k}_s = \mathbf{k}_s^0$. At an arbitrary subsequent moment of time t the wave function of a hole can be represented by

$$\psi^{(A,S)}(k', r, t) = \sum_{j=1}^{2} \int dk_E \, a_j^{(A,S)}(\mathbf{k}_s) \psi_j^{(A,S)}(\mathbf{k}_s, r) \delta(k_E - k_E^0 - eEt), \quad (12)$$

where j is the number of the two-dimensional subbands; k_E and k' are the components of $\mathbf{k}_s$ parallel and perpendicular to E. Substituting Eq. (12) into the secular Schrödinger equation, we obtain two systems of two equations for $a_j^{(A,S)}$:

$$i \frac{da_1^{(\lambda)}}{dk_E} + \left(\frac{i\varepsilon_1}{eE} + x_{11}^{(\lambda)} \right) a_1^{(\lambda)} + x_{12}^{(\lambda)} a_2^{(\lambda)} = 0,$$
$$i \frac{da_2^{(\lambda)}}{dk_E} + \left(\frac{i\varepsilon_2}{eE} + x_{22}^{(\lambda)} \right) a_2^{(\lambda)} + x_{21}^{(\lambda)} a_1^{(\lambda)} = 0 \quad (13)$$

with the boundary condition $a_1^{(\lambda)}(\mathbf{k}_s^0) = 1$, $a_2^{(\lambda)}(\mathbf{k}_s^0) = 0$, $\lambda = A,S$. The index h and the argument $\mathbf{k}_s$ in Eq. (13) are omitted for the sake of simplicity. The quantities $x_{ij}^{(\lambda)}$ are related to the matrix elements of the projection of the radius vector $\mathbf{r}$ along E:

$$\langle j, \mathbf{k}_s', \lambda | r_E | \lambda, \mathbf{k}_s, i \rangle = -i\delta_{ij} \frac{\partial}{\partial k_E} \delta(\mathbf{k}_s - \mathbf{k}_s') + x_{ji}^{(\lambda)} \delta(\mathbf{k}_s - \mathbf{k}_s'). \quad (14)$$

Figure 5 gives the probability of the tunneling of a hole in a Ge film from the first to the second subband in the course of its motion from $k_E = 0$ to $k_E = 17/d$ in a field $\mathbf{E} \| [100]$ plotted as a function of k_y when $\tilde{E} = 2m_0 d^3 eE / \gamma 2\hbar^2 = 10$ and as a function of $\tilde{E}$ for $k' = 0$, deduced by numerical solution of Eq. (13). In the case of a film with $d = 250$ Å in a field $E \leqslant 10^3$ V/cm the tunneling probability is $\lesssim 0.1$, i.e., it is low. The tunneling probability depends on the sign of the mixed product $\mathbf{k}_s \cdot [\mathbf{E} \times \langle \mathbf{J} \rangle]$, i.e., if $k' \neq 0$ it depends on the parity of the state because the matrix element $x_{ij}^{(\lambda)}$ is parity-dependent. If $k' = 0$, the probability is independent of the parity.

Figure 6 shows the dependences of the hole tunneling probability on the value of k_E in the final state obtained for $\tilde{E} = 4$ and 10 (when the initial value is $k_E = 0$). Clearly, the tunneling occurs mainly in the vicinity of the first minimum of $\Delta\varepsilon$ (Figs. 1 and 4). A hole passes practically without tunneling across the subband crossing region and this is decisive for a population inversion. The nonmonotonic dependence of the tunneling probability on k' is related mainly to the nonmonotonic dependence of the first minimum $\Delta\varepsilon$ on the direction of $\mathbf{k}_s$.

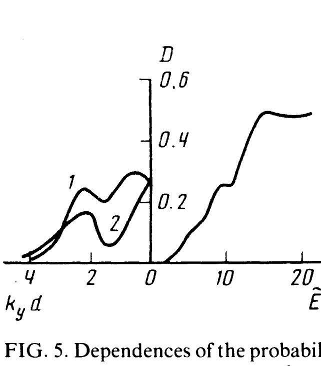

FIG. 5. Dependences of the probability of the tunneling of a hole from the first to the second subband on k_y ($\tilde{E} = 10$) and $\tilde{E}$ ($k_y = 0$) during the motion from $k_x = 0$ to $k_x = 15^{-1}$: 1) even states; 2) odd states.

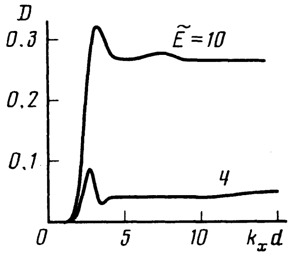

FIG. 6. Dependences of the probability of the tunneling of a hole from the first to the second subband on the final value of k_x; the initial value is $k_x = 0$ ($k_y = 0$), $\mathbf{E} \| [100]$.

