

Effect of Shear on Impurity Conduction in *n*-Type Germanium*

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Shear strains, which change the donor wave functions, greatly affect impurity conduction, which depends sensitively on the wave function overlap of neighboring impurity states. The change of impurity conduction of germanium containing 5.2×10^{15} antimony atoms per cc and about 3% compensation was measured at 1.9°K as a function of shear strains produced by uniaxial tension and compression along [110]. It is shown that the anisotropy and the saturation of the conductivity changes observed at stresses larger than 4×10^8 dynes/cm² can be understood from the strain-induced changes of the donor state wave functions.

ELECTRON spin resonance experiments on shallow donors in silicon¹ and germanium² have determined the magnitude of the donor wave function in the neighborhood of the donor. Kohn³ and Luttinger constructed a theory of the donor wave functions which agrees with the experiments except for some unresolved complications in germanium. Here we describe a method of studying the shape of the donor wave functions at large distances from the donor atom by means of the effect of shear stress on impurity conduction.⁴

Impurity conduction depends sensitively on the overlap of neighboring impurity states.⁵ Shear strains which lift the degeneracy of the conduction band valleys also lift the corresponding degeneracy of the donor levels and change the donor wave functions. The resultant change of the overlap strongly affects the electron transfer between neighboring donor sites and gives rise to a stress dependence of impurity conduction. The anisotropy of this piezoresistance effect enables one to deduce the anisotropy of the strain-modified donor wave functions.

As an example let us consider *n*-type germanium subjected to pure shear produced by uniaxial stress⁶ along [110]. Price⁷ calculated for this shear the splitting of the 1s-multiplet of shallow donors in germanium on the basis of the deformation potential theory.⁸ Treating the chemical shift⁷ $4\Delta_c$ and the shift of the valleys as perturbations, and labeling the four lowest-lying donor states from 1 to 4 in the order of decreasing energy, one obtains the following donor wave functions modified

by the strain

$$\begin{aligned}\Psi^{(1)} &= 2^{-\frac{1}{2}}(\Phi_1 - \Phi_2), \\ \Psi^{(2)} &= \frac{1}{2} \sum_{j=1}^4 [1 + \epsilon_j / (4\Delta_c^2 + \epsilon_j^2)^{\frac{1}{2}}] \Phi_j, \\ \Psi^{(3)} &= 2^{-\frac{1}{2}}(\Phi_3 - \Phi_4), \\ \Psi^{(4)} &= \frac{1}{2} \sum_{j=1}^4 [1 - \epsilon_j / (4\Delta_c^2 + \epsilon_j^2)^{\frac{1}{2}}] \Phi_j.\end{aligned}\quad (1)$$

Here $\Phi(\mathbf{r}) = F_j(\mathbf{r})\varphi_j(\mathbf{r})$ where the envelope function $F_j(\mathbf{r})$ is the solution of the effective mass equation³ for the *j*th valley and φ_j is the Bloch wave at the *j*th valley. The valleys are labeled from *j*=1 to *j*=4 according to the direction of their axes along [111], $[\bar{1}\bar{1}\bar{1}]$, $[\bar{1}11]$, and $[1\bar{1}\bar{1}]$. The deformation potential theory yields for the shear-induced shift of the valleys $\epsilon_1 = \epsilon_2 = -\epsilon_3 = -\epsilon_4 = E_2 S_{44} X / 6$, where E_2 =deformation potential for shear, S_{44} =elastic shear constant, and X =uniaxial stress along [110], taken positive for

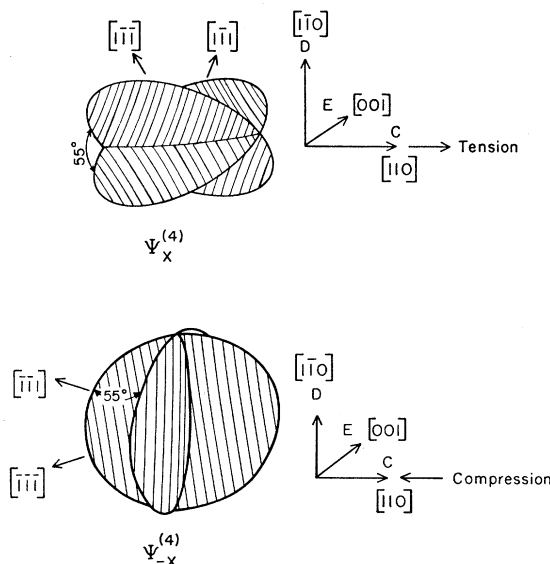


Fig. 1. Surfaces $\Psi^{(4)} = \text{constant}$ for donor ground state in the limit of large uniaxial stresses along [110].

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¹ R. C. Fletcher, W. A. Yager, G. L. Pearson, A. N. Holden, W. T. Read, and F. R. Merritt, Phys. Rev. **94**, 1392 (1954); A. Honig and A. F. Kip, Phys. Rev. **95**, 1686 (1954); G. Feher, Phys. Rev. **103**, 834 (1956).

² G. Feher, D. K. Wilson, and E. A. Gere, Phys. Rev. Letters **3**, 25 (1959).

³ W. Kohn, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 5, p. 257.

⁴ For references to papers on impurity conduction see H. Fritzsch, J. Phys. Chem. Solids **6**, 69 (1958).

