DEFORMATION POTENTIAL IN GERMANIUM FROM OPTICAL ABSORPTION LINES FOR EXCITON FORMATION

W. H. Kleiner and L. M. Roth
Lincoln Laboratory,* Massachusetts Institute of Technology, Lexington, Massachusetts
(Received March 26, 1959)

In their study of the direct exciton in germanium, Zwerdling *et al.*[1] observed a second absorption peak (1.5°K) about 0.005 ev above the absorption identified with the direct exciton. Since the separation of the two peaks was several times greater than the binding energy of the exciton, this could not be an excited state of the exciton in the ordinary sense, and no explanation has heretofore been given. However, recent experiments by Macfarlane *et al.*[2] have established that the ZLRB sample was strained, due to the difference in thermal contraction of the sample and its glass substrate, and that the strain accounted for the observed discrepancy in the position of the exciton line reported by the two groups, and for the presence of the second peak in the ZLRB data.

The appearance of the second peak should actually be expected in the presence of shear strain, since shear splits the valence band edge into two edges. There will then be two exciton levels, one associated with each valence band edge, as indicated in Fig. 1. The splitting and shift of the exciton with strain can, in fact, be used to obtain information about the deformation potential for the band edges. To analyze the data here we shall assume that the exciton binding energies ϵ_+ and ϵ_- are independent of strain, that is, equal to the binding energy in the absence of strain. This is reasonable since the binding energy is determined largely by the small electron mass. The splitting 2Δ of the valence band edge and the mean shift $\bar{E}-E_0$ of the gap are then determined from the position of the two exciton lines in the presence of strain[1] and the single exciton line in the absence of strain.[3]

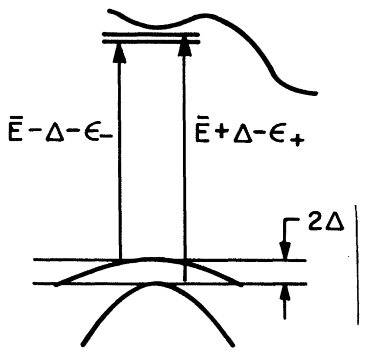

FIG. 1. An illustration of direct exciton formation transitions in Ge with general homogeneous strain present. (The exciton levels have been placed below the conduction band edge by an amount equal to their binding energies, and are not to be confused with one-electron levels.) 2Δ denotes the splitting of the valence band, $\bar{E}$ the mean gap between the valence bands and the conduction band ($\bar{E}=E_0$ in the absence of strain), and ϵ_+ and ϵ_- the binding energies of the two excitons.

The effect of a homogeneous strain S_i ($i=1$, 2, ..., 6, where $S_4=2S_{yz}$) on the conduction and valence band edges is conveniently described by Hamiltonians derived by symmetry consideration

$$\mathcal{H}^c=\mathcal{H}_0{}^c+D_d{}^c(S_1+S_2+S_3), \tag{1}$$

$$\mathcal{H}^v=\mathcal{H}_0{}^v+D_d{}^v(S_1+S_2+S_3)+\tfrac{2}{3}D_u\left[(J_x{}^2-\tfrac{1}{3}\vec{J}^2)S_1+\text{c.p.}\right]+\tfrac{2}{3}D_u{}'\left[\tfrac{1}{2}(J_yJ_z+J_zJ_y)S_4+\text{c.p.}\right], \tag{2}$$

where the D's are deformation potential coefficients, $\hbar\vec{J}$ is the angular momentum of the hole ($J=3/2$), and the $\mathcal{H}_0$'s describe the situation in the absence of strain; D_d is the shift per unit dilatation of the band edge, while $|2D_u|$ is the splitting of the band edge induced by uniaxial shear strain per unit extension along the [001] axis; $|2D_u{}'|$ gives the splitting similarly for the [111] axis.[4] Finally, "c.p." means "cyclic permutations of x, y, and z," referring to the crystallographic axes. The deformation potential parameters $D_d{}^c-D_d{}^v$, $|D_u|$, and $|D_u{}'|$ may be determined from the experimental splitting and mean shift measured for appropriate strains.

The data considered here[1] are for a Ge sample in the form of a very thin slab of uniform thickness with slab normal in the [110] direction. The sample is cemented to a supporting substrate at roughly room temperature. When the temperature is changed, the difference between the thermal expansion of Ge and the substrate induces a strain in the sample. If the sample, substrate and cementing are homogeneous and the substrate is elastically isotropic parallel to the interface, as assumed here, then the symmetry implies that the strain tensor in the sample is uniform,

Table I. Splitting of the valence band and mean shift of the direct energy gap for strains induced in thin slab samples, for three directions of the slab normal.