INVERTED DISTRIBUTIONS OF HOLES

We shall find the distribution of holes between the subbands in a strong electric field. We shall assume that the film is pure and that its lattice temperature is at absolute zero. As pointed out already, the main hole scattering mechanism is then spontaneous emission of optical phonons. Therefore, the holes from the subbands are accelerated by an electric field and acquire a momentum $k_{1,2}$ (Fig. 1) corresponding to the optical phonon energy $\hbar\omega_f = \varepsilon_{1,2}(k_{1,2})$ and then instantaneously (in the rigid phonon lid approximation) emit an optical phonon and are scattered to the minimum of the first subband characterized by $\mathbf{k}_s = 0$. This creates needle-shaped distributions of holes elongated along the field E (Ref. 9):

$$f_1(\mathbf{k}_s) \approx \frac{4\pi^2 nd}{k_1} [1 - D(k_E)] \theta(k_E) \theta(k_1 - k_E) \delta(k'),$$
$$f_2(\mathbf{k}_s) \approx \frac{4\pi^2 nd}{k_1} D(k_E) \theta(k_E) \theta(k_2 - k_E) \delta(k'), \qquad |k_1 - k_2| \ll k_1, \quad (15)$$

where n is the density of holes averaged over the film thickness and $D(k_E)$ is the probability (averaged over the parity) of the tunneling of a hole characterized by $k' = 0$ from the first to the second subband as it moves from $k_E = 0$ to k_E. Hence, as pointed out above, the tunneling is negligible in the subband crossing region and it follows that the function $f_{1,2}$ is practically independent of k_E in the interval $(k_0, k_{1,2})$. If $D(k_1) < 1/2$, which is easily satisfied, then the populations of the subbands are inverted in the interval (k_0, k_1). In the case of small values of D of interest to us the nondiagonal elements of the density matrix play no significant role and we shall therefore ignore them.

If $D > 1/2$, an inversion appears at $k < k_0$ after the first minimum of $\Delta\varepsilon$ (where strong tunneling occurs). This is an interesting case but it is difficult to achieve and we shall not consider it any further.

In reality the phonon lid is not absolutely rigid and holes penetrate this lid to a depth $\delta\varepsilon$ in excess of the energy of an optical phonon before emitting such a phonon. If this penetration is slight ($\delta\varepsilon < \varepsilon_{2\min} - \varepsilon_{1\min}$), so that after scattering a hole drops only to the first subband, and the result is simply swelling of the needle-like distribution and it can be allowed for approximately by making the substitution $\delta(k') \rightarrow \theta(k_1^2 s^2 - k'^2)/2k_1 s$ in Eq. (14); here s represents the dimensionless width of the hole distribution function in a plane perpendicular to **E**. An increase in s activates a third subband (which is the first light-hole subband) and we then have an equally interesting opportunity for a population inversion relative to the fourth subband (which is the third heavy-hole subband).

CONDUCTIVITY OF A FILM

We shall now consider the small-signal hf conductivity of a film in the presence of a strong static electric field **E**. For simplicity, we shall ignore the influence of this field on the photon emission and absorption processes.

An inversion of the subband populations in the region (k_0,k_1) is insufficient for a negative electrical conductivity in the frequency range $(0,\omega_0)$, since regions with a noninverted population $(0,k_0)$ absorb photons of these frequencies. The resultant sign of the conductivity depends on the relative values of the matrix elements of transition between the subbands, on the coordinate operator **r**, on the density of states, and on the intrasubband conductivity. Because of the alternating sign of the longitudinal and transverse effective masses of a hole, this intrasubband conductivity may also be both positive and negative. The frequency ω_0 corresponding to an infinite one-dimensional density of states is special in this context.

In this approximation the real part of the conductivity of a film averaged over its thickness is described by

$$\sigma_{\alpha\alpha}(\omega)=\frac{\pi\omega e^2}{d}\int d^2k_s|\tilde{r}_\alpha|^2\{\delta(\varepsilon_2-\varepsilon_1-\hbar\omega)-\delta(\varepsilon_1-\varepsilon_2-\hbar\omega)\}$$

$$(f_1-f_2)+\ \delta_{\alpha y}\frac{e^2nd}{\omega\hbar^2k_1}\int d^2k_s\sin\left(\frac{\omega}{\omega_E}\frac{k_E}{k_1}\right)\left(\frac{\partial^2\varepsilon_1}{\partial k'^2}f_1+\frac{\partial^2\varepsilon_2}{\partial k'^2}f_2\right)$$

$$=\sigma^{bs}_{\alpha\alpha}+\sigma^{is}_{\alpha\alpha},\quad k_2-k_1\ll k_1, \tag{16}$$

where we find from Eq. (14) that

$$\tilde{r}_\alpha\delta(\mathbf{k}_s-\mathbf{k}_s')=\int\psi_1^*(\mathbf{k}_s,r)r_\alpha\psi_2(\mathbf{k}_s',r)\,d^3r,\quad \omega_E=eE/\hbar k_1,$$

