Since it is unlikely that a transition from an ordered to a random state would occur with decreasing temperature, we propose that the low-temperature region possesses antiferromagnetic ordering rather than being paramagnetic. Preliminary results from neutron diffraction, obtained in cooperation with Battelle Memorial Institute, support this conclusion, and detailed results will be reported soon.

To account for the transition, we suggest that at least one of the exchange interactions changes sign near the critical dimension 6.53 A. Such a change in sign might occur because of possible opposing effects of certain superexchange and indirect exchange[3] interactions. It is not necessary to assume that a large change in either interaction must accompany the magnetic transition but only that their relative contribution is altered by the contraction of the crystal near the critical c-axis dimension. We propose to designate this temperature as the "exchange inversion temperature."

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[111] DIRECT TRANSITION EXCITON AND MAGNETOREFLECTION IN GERMANIUM

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From theoretical considerations of the g factor of electrons in germanium[1,2] and infrared[3] and microwave[4] experiments, it was deduced that a direct transition at an energy of ~2 ev[5] exists between the $L_{3'}$ and L_1 bands at the edge of the Brillouin zone along the [111] direction. (See Fig. 1.) This suggests the possibility of carrying out reflection experiments at liquid helium temperatures with magnetic fields and high-resolution grating spectrometers that could provide information about the $L_{3'}$ valence band. Under these experimental conditions it would be possible to observe a third exciton in germanium consisting of the [111] electron and a [111] hole. In addition the magneto-reflection would permit the observation of the fine structure of the Zeeman effect of this [111] exciton and also the direct transition between Landau levels of the $L_{3'}$ valence and L_1 conduction bands along two sets of principal crystal directions. The information to be obtained by these experiments consists of the effective-mass parameters of the $L_{3'}$ holes, the g factor of both electrons and holes and their anisotropies, an accurate determination of the energy gap between the two bands, and a measurement of the binding energy of the exciton. The purpose of this Letter is to predict theoretically some of these quantities and to specify those pertinent aspects of the experiments required for obtaining the desired information.

If second order perturbation theory using the $\vec{k}\cdot\vec{p}$ technique is applied to the L_1 conduction band, it can be shown that the matrix elements between this and the $L_{3'}$ band are essentially those that

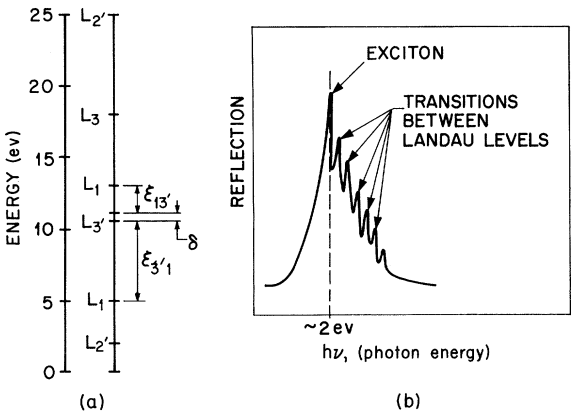

FIG. 1. (a) Approximate energy positions of band edges at the [111] zone edge in germanium. $\delta \approx 0.2$ ev is the spin-orbit splitting of the $L_{3'}$ band. (b) Sketch of expected [111] magnetoreflection spectrum. Fine structure is not indicated.

give rise to the transverse electron mass in germanium,[6] namely:

$$\alpha_t = \frac{m_0}{m_{t1}} \approx 1 + \frac{2M_{13'}^2}{m_0 \mathcal{E}_{13'}} = 12, \quad (1)$$

where $M_{13'} = |(L_1|p_x|L_{3'})|$.

