ing Letter, derives criteria for the assignment of the peaks to parabolic or saddle-point edges, confirming the early expectation[1] that the field-induced change in the density of states at critical points introduces a new parameter into band-structure analysis, which discriminates between these two types of transitions.

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OPTICAL-FIELD EFFECT ON THRESHOLDS, SADDLE-POINT EDGES, AND SADDLE-POINT EXCITONS

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Modulation of the potential barrier inside the reflecting surface of a semiconductor by means of an electric field[1-3] yields a phase-correlated reflectance response in the form of peaks and dips on the wavelength scale approximately 0.02 eV wide. The purpose of this note is to examine theoretically various mechanisms that may contribute to the observed lines and argue that three of these proposed mechanisms are present in Si in the narrow spectral range 3.35-3.50 eV.

The simplest mechanism is the modification of a direct absorption threshold by the electric field of the surface potential barrier. Although this Franz-Keldysh effect[4-7] is usually observed in transmission only,[8] the correlating reflectance effect is seen as a strong, narrow dip in $\Delta R/R$ at the 0.8-eV direct threshold in Ge.[9,10] Although the dominant effect is a shift of the edge with field because of photon-assisted tunneling, field enhancement of $\Phi(r_e-r_h)$ at $r_e=r_h$ also contributes enhanced absorption above the edge.[6] The center of the observed reflectance dip agrees with the direct magneto-optic edge[11] to within 0.005 eV.

Interband energy surfaces which contribute a saddle-point edge to ϵ_2 at $\omega=\omega_c$ may also exhibit a field effect. In general, one calculates $\Delta\epsilon_2$, the field-induced change of the imaginary part of the dielectric constant, rather than the change in n or k, and relates this to the experimentally observed quantity $\Delta R/R$ through the Kramers-Kronig integral. Confining ourselves to the neighborhood of the stationary point, we can then prove[12] the following duality theorem for the effect of an electric field F on simple nondegenerate M_1-type[13] saddle-point edges compared to parabolic thresholds when F is parallel to the principal axis of the isoenergetic saddle-point cone. The change in the former is obtained from the corresponding change in the latter by reversing the signs of $(\omega-\omega_c)$ and $\Delta\epsilon_2$. Thus, near an M_1-saddle-point edge ϵ_2 is decreased and the edge itself is shifted to higher frequencies by F.

We illustrate this theorem in Fig. 1(a) for

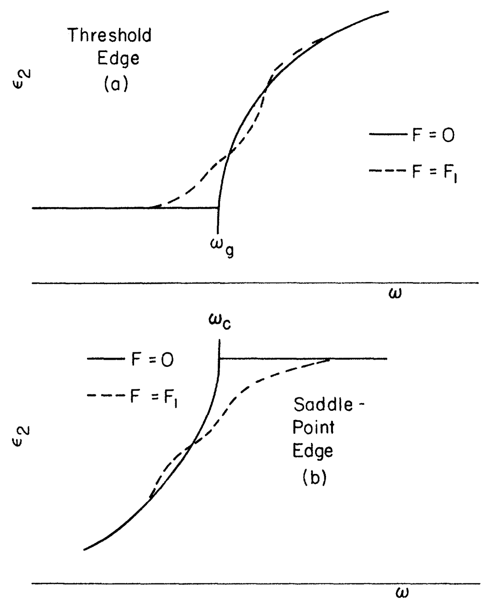

FIG. 1. (a) Sketch of the effect of an electric field F on an interband threshold. For Si at $F = 10^5$ V/cm the period of the oscillations above the edge is about 0.04 eV. (b) Similar to (a), but for a saddle-point edge at $\omega = \omega_c$ with F parallel to the principal axis.

thresholds and Fig. 1(b) for saddle-point edges. The sketches of ϵ_2 with $F = 0$ and $F = F_1 > 0$ are based on numerical evaluations (not asymptotic expansions) of the integrals over Airy functions which arise in computing oscillator strengths near either edge.[4-7] The oscillatory behavior (a) above or (b) below the edge is a consequence of semiclassical quantization of the wave-packet action.[7]

Because of different background levels and different ratios ϵ_2/ϵ_1 near the edge, the two reversals in sign of $\Delta\epsilon_2$ will in general not cancel each other completely in computing $\Delta R/R$. Whether a peak or a dip is observed —signifying by the sign the phase relation between reflectance response and modulating field—will depend upon the ratio of the imaginary to the real part of the dielectric constant and must be determined by separate analysis for every material.[14]