σ^{bs} and σ^{is} represent the components of the real part of the superconductivity due to transitions between subbands and inside a subband; $\alpha=x,y,z$. The contribution to σ^{bs}_{zz} comes from transitions between states of different parity, whereas the contributions to σ^{bs}_{xx} and σ^{bs}_{yy} are due to transitions between states of the same parity. The finite values of $\tilde{r}_\alpha$ are independent of the parity of states.

Substituting Eq. (15) into Eq. (16), assuming that the phonon lid is absolutely rigid, and using a tunneling coefficient $D(k_E)=\text{const}$ (as pointed out already, D depends strongly on k_E only near the first minimum where $\varepsilon_2-\varepsilon_1$), we find that the dimensionless conductivity because of transitions between the subbands (intersubband conductivity) is given by

$$\tilde{\sigma}^{bs}_{\alpha\alpha}(\omega)=\frac{\hbar k_1}{\pi nde^2(1-2D)}\sigma^{bs}_{\alpha\alpha}(\omega)$$

$$=\frac{\hbar\omega}{d}\left\{|\tilde{r}_\alpha|^2\left|\frac{d(\varepsilon_2-\varepsilon_1)}{dk_E}\right|^{-1}_{k_E=k_3}-|\tilde{r}_\alpha|^2\left|\frac{d(\varepsilon_2-\varepsilon_1)}{dk_E}\right|^{-1}_{k_E=k_4}\right\}, \tag{17}$$

where k_3 and k_4 obey the relationship $\Delta\varepsilon(k_3)=-\Delta\varepsilon(k_4)=\hbar\omega$. Figure 7 shows the dimensionless conductivity of a film of Ge of thickness $d=300$ Å subjected to a field $\mathbf{E}\|[100]$ calculated using Eq. (16) ($k_1d=15$, $\omega_0\approx1.2,\times10^{12}$ rad/s). In this case we find that (in the cgs esu system)

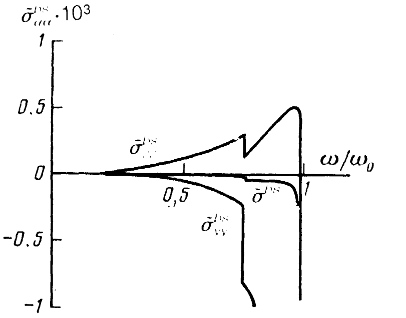

FIG. 7. Frequency dependences of the conductivity between subbands in a Ge film with $d=300$ Å, $\mathbf{E}\|[100]$.

$$\sigma_{\alpha\alpha}^{bs}\approx4.4\cdot10^{-4}(1-2D)n\tilde{\sigma}_{\alpha\alpha}^{bs}. \tag{18}$$

In view of the one-dimensional nature of the motion of a hole ($s=0$), we find that $\sigma^{bs}_{\alpha\alpha}\to-\infty$ in the limit $\omega\to\omega_0$. for a hole distribution of finite widths ($s\neq0$) the conductivity $\sigma^{bs}_{\alpha\alpha}$ is everywhere finite (when the influence of a static electric field on the process of phonon emission is allowed for, it is found that $\sigma^{ba}_{\alpha\alpha}$ is finite even when $s\to0$). In the case of the Ge film under discussion we find that the values of the conductivity components at $\omega=\omega_0$ are given by [the dimensions of the quantities in Eqs. 1(90), (20), (22), and (23) are the same as in Eq. (18)]:

$$\begin{aligned}\sigma_{xx}^{bs}&\approx5{,}0\cdot10^{-8}(0{,}8-s^{-1})(1-2D)n,\\ \sigma_{yy}^{bs}&\approx2{,}3\cdot10^{-6}(0{,}9-s^{-1})(1-2D)n,\\ \sigma_{zz}^{bs}&\approx2{,}8\cdot10^{-7}(23-s^{-1})(1-2D)n.\end{aligned} \tag{19}$$

These expressions are useful for estimating the order of magnitude of the negative conductivity. It is clear from them that in the case of a wide hole distribution function (large values of s) the negative conductivity is not observed. The discontinuities of $\tilde{\sigma}^{bs}_{\alpha\alpha}$ in Fig.7 correspond to the onset of phonon emission from holes with a wave vector $k_E=k_1$.