Since $L_{3'}$ is split by a spin-orbit coupling by ~ 0.2 ev, we need only consider just one half the interaction above, i.e., $M_{13'}^2/\mathcal{E}_{13'}$. However, in addition there are matrix elements of comparable magnitude between the $L_{3'}$ and L_3 bands and also between the $L_{3'}$ and lower L_1 valence bands. These make a smaller contribution since they are approximately 6 ev away. Using these results, one finds that the transverse effective mass of the $L_{3'}$ hole is given by

$$\beta_t = \frac{m_0}{m_{t3'}} \approx 1 - \frac{M_{13'}^2}{m_0 \mathcal{E}_{13'}} + \frac{M_{3'1}^2}{m_0 \mathcal{E}_{3'1}} - \frac{2M_{33'}^2}{m_0 \mathcal{E}_{33'}} \approx -6.3, \quad (2)$$

where $M_{3'1}$ is the matrix to the lower L_1 band. It is assumed that the matrix elements $M_{13'}$, $M_{3'1}$, and $M_{33'}$ are of the same order of magnitude and that $\mathcal{E}_{13'} \approx 2$ ev, $\mathcal{E}_{3'1} \approx \mathcal{E}_{33'} \approx 6$ ev.

The longitudinal mass is obtained by taking the matrix elements for the coordinate along the [111] direction. From symmetry considerations, no matrix elements exist between the $L_{3'}$ and L_1 bands but the most important one is between the L_3 and $L_{3'}$ bands. The result is

$$\beta_l = \frac{m_0}{m_{l3'}} \approx 1 - \frac{2M_{33'}^2}{m_0 \mathcal{E}_{33'}} \approx -2.6, \quad (3)$$

where $M_{33'} = |(L_3|p_z|L_{3'})|$.

From these estimates it appears that the holes of the $L_{3'}$ band move on ellipsoids of revolution with masses $m_t \approx 0.16 m_0$ and $m_l \approx 0.4 m_0$. With these values and those obtained from cyclotron resonance for electrons, the binding energy of the exciton can be readily estimated. From the effective-mass Schrödinger equation for the exciton moving on spheroidal energy surfaces, the reduced effective masses become

$$\frac{1}{\mu_t} = \frac{1}{m_{t1}} + \frac{1}{m_{t3'}} \approx 18,$$

$$\frac{1}{\mu_l} = \frac{1}{m_{l1}} + \frac{1}{m_{l3'}} \approx 3.2. \quad (4)$$

From a variational calculation of the binding energy for an ellipsoidal hydrogenic structure from Lampert's curves[7] for the above values and a value of the dielectric constant $K = 16$, we obtain that this becomes $\mathcal{E}_{ex} \approx 0.0048$ ev. This value is larger than that of the direct exciton[8] ($\mathcal{E}_{ex} \approx 0.0015$ ev) or that of the indirect exciton[8] ($\mathcal{E}_{ex} \approx 0.0025$ ev).

The magnetoreflection spectrum can most distinctly be observed with the magnetic field parallel to a [111] direction or perpendicular to it, i.e., a [110] direction. For other directions no selection rules for Δn, the magnetic quantum number, exist since the magnetic field is not along a principal axis of an ellipsoid.[9] Hence along the [111] axis for a magnetic field of approximately 40 000 gauss, the interband transition between two sets of Landau levels of the same quantum number n for one of the four ellipsoids of each band will give an energy separation $\Delta\mathcal{E}_t = \hbar\omega_t$, where $\omega_t = eH/\mu_t c$. The value of $\Delta\mathcal{E}_t \approx 0.007$ ev. For the [110] direction $\Delta\mathcal{E} = \hbar\omega_c$, $\omega_c = eH/\mu_{lt}c$, where $\mu_{lt} = (\mu_\Delta \mu_t)^{1/2} = 0.13 m_0$ or $\Delta\mathcal{E} \approx 0.003$ ev. This time two sets of ellipsoids of each band will contribute to the magnetoreflection. There should be fine structure associated with the splitting of the lines due to spin for the magnetic field along the [111] direction with a separation $\Delta\mathcal{E}_m = g_{\parallel}\beta H$, where $g_{\parallel}$ is a combination of two g factors of the L_1 and $L_{3'}$ bands. Similarly for the [110] direction $\Delta\mathcal{E}_s = g_{\perp}\beta H$. These separations, which are of the order of $10^{-4} - 10^{-3}$ ev, should be resolvable with good accuracy spectroscopically. From the known g values of the L_1 band obtained from spin resonance,[1,4] those of the $L_{3'}$ band can be readily deduced.

