Effect of quantization on electrical-reflection spectra in the surface region of a semiconductor

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Singularities associated with the effect of size quantization on interband optical transitions in the region of the space charge of a semiconductor were observed for the first time in the electrical-reflection spectra for germanium.

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In sufficiently thin layers of a space charge, whose thickness is comparable with the wavelength of mobile carriers, the motion of these carriers is quantized in the direction perpendicular to the surface. This leads to the formation of two-dimensional surface subbands. Duke[1] developed a theory of optical transitions to the state of such a size-quantized band according to which the electric field of a space charge introduces a series of broadened steps into the dependence of the absorption coefficient on the frequency as a result of interband transitions. Each of these steps is described by a spectral function $G(\omega, E_n)$ for spherical bands of the form

$$G(\omega, E_n) \approx \frac{2}{\pi}(r_m E_n)\int_0^{\hbar\omega - E_g - E_n}\frac{E^{1/2}dE}{(E + r_m E_n)^2}$$

$$= \frac{2}{\pi}\left[\arctan\left(\frac{\hbar\omega - E_g - E_n}{r_m E_n}\right)^{1/2} - \frac{[r_m E_n(\hbar\omega - E_g - E_n)]^{1/2}}{\hbar\omega - E_g - E_n + r_m E_n}\right], \qquad (1)$$

where E_n is the energy of the nth quantum level, E_g is the width of the forbidden band, $\hbar\omega$ is the quantum energy, and $r_m = m_c/m_v$ or m_v/m_c in the case of quantization of the conduction band or of the valence band, respectively.

The reduced density of states, which is responsible for the interband optical transitions, can be written in this case as a relation:

$$\rho_{cv}(\omega, E_n) \sim \sum_n G(\omega, E_n)\, H(\hbar\omega - E_g - E_n), \qquad (2)$$

where $H(\hbar\omega - E_g - E_n)$ is a unit step function.

We can see in Eq. (1) that the reduced density of states consists of sharp steps as $r_m \to 0$, which are smoothed out as a result of increasing r_m. Figure 1 shows reduced density of states for germanium for different ratios of the effective masses of charge carriers which can participate in the interband transitions at the center of the Brillouin

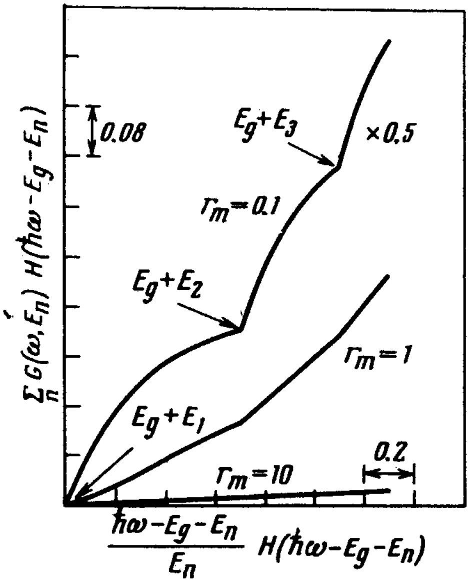

FIG. 1. Reduced density of states with allowance for quantization of the different ratios of the effective masses r_m.

zone, with allowance for quantization in the space-charge region (SCR). If a conduction band is quantized, then r_m will be equal to 0.1 and 1 for the transitions from the band of heavy and light holes, respectively; if, however, a valence band is quantized, then r_m will be equal to 10 and 1 for the same transitions. We can see that for photon energies of $E_g + E_n$ the reduced density-of-states function clearly shows the presence of singularities at $r_m = 0.1$; these singularities are less clearly evident at $r_m = 1$ and disappear entirely at $r_m = 10$. Weakly manifested singularities such as those in the

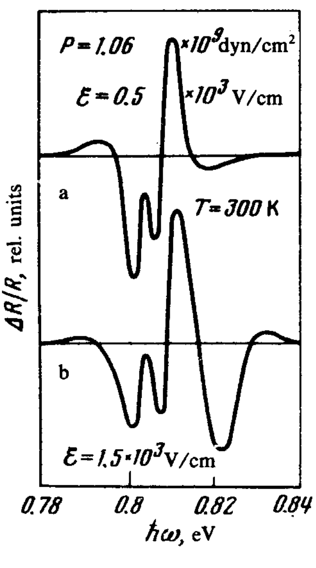

FIG. 2. (a) ER spectrum for germanium produced as a result of uniaxial deformation of the sample and (b) ER spectrum for the Schottky barrier in the presence of quantization.

