VALENCE BAND PARAMETERS IN SILICON FROM CYCLOTRON RESONANCES IN CRYSTALS SUBJECTED TO UNIAXIAL STRESS

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Cyclotron resonance[1,2] has been highly effective in the elucidation of the shapes of conduction band edges for silicon and germanium. The situation is less satisfactory for holes due to the degeneracy of the valence band at $\vec{k}=0$. Here the coupling between bands gives rise to fluted energy surfaces which broaden and shift the resonance lines, making an accurate determination of their centers difficult. An even more fundamental drawback is the fact that from "classical" cyclotron resonance data one cannot specify the signs of two of the three valence band inverse mass parameters. This ambiguity, in principle, could be resolved by investigations of the quantum effects[3,4] arising from the anomalous spacing of the low-lying Landau levels. The present Letter outlines another procedure to determine all three parameters directly by utilizing a uniaxial stress to decouple the degenerate bands. Preliminary results have been obtained for cyclotron resonance in silicon single crystals subjected to stress in the [001] and [111] crystallographic directions.

At $\vec{k}=0$ the valence band of silicon has the character of a $p_{3/2}$ multiplet with 4-fold degeneracy. If the cubic symmetry of the crystal is removed by the application of a uniaxial stress, the 4-fold degeneracy is lifted and two doubly degenerate bands are obtained. For a stress along [001] and [111] directions, the energy surfaces become ellipsoids near $\vec{k}=0$ with their principal axes in the direction of the applied stress. For quantization in these stress directions, the magnetic quantum number M_J becomes a good quantum number when the bands decouple. The energy surfaces are given by the dispersion relations

$$E(k)=(A\pm\tfrac{1}{2}B)k_{\perp}^{2}+(A\mp B)k_{\parallel}^{2}\pm\epsilon, \qquad (1)$$

and

$$E(k)=(A\pm\tfrac{1}{6}N)k_{\perp}^{2}+(A\mp\tfrac{1}{3}N)k_{\parallel}^{2}\pm\epsilon', \qquad (2)$$

for uniaxial stress along the [001] and [111] directions, respectively. The A, B, and N are the valence band inverse-mass parameters.[1] The upper choice of signs correspond to the band identified by $M_J=\pm 3/2$ and the lower choice by $M_J=\pm 1/2$. The splitting energies are $\epsilon=\frac{2}{3}D_u S$ and $\epsilon'=\frac{2}{3}D_u' S'$ in terms of the deformation potentials D_u and D_u' of Kleiner and Roth[5] and strains

$$S=T/(c_{11}-c_{12}), \quad S'=T/c_{44}, \qquad (3)$$

where T is the stress and c_{11}, c_{12}, and c_{44} are the elastic constants.

From (1) and (2) it is evident that measurements of the anisotropy of the cyclotron effective mass m^* under conditions of high strains will yield the values of the three inverse-mass parameters A, B, and N. The choice of sign for B and N, however, is contingent upon knowing the signs of D_u and D_u'. The latter determine whether the $M_J=\pm 3/2$ band or the $M_J=\pm 1/2$ band moves "up" and thus gives rise to the observed cyclotron resonance. The descending band depopulates and does not contribute to the resonance.

The cyclotron resonance experiment was done at ~9000 Mc/sec and at a temperature of 1.26°K on silicon samples subjected to uniform, compressive stresses up to 1000 kg/cm^2 applied either in the [001] or the [111] directions. The rectangular-shaped samples, cut from a single crystal of 5000 ohm-cm Merck p-type silicon, were mounted in a TE_{101} cavity near the ends of the cavity in regions of low electric field strength. The cavity was operated at very low power levels between 10^{-8} and 10^{-7} watt to avoid microwave heating of the carriers. To produce the carriers, chopped white light from a tungsten lamp illuminated the sample via a quartz light pipe.

Figure 1 shows a comparison of typical recorder tracings with and without strain. The light- and heavy-hole lines disappear under stress whereas a new line of intermediate mass forms.[6] This line is broadened at low strains due to incomplete decoupling of the bands so that some of the carriers have sufficient energy to move into regions of k space where the energy surfaces begin to depart from ellipsoidal shape. Furthermore, the line was also observed to broaden and shift to higher mass when the microwave power was increased above 10^{-6} watt.