The line shape of the magnetoreflection spectrum can be theoretically approximated by the following expressions for the change in reflection coefficient if we assume that the magnetic effects are a small perturbation on the zero-field background of the [111] direct transition:

$$\Delta R \approx 4 \frac{[(n_0^2 - 1) - k_0^2]\Delta n + 2n_0 k_0 \Delta k}{[(n_0+1)^2 + k_0^2]^2}. \quad (5)$$

For germanium the index of refraction and the extinction coefficient are $n_0 \approx 5$ and $k_0 \approx 2$ so that to a reasonable approximation,

$$\Delta R \sim (\Delta n + \Delta k) = (n_0 - k_0)\sigma_i + (n_0 + k_0)\sigma_r, \quad (6)$$

where[10]

$$\sigma_r \sim \left[\frac{(x_n^2+1)^{1/2} + x_n}{2(x_n^2+1)}\right]^{1/2}, \quad \sigma_i \sim \left[\frac{(x_n^2+1)^{1/2} - x_n}{2(x_n^2+1)}\right]^{1/2}, \quad (7)$$

and $x_n = (\omega - \omega_n)$ and $\hbar\omega_n = \mathcal{E}_g + (n + \frac{1}{2})\hbar(\omega_{c1} + \omega_{c3'})$.

The line shape therefore should consist of maxima corresponding to the transitions between Landau levels. The exciton line shape is also similar and is hence favorable for accurate determination of the various parameters. The exciton Zeeman pattern should give discrete resolvable lines for all crystal directions and allow the measurement of the anisotropic g factors. This pattern in the [110] plane will have three branches due to the spin alone.

The above transition should be extremely attractive for use in an optically excited cyclotron resonance maser since the fundamental excitation is in a very desirable range of the optical spectrum where pulsed line sources of the order of several watts or more are possible. Furthermore, this transition fulfills the necessary requirements for such a maser.[11] The direct transition permits selective excitation to discrete magnetic levels deep into the bands allowing population inversion of holes or electrons relative to Landau levels of lower quantum number. Due to the interaction of the spin-orbit split L_3, valence bands, these should have large change of curvature. This will permit unequally spaced magnetic levels so that selective transitions downward in energy between only two unique levels can be chosen by the resonant radiation in an interferometer tuned to this frequency. Thus the induced electric dipole cyclotron resonance transition will be emissive. From the values estimated in this paper for H along a [111] direction, with fields of the order of 4×10^4 gauss or larger which are available and desired for the interband transitions, the maser should be operable in the submillimeter or far infrared region at approximately 600 microns.

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DIRECTION OF THE EFFECTIVE MAGNETIC FIELD AT THE NUCLEUS IN FERROMAGNETIC IRON†

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In a recent experiment[1] it was shown that in ferromagnetic iron the effective magnetic field at the iron nucleus is strongly correlated with the magnetization. The sense of the correlation, however, was not determined, i.e., it was not known whether the effective field was parallel or antiparallel to the magnetization. The sense of the correlation has now been established by observing the change in the hyperfine splitting of the nuclear energy levels of Fe^{57} on application of an external field of 17 to 20 koe.

In an earlier paper[2] we presented the hyperfine spectrum obtained in the resonant Mössbauer[3] absorption in Fe^{57}. The interpretation given to the spectrum has since been confirmed in detail. Several groups have shown the correctness of the hyperfine pattern by observing the spectrum when different alloys and compounds of iron are used.[4] Gossard, Portis, and Sandle[5] have observed the nuclear magnetic resonance in the ground state of Fe^{57} at a frequency corresponding to a value of the effective field in close agreement with the value of 333 koe deduced in reference 2. In addition, Ewan, Graham, and Geiger[6] have