Slab normal	[001]	[111]	[110]
Strain components	$S_1=S_2=S$, $S_3=-\lambda S$, $S_4=S_5=S_6=0$	$S_1=S_2=S_3=\frac{1}{3}(2-\lambda)S$, $S_4=S_5=S_6=-\frac{2}{3}(1+\lambda)S$	$S_1=S_2=\frac{1}{2}(1-\lambda)S$, $S_3=S$, $S_4=S_5=0$, $S_6=-(1+\lambda)S$
λ	$2c_{12}/c_{11}$	$2(c_{11}+2c_{12}-2c_{44})/(c_{11}+2c_{12}+4c_{44})$	$(c_{11}+3c_{12}-2c_{44})/(c_{11}+c_{12}+2c_{44})$
Δ	$\frac{2}{3}(1+\lambda)\lvert D_u\rvert\lvert S\rvert$	$\frac{2}{3}(1+\lambda)\lvert D_u'\rvert\lvert S\rvert$	$\frac{2}{3}(1+\lambda)(\frac{1}{4}D_u^2+\frac{3}{4}D_u'^2)^{1/2}\lvert S\rvert$
$\bar{E}-E_0$	$(2-\lambda)(D_d^c-D_d^v)S$	$(2-\lambda)(D_d^c-D_d^v)S$	$(2-\lambda)(D_d^c-D_d^v)S$
R	$\lvert D_u\rvert/\lvert D_d^c-D_d^v\rvert$	$\lvert D_u'\rvert/\lvert D_d^c-D_d^v\rvert$	$(\frac{1}{4}D_u^2+\frac{3}{4}D_u'^2)^{1/2}/\lvert D_d^c-D_d^v\rvert$

diagonal with respect to coordinate axes in the plane of the slab (x', y') and perpendicular to the slab (z'), and isotropic in the plane of the slab. We denote the principal strain components by S, S, $-\lambda S$, where λ is determined by the condition that the normal stress vanish. When referred to crystallographic coordinates, the strain components are $S_1=S_2=\frac{1}{2}(1-\lambda)S$, $S_3=S$, $S_4=S_5=0$, $S_6=-(1+\lambda)S$. With these values of the strain, Δ and $\bar{E}-E_0$ are readily determined from the eigenvalues of (1) and (2). The results are given in Table I together with corresponding results for the slab normal in the [001] and [111] directions. The sign of $D_d^c-D_d^v$ is determined by the sign of S. If the magnitude of S is unknown, valuable information can still be obtained in the form of the ratio,

$$R=\frac{3(2-\lambda)}{2(1+\lambda)}\frac{\Delta}{\lvert\bar{E}-E_0\rvert}, \tag{3}$$

of shear to dilatation deformation potential coefficients (See Table I).

Values of R derived from the ZLRB and the MMQR[3] data are given in Table II and are probably in error by less than 10%.[5] The close agreement between the values of R at the two temperatures supports our interpretation of the data.

If we use the value -9 ev per unit dilatation for $D_d^c-D_d^v$ obtained from pressure measurements,[6] we can deduce from R the value 4.5 ev per unit strain for $(D_u^2/4+3D_u'^2/4)^{1/2}$. This is somewhat larger than the result $E_2=1.66$ ev per unit strain obtained by Brooks,[4] from piezoresistance data, where $-E_2$ is an average of D_u and D_u'. The agreement is slightly improved if we use Brooks' formula (6.34) to calculate D_u and D_u' separately from the piezoresistance coefficients $(m_{11}-m_{12})/2$ and m_{44}, respectively, giving $D_u=0.3$ ev and $D_u'=-2.9$ ev, which yields $(D_u^2/4+3D_u'^2/4)^{1/2}=2.5$ ev. This may not be significant, however, as the piezoresistance calculation neglects anisotropy of the energy surfaces.

Further strain measurements on samples with [001] and [111] slab normals would give D_u and D_u' separately, and in addition it should be possible to determine the signs of D_u and D_u' by analyzing the magnetic spectrum. Finally, measurements should be made on substrates with known thermal expansion (so that S can be accurately determined).

Table II. The ratio R of shear to dilatation deformation potential coefficients derived from splitting and mean shift of exciton lines.[a]

T(°K)	λ	Splitting 2Δ (milli-ev)	Mean shift $\lvert\bar{E}-E_0\rvert$ (milli-ev)	R
1.5	0.442	4.9	8.9	0.46
77	0.442	4.1	6.9	0.48

[a] Elastic constant data were taken from M. E. Fine, J. Appl. Phys. 26, 862 (1955).