The results of the anisotropy measurements of

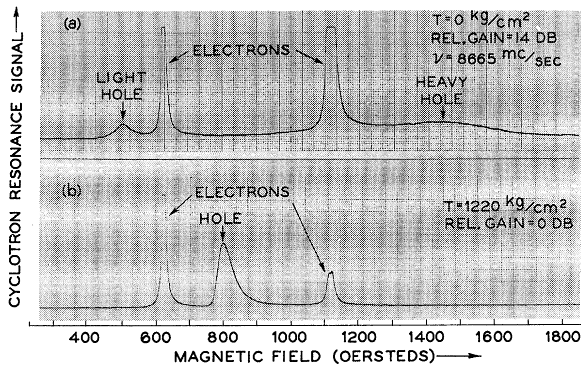

FIG. 1. Typical recorder tracings of cyclotron resonance lines for silicon, (a) without strain and (b) with strain. For both tracings the magnetic field was in the (110) plane and inclined 20° from the [001] axis. The stress in (b) was parallel to the [001] axis. The higher mass electron line has been split by a slight misorientation of H_0 out of the (110) plane. For the electron lines, $\omega\tau = 200$ at 9000 Mc/sec and 1.26°K.

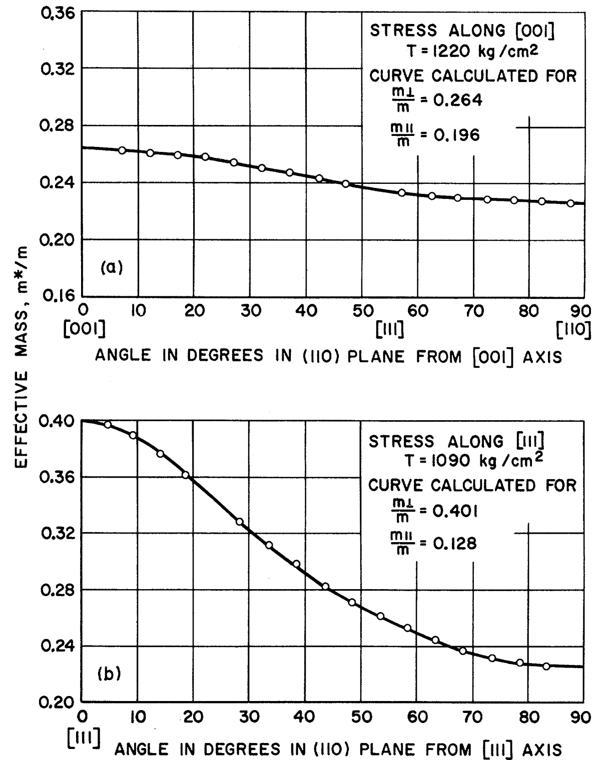

FIG. 2. Effective mass for holes in silicon subjected to uniaxial stress, (a) along the [001] axis and (b) along the [111] axis. The curves were calculated assuming ellipsoidal energy surfaces with the principal axis along the stress direction.

the effective mass m^* are shown in Fig. 2 for two cases having stress parallel to [001] and [111]. The magnetic field was rotated from perpendicular to parallel positions with respect to the stress direction—the anisotropy being independent of the crystallographic plane in which the magnetic field was moved. The effective mass was found to be isotropic in a plane perpendicular to the stress direction, suggesting that the bands were well decoupled and the energy surfaces were axially symmetric.

Our results are summarized in Table I. Since the question of signs of B and N rests upon the yet unknown deformation potentials D_u and D_u', we have reported only the absolute values for these parameters. However, the following two conjectures can be made. The parameter N is almost certainly negative,[7] so the data imply that the $M_J = \pm 1/2$ band is "up" for a [111] stress and $D_u' > 0$. Likewise a positive sign[7] is favored in silicon for B, leading to the conclusion that the $M_J = \pm 3/2$ band lies higher for a [001] stress and $D_u < 0$. Corrections have not yet been measured for the shift in effective mass with increasing stress which presumably accounts for the small discrepancy between the two values of A. Experiments are presently being carried out to extrapolate m^* to zero stress.

Table I. Effective masses for valence band ellipsoids and inverse-mass parameter for stress along the [001] and [111] directions.

[001] $T = 1220$ kg/cm²	[111] $T = 1090$ kg/cm²
$m_\parallel/m = 0.196 \pm 0.001$	$m_\parallel/m = 0.128 \pm 0.001$
$m_\perp/m = 0.264 \pm 0.001$	$m_\perp/m = 0.401 \pm 0.001$
$A = (-4.23 \pm 0.02)\hbar^2/2m$	$A = (-4.26 \pm 0.02)\hbar^2/2m$
$\lvert B\rvert = (0.87 \pm 0.02)\hbar^2/2m$	$\lvert N\rvert = (10.64 \pm 0.04)\hbar^2/2m$

As a final note, the cyclotron hole line in strained germanium has also been observed and a systematic study is in progress.

We would like to express our appreciation to Professor W. Kohn whose suggestions initiated this study and also to Dr. Y. Yafet for many invaluable discussions on these subjects. E. A. Gere and D. H. Sweet assisted in making the measurements.