More complex situations arise when F is not parallel to the principal axis or when several bands are degenerate at the saddle point so that the isoenergetic surface passing through it consists of several cones.[13] Then introducing the interband energy E_t transverse to F, one can see that $(\omega_c - \omega - E_t/\hbar)$ changes sign in the neighborhood of the saddle point when ω is near ω_c. This yields a field effect which is a mixture of the parabolic and simple saddle-point effects. The extent of the mixing —e.g., whether the edge shifts to higher or lower energies—depends on μ_l/μ_t, where μ is an appropriate interband mass. Qualitatively, however, we note that pronounced dependence of $\Delta R/R$ on the orientation of F certainly requires saddle-point rather than parabolic interband energy surfaces. Moreover, with simple hyperbolic surfaces the magnitude of the field effect should be largest when F is parallel to the principal axis of at least one saddle-point edge.

In both diamond and silicon the direct threshold is expected to occur near $\Gamma_{25'} \rightarrow \Gamma_{15}$. Neglecting spin-orbit splitting, the interband energy surfaces are sixfold degenerate and clusters of critical points may arise not only at but also near Γ along symmetry axes.[15] In discussing this structure theoretically and also in considering the reflectance[16] of natural diamond surfaces at 80 and 300°K, one of us proposed[17] that a strong exciton was present below this edge in diamond, and that a similar exciton could be expected in Si. It was also noted that a threshold was expected near Γ and that in Si it should be followed at a 0.1-eV higher energy by a saddle-point edge associated either with $L_{3'} - L_1$ or with the neighborhood of $k = \Gamma$.

Because of the high resolution of the data presented in the preceding Letter, we can confirm these predictions for silicon in their entirety. We begin by separating exciton and edge effects. Although the spectral range is narrow, the temperature dependence of the three lines shown in Fig. 2 of the preceding note gives no indication of configuration repulsion.[18,19] That means that there is at most one exciton present. That peak II is actually an exciton is attested to by the strong temperature dependence of its size, which is one of the surest indications of the presence of an exciton resonance which overlaps a continuum.[20] The field effect on a resonance contributes a shift (polarization energy) and through tunneling enhances the rate of autoionization into the continuum background.[18,19]

In Si, exciton binding energies are generally small because of the large value of $\epsilon_1(0) = 12$. Here we apparently have a saddle-point exciton with a binding energy of 0.07 eV, which is not inconsistent with the value $\gtrsim 1$ eV estimated for diamond.[17] Below peak I we expect a conventional parabolic exciton. However, the binding energy of a saddle-point exciton (including dielectric breakdown in the central cell) is expected to be 5-10 times larger than that of a parabolic exciton, while oscillator strengths vary in the hydrogenic model as the cube of the binding energy. Thus we would not expect to resolve the parabolic exciton associated with line I in the preceding Letter. However, the optical-field effect may prove valuable in studying hitherto unresolved parabolic excitons in the fundamental absorption region of other semiconductors and insulators with smaller values of $\epsilon_1(0)$.

Peak III shows a temperature shift of the wavelength position quite different from peak I. The latter shifts slowly, as expected for a threshold near $k=\Gamma$. The greater temperature dependence of III suggests an $L_{3'} \rightarrow L_1$ transition.[21,22] Finally, the dependences of II and III on the magnitude and orientation of F as well as their temperature shifts are almost the same, which is what one would expect if II is indeed an exciton derived from the saddle-point edge III.

Because of orbital degeneracies, theoretical analysis of the sign of a positive peak or negative dip is complex (see discussion below). However, there is one relation which may be true quite generally for both M_0 thresholds and M_1 edges, regardless of orbital degeneracies. This concerns the relative sign of structure associated with an exciton and its parent edge. For peaks II and III in Si,[3] the sign of the exciton structure is reversed from that of the parent interband edge. This will be the case if the dominant field effect on the exciton is one of quenching through enhanced autoionization.[18,19]

We conclude by drawing an analogy between structure observed in the electro-optic effect discussed here and the piezo-optic effect.[23,24] Phase-sensitive detection of these effects offers high resolution; in the electro-optic effect $\Delta R/R$ can be measured[3] with a signal-to-noise ratio of 10 and a slit width of 0.003 eV at 3 eV. (The resolution of the piezo-optic effect depends ultimately on the acoustic driver used, and with quartz transducers[24] may be 2-4 times smaller in Si than that of the electro-optic effect.) In many other respects the two effects are quite similar,[12] if one discounts factors of proportionality associated with elastic constants and the difference between deformation potentials in the deformable and rigid-ion models.[25,26] The line shape in the electro-optic effect is somewhat more complex, but one can calculate $\Delta R/R$ from Eq. (1) of the preceding Letter starting from Fig. 1 here. The results, including wings of opposite sign to the central peak, have shown[9,10] to be in good agreement with experiment for the direct edge in Ge.

