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STRESS-INDUCED SHIFTS OF SHALLOW DONOR POLARIZABILITIES IN n-TYPE SILICON*

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Piezocapacitance measurements on high-purity and n-type silicon versus uniaxial stress have yielded strain-dependent donor polarizabilities $\alpha_D(x)$. The valley repopulation model with strain-dependent Bohr radii is inadequate to explain the data. A many-valley approach featuring strain-dependent valley-valley coupling is more successful.

I. Introduction

Previous experimental studies have yielded useful information on the strain-dependence of shallow donor wave functions in Si and Ge. These have included measurements of piezoresistance[1], piezohyperfine Fermi contact constants of the donor nucleus[2], and piezohyperfine constants of Si^{29} nuclei[3] obtained by the ENDOR technique. At liquid He temperatures on the insulating side of the insulator-metal transition the piezoresistance depends on the transfer or hopping matrix between a filled and empty donor site. The donor Fermi contact constant measures $|\psi(\vec{r}=0,x)|^2$ of the donor ground state versus the reduced valley strain x. The ENDOR measurement for a specific Si^{29} site at $\vec{r}_\ell$ from the donor determines $|\psi(\vec{r}_\ell,x)|^2$. New piezocapacitance measurements on both high-purity Si and n-type Si samples yield donor polarizabilities $\alpha_D(x)$ which give a direct measure of how the size of a donor wave function changes with strain. The experimental results for Si:P cannot be explained with a conventional theory based on the valley repopulation model (VRM) and strain-dependent Bohr radii associated with each valley. A new theoretical approach incorporating different Bohr radii for the strain-admixed $1s\text{-}A_1$ and $1s\text{-}E_a$ states, rather than with the stress-raised and stress-lowered valleys, gives good agreement with the data. However, one must include strain-dependent valley-valley coupling matrix elements.

II. Experiment and Experimental Results

Piezocapacitance measurements, for both [100] and [110] axis uniaxial tensile stresses, have been made on high-purity Si, P-doped and Sb-doped Si samples in the temperature range 4.2K to 1.1K for stresses σ_s up to 1000 Kgm/cm^2. The doped samples have donor concentrations (N_D) in the range 6×10^{16} to 1.9×10^{18}/cm^3. For all samples the electric field is applied transverse to the stress axis along [001]. The capacitance, after edge corrections, yields the component $\varepsilon_{zz}(x,N_D,T)$ of the dielectric tensor. Using the Clausius-Mossotti relationship we obtain an effective donor polarizability component

$$\alpha_{D,zz}(x,N_D,T) = \frac{3\varepsilon_{h,zz}(x,T)}{4\pi N_D}\left[\frac{\varepsilon_{zz}(x,N_D,T)-\varepsilon_{h,zz}(x,T)}{\varepsilon_{zz}(x,N_D,T)+2\varepsilon_{h,zz}(x,T)}\right], \qquad (1)$$

where ε_h is the host dielectric constant, and has been found to be 11.40±0.06 as T→0K, in excellent agreement with Faulkner's value (4). The high purity Si data show a linear decrease of ε_{zz} with stress yielding the result $(1/\varepsilon_h(0))(\Delta\varepsilon_{h,zz}/\Delta\sigma_s) = -(3.37\pm0.07)\times10^{-7}$ cm²/Kgm, which is intermediate between values obtained with hydrostatic pressure[5] near room temperature [the uniaxial tension produces a transverse contraction along the electric field].

Figure (1) shows $\alpha_{D,zz}(x)$ (we now drop the zz subscript) versus the valley strain x ($x_{100}=\frac{1}{3}(\Xi_u/\Delta)(S_{11}-S_{12})\sigma_s$, $x_{110}=\frac{1}{2}x_{100}$; Ξ_u is the shear deformation potential, Δ is the adjacent valley coupling, S_{11} and S_{12} are the elastic compliance constants). For the [100] axis tension F $\alpha_D(x)$ decreases, passes through a minimum for $x_{100}\approx0.6$, and subsequently increases. The hopping contribution to $\alpha_D(x,T)$ decreases rapidly with temperature T as T→0K. The $\alpha_D(x,T)$ curves move down rigidly showing that the strain dependence of $\alpha_D(x,T)$ is independent of T. One can extract $\alpha_D(x,T\to0K)$ from the data. The [110] axis tension data show a decrease with x_{110} that is almost linear, but yields a slight upward deviation from linearity. The slope $(1/\alpha_D(0))(\partial\alpha_D/\partial x)_{x=0}$ is twice that for the [100] data in agreement with the prediction of the VRM. Other Si:P samples ($N_D\sim2.3\times10^{17}$/cm³) show behavior identical to that in Fig. (1) while more concentrated samples (1.4 to 1.9×10^{18}/cm³) show the same initial slope but with $x_{100}^{min}\sim0.4$. A Si:Sb sample ($N_D\sim6\times10^{16}$/cm³) exhibits smaller slope at x=0 and gives $x_{100}^{min}\sim0.9$.