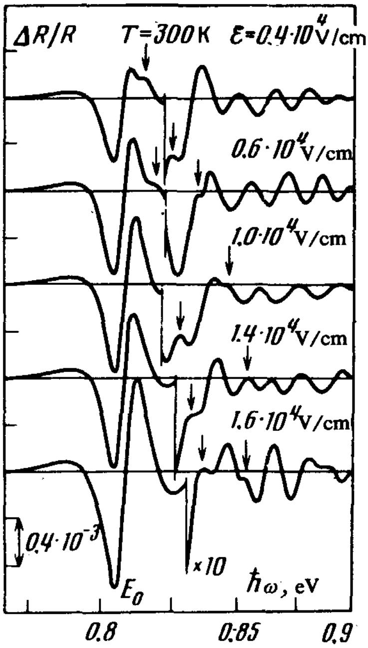

FIG. 3. ER spectra for a Schottky barrier in germanium for different values of the field in the SCR. The arrows indicate the locations of additional singularities.

case of $r_m = 1$ can be enhanced and can probably be recorded experimentally by using a differential electrical-reflection (ER) technique.

A convenient object of investigation for this purpose is the Schottky germanium barrier which has a tunnel-thin, natural oxide layer under the metal layer of thickness capable of having quantum levels, and which has minority carriers that can filter through this layer without shielding the electric field. Such samples have a highly uniform electric field at the level of formation of a reflected ray of light, an important factor for recording high-quality ER spectra, since the singularities in the spectra are smoothed out in a nonuniform field and hence become indiscernible.[2] The experimental technique and preparation of the samples were described elsewhere.[3]

Good Schottky barriers can be obtained in *n*-Ge, and the bands in the SCR can be bent only in the direction of depletion, i.e., we could quantize only the valence band. It seems that the degeneracy of the bands of light and heavy holes at $\mathbf{k} = 0$ in this case must be eliminated. To demonstrate that degeneracy can be eliminated, we compared one of our spectra, obtained for small fields (Fig. 2b), with the ER spectrum obtained as a result of uniaxial deformation of the sample, which latter fully eliminated the degeneracy (Fig. 2a).[4] We can see that the main peak in our spectrum at $E_g = 0.8$ eV, is split into two peaks, just as in the spectrum with a uniaxial deformation. We should note that the levels, which are separated from each other by an amount that is smaller by a factor of four than the value kT, are fairly well resolved. If the electric field strength is increased, then the strain needed to eliminate the degeneracy must be increased and the singularities associated with quantization will be shifted in the direction of higher energies. Figure 3 shows the ER spectra produced as a result of increasing the electric field strength, in which there is evidence of motion of these singularities (indicated by arrows). As a result of removal of the degeneracy at the point $\mathbf{k} = 0$, the effective masses of the bands of light and heavy holes are shifted in a complicated way and become different from their bulk values. The search for the effective masses in the quantization of the "undulating" hole bands so far has not produced any results. Therefore, if the electric field strength in the spectra is known and the triangular potential-well model is used, we can show that the energies of the singularities in the spectra coincide with the energy locations of the first two levels of the band with an effective mass of $(0.04 \pm 0.01)m_0$. This value of the effective mass will coincide with good accuracy with the volume mass of the band of light holes, if we approximate the constant-energy surfaces by using average spheres. It should be noted that the second singularity in the spectrum with $\vec{\mathscr{E}} = 1.6 \times 10^4$ V/cm was not shifted as much as the calculation indicates. This may be attributed to the fact that the potential well expands faster than the triangular well, a factor that was used in the calculation.

The vibration periods in the ER spectra and the type of "beats" observed in them are sensitive functions of the reduced masses of the bands of light and heavy holes and of their ratios.[3] We can see that the vibrating parts in the spectra, beginning with $\vec{\mathscr{E}} = 1.4 \times 10^4$ V/cm, change their shape sharply, indicating that the masses of the bands of light and heavy holes change. There was no evidence for the existence of singularities associated with the transitions from the quantized band of heavy holes, since we can see in Fig. 1 that the reduced density-of-states function has no singularities at $r_m = 10$. Moreover, to resolve the quantum levels in the ER spectra, the distance between them must be larger than the uncertainty introduced by the electric field into the energy levels, $\hbar\theta = (e^2\mathscr{E}^2\hbar^3/2\mu_{\parallel})^{1/3}$, where $\vec{\mathscr{E}}$ is the electric field strength and $\mu_{\parallel}$ is the reduced mass in the direction of the electric field. This condition is satisfied for the band of light holes but not for the band of heavy holes.

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