In treating orbital degeneracies the foregoing analogy is useful because the piezo-optic effect can be discussed for an n-fold degenerate edge in terms of n deformation parameters; a matrix analysis of the Franz-Keldysh type can be made, at least for the central peak, in terms of n similar parameters. Combining this analysis with polarization and orientation studies to obtain the independent components of the electro-optic or piezo-optic tensor[24] should establish the location of interband edges at or near symmetry directions in the Brillouin zone. Because the temperature dependence of peak III in Si suggests an $L_{3'} \rightarrow L_1$ edge while the tensorial dependence has been used[24] to support a hypothetical nondegenerate $\Delta_5 \rightarrow \Delta_1$ edge, this peak should furnish an interesting proving ground for these effects.

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[21]Another "sensitive" candidate is $\Gamma_{25'} \rightarrow \Gamma_{2'}$. However, from second-order perturbation theory we believe this edge shifts rapidly only for crystals such as Ge, GaAs, etc., where $\Gamma_{2'}$ is near the bottom of the conduction band. When $\Gamma_{2'}$ is near Γ_{15}, its temperature dependence should be similar to that of Γ_{15} itself.

[22]Another question that arises is why $L_{3'} \rightarrow L_1$ is detected as a saddle-point edge in Si, but not as a threshold in Ge. But note that the strength of either edge is roughly proportional to $(\mu_l)^{1/2}$, where μ_l is the reduced interband mass along (111) axes near L. Si-Ge alloy data [J. Tauc and A. Abraham, J. Phys. Chem. Solids 20, 190 (1961)] show that $\mu_l \rightarrow \infty$ near 0.8-0.9 Si, which suggests much stronger intensities for $\Delta R/R$ in Si than in Ge.

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SCHUBNIKOW-de HAAS TYPE PHENOMENA IN PYROLYTIC CARBONS AT LIQUID-NITROGEN TEMPERATURES

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Two years ago, we noticed some unusual behavior in the low-temperature galvanomagnetic effects in pyrolytic carbons.[1,2] One of the features we noticed then was that the field depandence of the negative magnetoresistance $\Delta\rho/\rho_0$ observed in pyrolytic carbons is not monotonic, as had been reported, but turns to positive at higher fields. It was found that the character of field dependence is sensitive to the crystalline structure, varying from sample to sample.

Later work revealed that the curves are also nonmonotonic in the positive magnetoresistance region; as the field intensity increases the values of $\Delta\rho/\rho_0$ in all samples begin to show evidence of gradual saturation. In some samples we could even observe the magnetoresistance reaching peak values and then falling off to negative values. At the same time, further precise measurements along this line revealed the detailed shape of the curves in the low-field region. The over-all shape of the field dependence seems to be of oscillatory nature (Fig. 1).

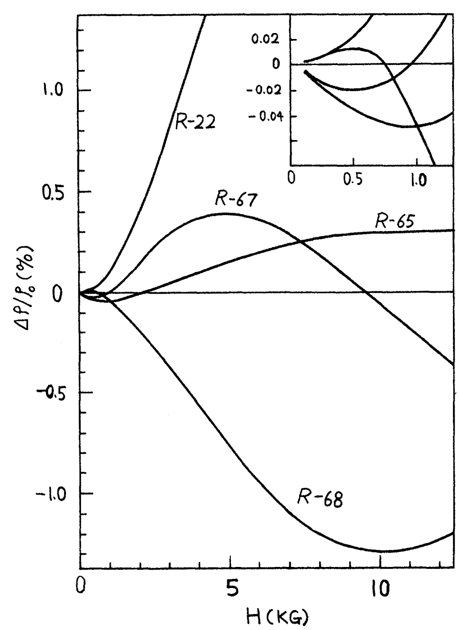

FIG. 1. Field dependence of the magnetoresistance in pyrolytic carbons. Note a small positive magnetoresistance region at low field strengths observed in sample No. R-68. These curves suggest an oscillatory nature for the over-all shapes.

The fabricating conditions of the deposits used in these experiments are listed in Table I. The samples are cut in a bridge shape 30 mm long with the flat faces parallel to the layer planes of the deposits. Most of our measurements were made with current densities of 100 mA/mm^2 or less.

Just as in the case of negative magnetoresistance, so in the case of positive magnetoresistance the character of the field dependence is structure sensitive. The field intensities for which the peak values are observed vary from