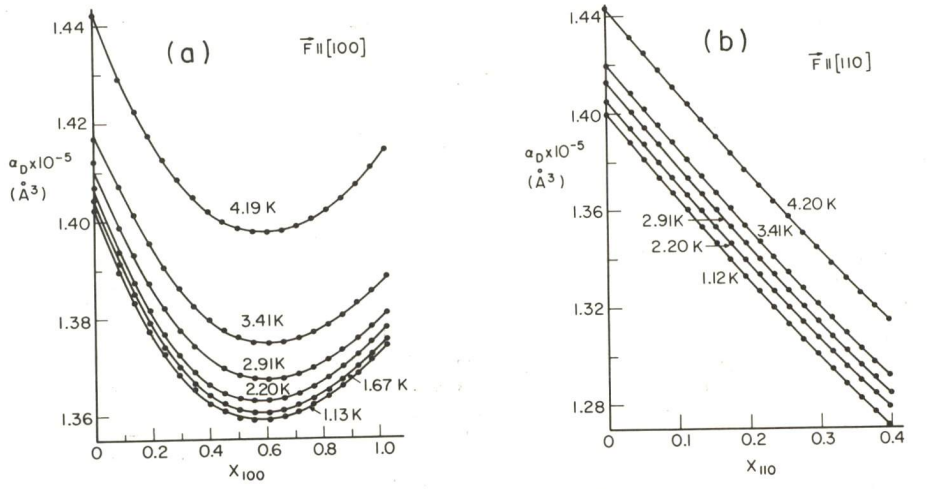

Fig. 1 $\alpha_D(x)$ versus x for Si:P ($N_D\sim5\times10^{17}$/cm³), a)[100], b)[110]

III. Theory of the Strain-Dependent Donor Polarizability

Using the VRM, with valley occupation coefficients $C_j(x)$ for a [100] axis stress of the form $(C_B,C_B,C_A,C_A,C_A,C_A)$ {$C_B(x)$ and $C_A(x)$ given in [2]}, and strain-dependent Bohr radii $a_j(x)$ for the stress-raised and stress-lowered valleys [1] we have shown[6] that

$$\alpha_D(x_{100}) = f_u\,\alpha_\perp + 2C_A^2\,[f_\ell(\alpha_\parallel+\alpha_\perp)] \quad , \qquad (2)$$

where $f_u=[a(x_{100})/a(0)]_u^3$ and $f_\ell=[a(x_{100})/a(0)]_\ell^3$ are factors giving the contribution to $\alpha_D(x_{100})$ from the $a_j(x)$ for the upper and lower valleys respectively. $\alpha_\parallel$ and $\alpha_\perp$ are the single valley polarizability components parallel and perpendicular to the valley axis. For the

effective mass approximation (EMA) case Dexter[7] found that $\alpha_{EMA}=\frac{1}{3}(\alpha_{\parallel}+2\alpha_{\perp})=4.328\times10^5$ Å^3, with $\alpha_{\perp}/\alpha_{\parallel}=2.123$ for $\varepsilon_h=11.4$, $m_{\parallel}/m=0.9163$, and $m_{\perp}/m=0.1905$. Using a series expansion and valley coupling parameters for Si:P we obtain[6] $\alpha_D(x)/\alpha_D(0)=[1-0.0866x+0.0560x^2-0.0072x^3+\ldots]$. This result yields an initial slope at x=0 only 2/3 of the experimental slope and produces a minimum at x~1.3, or more than twice the experimental value for Si:P. Neglecting the strain-dependent Bohr radii ($f_u=f_\ell=1$) the comparison with the data is even worse. Although the initial slope can be forced equal to the experimental slope by setting $\alpha_{\perp}/\alpha_{\parallel}=3.7$ this pushes the minimum out to x~2 and makes the overall agreement poorer. A strain-dependent $\Delta(x) = \Delta(0)[1+ax+bx^2+cx^3+\ldots]$ can be introduced to force-fit Eq. (2) to the data but the coefficients are large and arbitrary.