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PARAMAGNETIC RESONANCE ABSORPTION FROM ACCEPTORS IN SILICON

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In the past, several attempts to observe the paramagnetic absorption from acceptors in silicon were unsuccessful. The reasons for this failure were pointed out by Kohn[1] and are associated with the degeneracy of the valence band in silicon. We wish to report in this Letter the observation of the paramagnetic resonance signal from p-type silicon subjected to a uniaxial stress which removes this degeneracy and thereby eliminates the difficulties encountered in previous experiments.

The structure of the valence band in silicon is shown in Fig. 1(a). In the absence of strains the bands are degenerate at $k=0$ and the energy surfaces are fluted as indicated at the bottom of Fig. 1(a). In the presence of a uniaxial stress the degeneracy is lifted and for large enough strains the bands become decoupled and ellipsoidal [see Fig. 1(b)]. Local random strains due to dislocations, imperfections, and lattice vibrations are always present in a sample and will split the valence band by an amount $\Delta E = DS$, where D is the appropriate deformation potential and S the internal strain. In an external magnetic field H, the spin degeneracy is also lifted and each band is split by the Zeeman energy $g_h \mu H$, where μ is the Bohr magneton and g_h the hole g value. We may distinguish the following two cases:

$\Delta E \approx g_h \mu H$: This situation is illustrated in Fig. 1(c). Since the bands are not characterized by a given M_J quantum number, all the six spin transitions indicated are allowed, which will result in a very short spin-lattice relaxation time. A sample with random internal strains will have a distribution of ΔE values and hence a multitude

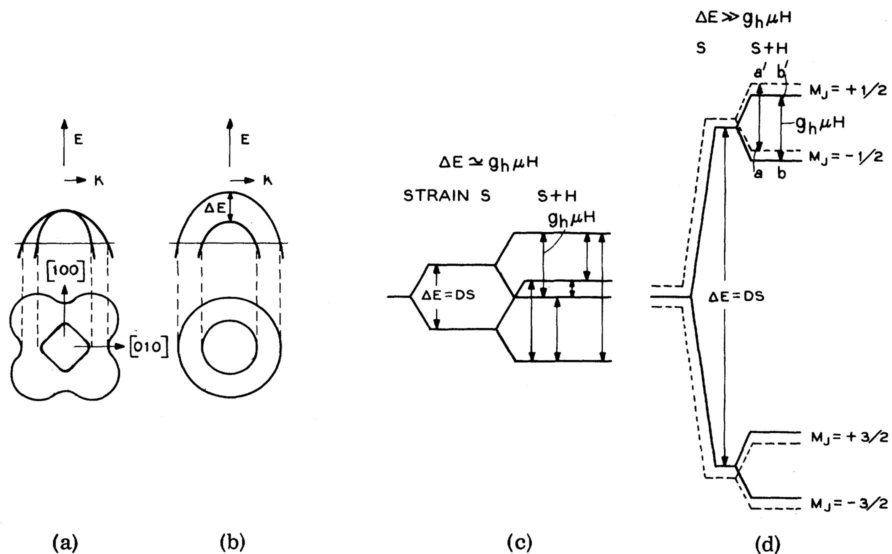

FIG. 1. Valence band in silicon: (a) in the absence of stress; (b) with applied uniaxial stress. (c) Energy levels with $\Delta E \approx g_h \mu H$. All six transitions indicated are allowed. Resonance line will be broadened and difficult to observe. (d) Energy levels with $\Delta E >> g_h \mu H$. Transition frequencies $aa' = bb'$. Lines will not be broadened by random internal strains and paramagnetic resonance is observable.

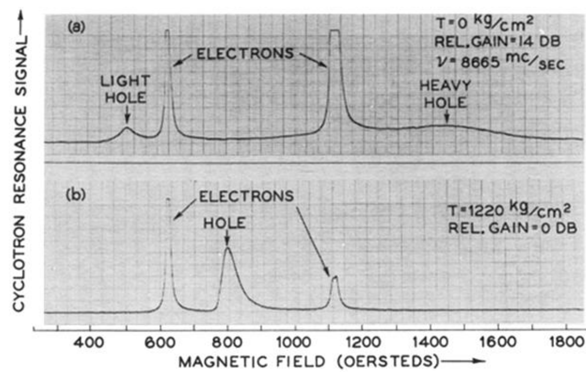

FIG. 1. Typical recorder tracings of cyclotron resonance lines for silicon, (a) without strain and (b) with strain. For both tracings the magnetic field was in the (110) plane and inclined 20° from the [001] axis. The stress in (b) was parallel to the [001] axis. The higher mass electron line has been split by a slight misorientation of H_0 out of the (110) plane. For the electron lines, $\omega\tau = 200$ at 9000 Mc/sec and 1.26°K.