FIG. 1. Thermoelectric power of p-type germanium samples.

and Hull[7] in their work in the same temperature region. $S1$ is a polycrystalline p-type sample with a resistivity of $\sim$30 ohm cm at 295°K. It is 2.23 mm$\times$2.20 mm in cross section, 55 mm in length, and contains about six crystallites. $S2$ is an n-type single crystal with a resistivity of $\sim$50 ohm cm at 295°K and has dimensions 2.26 mm$\times$1.74 mm$\times$39.5 mm.

The samples were mounted in a cryostat described previously by White and Woods[8] and the thermoelectric voltage was measured with an electrometer (necessary because of the high sample resistance). One end of the sample was connected to the earthed cryostat, while the heater and thermometers were connected to the sample through junctions of resistance greater than 5×10^9 ohms. The electrometer, having an input resistance of $\sim$10^{10} ohms, was connected to the sample at the thermometer junctions and was earthed only through the sample.

The variation of the thermoelectric power of $S1$ with temperature is shown in Fig. 1 together with a curve taken from the results of Geballe and Hull for an indium-doped p-type sample with a resistivity of 21.5 ohms at 300°K. The general features of the two curves are similar and are in good agreement with Herring's theory; the differences are almost certainly due to differing dimensions and impurity content.
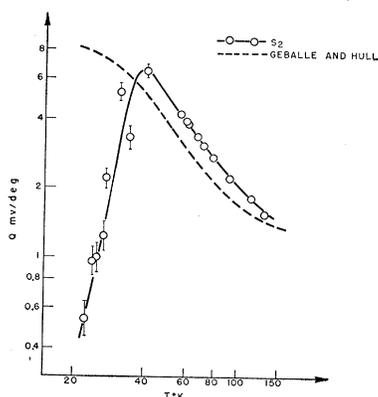

FIG. 2. Thermoelectric power of n-type germanium samples.

Figure 2 shows the results obtained for sample $S2$ and a curve, taken from Geballe and Hull, for an n-type sample with a resistivity of 18.5 ohm cm at 300°K. It is evident that the two curves agree well down to about 40°K, below which temperature the thermoelectric power of our sample decreases abruptly. Since the results are reproducible within the experimental error, which is relatively large because of the small temperature differences used ($\sim$2 percent of the mean sample temperature), we believe the effect is real, but it does not seem to be accounted for by the present theories. A satisfactory theoretical interpretation must await measurements of other properties of this sample, such as, for example, the Hall voltage and electrical resistivity at these low temperatures.

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Excited Donor Levels in Silicon*

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EXCITED energy levels of a monovalent donor impurity have been calculated approximately in the effective mass approximation taking account of anisotropy of the effective mass. The results lead to an identification of observed[1] infrared absorption lines in which the mass anisotropy is an essential feature. We use the effective mass approximation, in spite of the many and great difficulties involved in its theoretical justification, because its relative simplicity allows calculations to be completed in a reasonable time and the results give at least qualitative insight.

Our treatment is based on the effective-mass Schrödinger equation:

$$H\psi=E\psi, \quad H=(p_x^2+p_y^2)/2m_\perp+p_z^2/2m_{\parallel}+V(\mathbf{r}), \quad (1)$$

for the donor impurity electron in silicon, interaction between the six degenerate $\mathbf{k}$ values being neglected. $m_\perp$ and $m_{\parallel}$ are the transverse and longitudinal effective masses taken from experiment; for[2] Si, $m_\perp/m_0=0.19$, $m_{\parallel}/m_0=0.98$ and $\gamma=m_{\parallel}/m_\perp=5.2$. m_0 is the free electron mass; V is the difference between the potential energy of

the impurity electron in the crystal containing one impurity ion and the potential energy in the perfect crystal. $V(\mathbf{r})$ is here assumed spherically symmetrical. H then has cylindrical and inversion symmetry, and the z-component of the angular momentum is a constant of the motion. In the limit $\gamma \equiv m_{\text{II}}/m_{\perp} \to 1$ the symmetry becomes spherical.

As a calculational and conceptual aid we separate the problem into two parts: (1) a consideration of the effect of the effective mass anisotropy, and (2) a consideration of the effect of the detailed shape of $V(r)$. The procedure is: Partition the eigenstates of (1) into sets which become degenerate as $\gamma \to 1$ and find the mean energy $\bar{E}_{nl}$ of the $2l+1$ eigenstates of a set. Fit the spectrum of the $\bar{E}_{nl}$'s to the eigenspectrum of $H_0\psi = E_{nl}\psi$, where

$$H_0 = (p_x^2 + p_y^2 + p_z^2)/2m(\gamma) + V(r), \qquad (2)$$

and thereby determine an effective isotropic mass $m(\gamma)$. It is assumed that the $m(\gamma)$'s determined from different pairs of levels will be nearly the same at least in the region of the spectrum that is of interest, and further that the value of $m(\gamma)$ is sufficiently independent of choices of $V(r)$ for the choices considered. $m(\gamma)$ is given quite generally in the limit $\gamma \to 1$ by $3/m(1) = 2/m_{\perp} + 1/m_{\text{II}}$.