Figure 8 gives the value of $\sigma^{bb}_{\alpha\alpha}$ calculated for a Ge film of thickness 350 Å in a field $\mathbf{E}\|[110]$ ($k_1d=23.3$). In this case we have $\omega_0\approx3.5\times10^{11}$ rad/s, $\Delta\varepsilon(k_1)=\hbar\omega_0$, and

$$\sigma_{\alpha\alpha}^{bs}\approx5{,}0\cdot10^{-4}(1-2D)n\tilde{\sigma}_{\alpha\alpha}^{bs}. \tag{20}$$

The quantity $\tilde{\sigma}_{11}$ in Fig. 8 denotes the dimensionless conductivity along **E**, i.e., along [110], whereas σ_{22} is the conductivity along [$1\bar{1}0$], i.e., at right-angles to **E**.

There are contributions to the conductivity σ_{yy} (σ_{22}) from intrasubband motion of holes, which is in contract to σ_{xx} (σ_{11}) and σ_{zz}. The conductivity averaged over the thickness of the film, calculated in the approximation $s\to0$ and $D\to0$ is

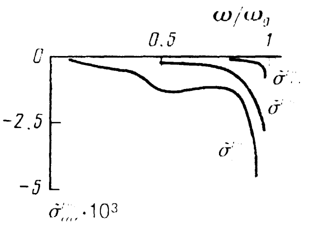

FIG. 8. Frequency dependences of the conductivity between subbands for a Ge film with $d=350$ Å, $\mathbf{E}\|[110]$.

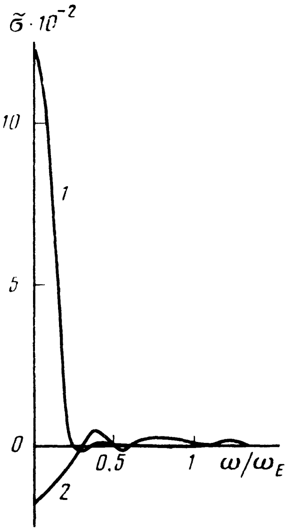

FIG. 9. Frequency dependence of the intrasubband conductivity of a Ge film: 1) E||[110]; 2) E||[100].

$$\sigma_{yy}^{A} = \frac{e^2\gamma_2 n}{2m_0 d k_1 \omega_E}\tilde{\sigma}\left(\frac{\omega}{\omega_E}\right),$$
$$\tilde{\sigma}(x) = \frac{2m_0 d}{\gamma_2 \hbar^2 x}\int_0^{k_1} \frac{\partial^2 \varepsilon_1}{\partial k'^2}\bigg|_{k'=0} \sin(x k_E d)\, dk_E. \qquad (21)$$

Figure 9 shows the dependence $\tilde{\sigma}(\omega/\omega_E)$ for two Ge films with the parameters given above. In the case when **E**||[100], we have

$$\sigma_{yy}^{A} \approx 3.3\cdot 10^7 \frac{n}{\omega_E}\tilde{\sigma}\left(\frac{\omega}{\omega_E}\right), \qquad (22)$$

whereas for **E**||[100], we obtain

$$\sigma_{yy}^{A} \approx 2.4\cdot 10^7 \frac{n}{\omega_E}\tilde{\sigma}\left(\frac{\omega}{\omega_E}\right). \qquad (23)$$

A numerical analysis shows that the y polarization of an alternating field (σ_{yy}) in the case when **E**||[100] and the z polarization (σ_{zz}) in the case when **E**||[100] are the most favorable configurations for NDC of Ge. The former case corresponds to higher frequencies.

The estimates given for Ge can also be applied to GaAs, since the case of these two materials the ratios γ'_1/γ'_2 and γ'_3/γ'_2 are similar and they determine the following dimensionless quantities: the spectrum of holes, the conductivity, and the tunneling probability. However, $\gamma_2'^{(\mathrm{Ge})}/\gamma_2'^{(\mathrm{GaAs})} = 1.8/1$ and the energies of optical phonons are approximately the same. Therefore the corresponding dimensional thickness and conductivity of a GaAs film are 1.8 times less than for Ge.

Our analysis demonstrates that thin semiconductor films may exhibit a new mechanism for an inversion of the distribution of holes as a result of crossing a size-quantization subbands. Under certain conditions this may give rise to a negative hf conductivity. The magnitude and the frequency dispersion of this negative conductivity can be controlled by altering the shape and magnitude of the potential well represented by the film.

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