---

[*] A center for research operated by the Massachusetts Institute of Technology with the joint support of the U. S. Army, Navy, and Air Force.

[1] Zwerdling, Lax, Roth, and Button, Phys. Rev. (to be published).

[2] Macfarlane, McLean, Quarrington, and Roberts, Phys. Rev. Lett. 2, 252 (1959).

[3] Macfarlane, McLean, Quarrington, and Roberts, Proc. Phys. Soc. (London) 71, 863 (1958).

[4] H. Brooks, Advances in Electronics and Electron Physics (Academic Press, New York, 1955), Vol. 7, p. 85. Brooks uses $E_1=-D_d^v$, $E_2=-D_u=-D_u'$ in

Eq. (6.29).

[5] Since the magnitude of S is unknown for the ZLRB data, only values of R can be derived. The sign of S is known,[2] however, implying $D_d^c - D_d^v < 0$ as expected.

[6] W. Paul and D. M. Warschauer, J. Phys. Chem. Solids 5, 89 (1958).

ELECTRICAL AND THERMAL RESISTIVITY OF DISLOCATIONS

Peter Carruthers*
Department of Physics, Cornell University, Ithaca, New York

(Received February 26, 1959)

For a long time it has been known that mechanical deformation greatly reduces the electrical conductivity of metals.[1-3] Since the change in resistivity was consistently found to be one to two orders of magnitude greater than expected theoretically[4-8] for scattering by the strain field of a dislocation, various authors have invoked scattering by stacking faults,[9] or the dislocation core,[10] to explain the discrepancy. Because of the difficulty of the latter calculations, the reliability of such explanations has not been determined.

Recently, observations of the effect of dislocations on the thermal conductivity of LiF at low temperatures by Sproull, Moss, and Weinstock[11] have shown that the thermal conductivity is about 100 times less than that predicted by Klemens.[12] It seems that this discrepancy may be intimately related to that of the electrical resistivity caused by dislocations. The author[13] has proposed an explanation of the high thermal resistivity caused by dislocations. The purpose of the present note is to suggest that the scattering of electrons by the strain field of an edge dislocation may be much larger than found in previous calculations.[4-8] Also, recent experimental results are compared to the author's theory[13] of thermal resistance of dislocations.

The raison d'être of the electron problem may be best understood by comparing the author's theory of the strain field scattering of phonons with that of Klemens.[12] In both treatments the scattering proceeds by the anharmonic forces. The energy-conserving perturbation is then linear in the displacement field and quadratic in the phonon creation and annihilation operators. The author's theory is atomic in character; the complicated sums are rearranged and simplified without approximation. The approximation necessary to work out a given problem are made after the pertinent physical quantities have been separated out. The essential feature is that the Fourier component of the strain field displacement enters into the matrix elements.

Klemens,[12] proceeding from a Grüneisen model of the anharmonicities, obtains in the pertinent matrix elements the Fourier component of the dilatation (or rotation). In deriving this result (for a simple cubic lattice), the approximation was made that the component of the difference of displacements $\vec{v}$ at lattice sites $\vec{m}$ and $\vec{m}-\vec{l}$ in the direction of the linkage l_i is equal to $(dv_i/dx^i)a$, where a is a lattice constant. The details of the calculation are such that the (two-dimensional) Fourier component of this function is then taken. (That is, the approximation is made before the sum over all lattice positions is taken.) It is easy, using the exact difference of y-displacements due to an edge dislocation, to demonstrate that the integrand is not uniformly convergent to Klemens' approximation. Thus the author's calculation for the relaxation time τ of a phonon in the strain field of an edge dislocation differs from Klemens' result essentially by the factor $\frac{1}{2}[\ln(R/r_0)]^2$. This result is

$$\tau^{-1} = \tfrac{1}{2}\sigma[\ln(R/r_0)]^2 b^2\gamma^2 c q. \tag{1}$$

Here σ is the dislocation density, r_0 is the core radius, b is the Burgers vector, R is the mean range of the dislocation strain field, γ is Grüneisen's constant, c is the velocity of sound, and q is the wave vector of the phonon. The logarithm factor directly reflects the long-range (logarithmic) nature of the displacement field, i.e., the scattering "center" is not localized.

We now return to the problem of electron scattering by the strain field of a dislocation. In this case it is not evident that the core scattering is negligible, since the wavelengths of the electrons in conductivity are much smaller than those of the phonons considered above. Further complications arise from the redistribution of the electrons in a dilated lattice.[4] Harrison[10] has shown that for a hollow-core dislocation model, the scattering is almost enough to account for the experimental results. However, it seems that such