⁵ W. D. Twose, Ph.D. thesis, Cambridge University, 1959 (unpublished); A. H. Miller, Ph.D. thesis, Rutgers University, 1960 (unpublished).

⁶ The isotropic strain produced by this stress has been found not to affect impurity conduction.

⁷ P. J. Price, Phys. Rev. **104**, 1223 (1956).

⁸ C. Herring and E. Vogt, Phys. Rev. **101**, 944 (1956).

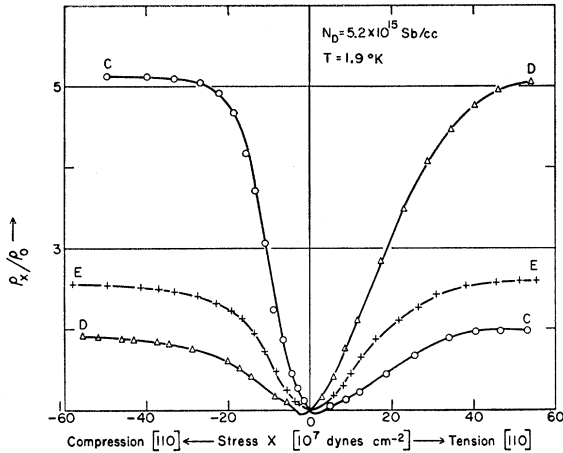


FIG. 2. Ratio of the resistivities of stressed and unstressed n -type germanium for the principal directions as a function of stress.

tension and negative for compression. For compression interchange $\Psi^{(1)}$ and $\Psi^{(3)}$ in Eq. (1).

Two effects contribute to the piezoresistance of impurity conduction, (1) the redistribution of electrons as the $1s$ donor states split under shear strain, and (2) the change of the wave functions according to Eq. (1). The redistribution effect is negligible when $kT \ll 2\Delta_c$. This condition is satisfied below 4°K for arsenic and phosphorus donors for which $2\Delta_c = 2.1$ milliev^{9,10} and $2\Delta_c = 1.45$ milliev¹⁰ respectively. In these cases only the ground state $\Psi^{(4)}$ is occupied. For strains large enough so that $|\epsilon_j| \gg 4\Delta_c$, all $\Psi^{(i)}$ become strain independent and hence the piezoresistance of impurity conduction saturates. In this limit $\Psi^{(4)}$ approaches the form $\Psi_X^{(4)} = 2^{-\frac{1}{2}}(\Phi_3 + \Phi_4)$ for uniaxial tension and $\Psi_{-X}^{(4)} = 2^{-\frac{1}{2}}(\Phi_1 + \Phi_2)$ for uniaxial compression.

Figure 1 shows schematically the two forms $\Psi_{\pm X}^{(4)}$. Only the envelope functions $F(\mathbf{r})$ are shown since they determine the electron transfer between donor centers.

⁹ H. Fritzsche, Phys. Rev. **115**, 336 (1959).

¹⁰ D. K. Wilson and G. Feher, Bull. Am. Phys. Soc. **5**, 56 (1960).

At large distances from the donor $F(\mathbf{r}) = (\pi a^2 b)^{-\frac{1}{2}} \times \exp -[(x^2 + y^2)/a^2 + z^2/b^2]^{\frac{1}{2}}$, where for germanium $a = 64.5$ Å and $b = 22.7$ Å and the particular valley axis is chosen as z axis.⁸

The principal axes of the resistivity tensor are indicated by C , D , and E . Since the shear strains caused by tension and compression along $[110]$ are identical except for a rotation around $[001]$ by 90° , the following relations are required by symmetry

$$\begin{aligned} \rho_D(X) &= \rho_C(-X), \quad \rho_E(X) = \rho_E(-X), \\ \rho_C(X) &= \rho_D(-X). \end{aligned} \quad (2)$$

Because for zero strain $\Psi_0^{(4)} = 2^{-\frac{1}{2}}(\Psi_X^{(4)} + \Psi_{-X}^{(4)})$, it follows from the reduction of the wave function in the various directions that

$$\rho_D(X) > \rho_E(X) > \rho_C(X). \quad (3)$$

The change of impurity conduction of germanium containing 5.2×10^{15} Sb atoms per cc and about 3% compensation was measured at 1.9°K as a function of uniaxial tension and compression along $[110]$. Antimony was chosen as donor impurities because its small chemical shift, $4\Delta_c = 0.57$ milliev,¹¹ enables one to reach saturation of the piezoresistance at relatively small stresses. Figure 2 shows the resistivity ratios of the strained to the unstrained sample for the three principal directions. The relative magnitudes of the piezoresistance in the principal directions agree with Eq. (3). The symmetry conditions, Eq. (2), are fulfilled by the saturation values but not by the piezoresistances at smaller stresses. This discrepancy may partly be caused by experimental difficulties with the transverse piezoresistance measurements at small stresses.

For Sb donors the magnitude of the piezoresistance is affected by the redistribution effect. A rough estimate of $\rho_C(-X)/\rho_0$ at saturation based on Twose's theory yielded the value 4, the experimental value is 5.05. Experiments on As-doped germanium and with different strain orientations are in progress.

¹¹ H. Fritzsche (to be published).