With $V = -e^2/\kappa r$ (the static dielectric coefficient κ is 12 for Si), we find approximate eigenvalues of (1) by the variational method using analytic trial functions derived from hydrogenic eigenfunctions. For example, the hydrogen $1s$ eigenfunction is proportional to $\exp[-A(x^2+y^2+z^2)^{\frac{1}{2}}]$ and the corresponding trial function is proportional to $\exp[-(B^2x^2+B^2y^2+D^2z^2)^{\frac{1}{2}}]$, where B and D are variable parameters chosen to minimize the energy. All trial functions are mutually orthogonal. Lampert[3] has calculated the $1s$ level by this method, and we have extended his calculations to excited states with the following results for Si:

Energy level designation	$1s$	$2p_0$	$2s$	$2p_{\pm}$	$3p_0$	$3p_{\pm}$
Binding energy (ev)	0.0284	0.0106	0.0071	0.0058	0.0047	0.0026

We identify the four observed absorption lines[1] for As in Si as the transitions: $1s \to 2p_0$, $1s \to 2p_{\pm}$, $1s \to 3p_0$, $1s \to 3p_{\pm}$. Comparison between theory and experiment (Table I) indicates that this identification is consistent with the observed lines, that the calculation represents the splitting in the np levels associated with the anisotropic effective mass to reasonable accuracy, but that the scale of the calculated mean energy levels $\bar{E}_{nl}$ is too small. $\bar{E}_{3p} - \bar{E}_{2p}$ is small by a factor 0.71 while $\bar{E}_{3p} - \bar{E}_{1s}$ and $\bar{E}_{2p} - \bar{E}_{1s}$ are small by factors 0.49 and 0.46, indicating that the solution is better for excited than for ground energies, as might be expected. The region near $r = 0$, which is the presumed source of the major discrepancies, is less important for the excited states because of their larger orbits.

The small difference between the $m(5.2)$'s from the calculated $1s \to 2p$ and $1s \to 3p$ transitions (Table I),

TABLE I. Comparison between theory and experiment. ΔE is the energy difference in ev of the designated transition; $\delta(\Delta E)$ is the energy difference of adjacent transitions, equivalent to the level separation; $\Delta \bar{E}_{nl}$ is the mean transition energy.

Transition	Experimental			Calculated		
	ΔE(ev)	$\delta(\Delta E)$	$\Delta \bar{E}_{nl}$	ΔE(ev)	$\delta(\Delta E)$	$\Delta \bar{E}_{nl}$
$1s \to 3p_{\pm}$	0.0521			0.0258		
		0.0015	0.0516		0.0021	0.0251
$1s \to 3p_0$	0.0506			0.0237		
		0.0031			0.0011	
$1s \to 2p_{\pm}$	0.0475			0.0226		
		0.0050	0.0458		0.0048	0.0210
$1s \to 2p_0$	0.0425			0.0178		

0.296 and 0.299, supports our assumption of the existence of an $m(\gamma)$, while the larger difference between the corresponding experimental values, 0.648 and 0.614, points to a deviation of V from hydrogenic form. Changes in the $\bar{E}_{nl}$ from use of a more realistic V than $-e^2/\kappa r$ are being investigated with a view to improving the poor agreement between the experimental and the calculated values of $\bar{E}_{nl}$ shown in Table I.

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Theory of Melting and Yield Strengths

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THE theory of melting proposed by Fürth,[1] which has been related to the rupture strength, has been criticized as yielding fortuitous results largely because rupture strengths have been associated more definitely with surface phenomena.[2] It may therefore be of interest to try to relate Fürth's theory or a modification thereof to the yield strength, which is less surface-dependent.

If we restrict ourselves to single crystals of high purity, the Frank-Read mechanism for yielding presumably applies. The increase in energy, U, in forming a semicircular dislocation of radius R from an edge dislocation of width ζ may be written as

$$U = -\tfrac{1}{2}\pi R^2 \tau b + U_e + U_m, \qquad (1)$$

where τ is the applied shear stress, b is the Burgers vector, and U_e and U_m represent, respectively, the in-