A new calculation of $\alpha_D(x)$ has been made using the Hassé variational approach employed for the donor polarizability enhancement[8] $\alpha_D(N_D)/\alpha_D(0)$ as $N_D\to N_c$ [N_c is the concentration for the insulator-metal transition]. The strain-dependent ground state wave function for a [100] axis strain will be

$$\psi_{GS}(\vec{r},x) = \gamma(x)\psi_{A1}(\vec{r},\, a_A(x)) + \beta(x)\psi_{Ea}(\vec{r},\, a_E(x)) \ , \qquad (3)$$

where the c_j are $(1/6)^{\frac{1}{2}}(1,1,1,1,1,1)$ for the ls-A_1 state and $(1/12)^{\frac{1}{2}}(-2,-2,1,1,1,1)$ for the ls-E_a state and $\gamma(x)$ and $\beta(x)$ are related to $C_A(x)$ and $C_B(x)$ of the VRM by $\gamma(x)=(2/3)^{\frac{1}{2}}(2C_A+C_B)$ and $\beta(x)=(4/3)^{\frac{1}{2}}(C_A-C_B)$. $a_A(x)$ and $a_E(x)$ are strain-dependent Bohr radii for the ls-A_1 and ls-E_a states. Calculating $\alpha_D(x)$ with the trial wave function $\psi_t=\psi_{GS}(\vec{r},x)(1+bz+crz)$ for an electric field along the z-axis yields the results for $\alpha_D(x)/\alpha_D(0)$ shown in Fig. (2) for Si:P. The VRM-EMA curve for $E_{1s}=E_{EMA}$=constant has too small a slope and shows no sign of a minimum. The lower VRM]$_{\Delta(0)}$ curve with $E_{GS}(x)$, $a_A(x)$ and $a_E(x)$ has almost the correct slope at x=0, but falls too steeply. The calculated curve (×) with $\Delta(x)=\Delta(0)[1+0.01x-0.145x^2+0.042x^3]$ gives an excellent fit to the data (●). For the [110] axis case $\alpha_D(x)/\alpha_D(0)$ is well fit by $\Delta(x)=\Delta(0)[1+0.04x-0.115x^2]$, which differs slightly from the [100] axis results. The [100] axis data for a Si:Sb sample can be fit with $\Delta(x)=\Delta(0)[1-0.0635x-0.050x^2+0.004x^3]$.

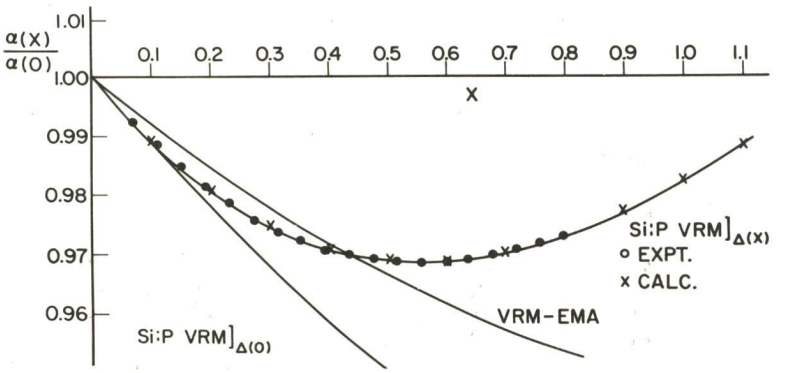

Fig. 2 Calculated $\alpha_D(x_{100})/\alpha_D(0)$ versus x compared with Si:P data

The $\psi_{GS}(\vec{r},x)$ in Eq. (3) yields a donor Fermi contact piezohyperfine interaction proportional to $|\psi_{GS}(r=0,x)|^2\propto\gamma^2(x)(1/a_A(x))^3$ since $\psi_{Ea}(\vec{r}=0,x)=0$. Previous work[2] considered only the VRM with a constant $a_A(0)$ and thereby inferred too large a value of Ξ_u. With a small increase on $a_A(x)$ with x_{100} one can explain the donor piezohyperfine

interaction with E_u=8.6 eV, in agreement with an optical result[9]. In Fig. (3a) $a_A(x)$ and $a_E(x)$ are shown versus x_{100} for the two cases $\Delta(0)$ and $\Delta(x)$, the latter for the results above yielding good agreement for $\alpha_D(x)/\alpha_D(0)$. $a_E(x)$ shows a significant increase which decreases slightly at large x for the $\Delta(x)$ case. However, $a_A(x)$ gets

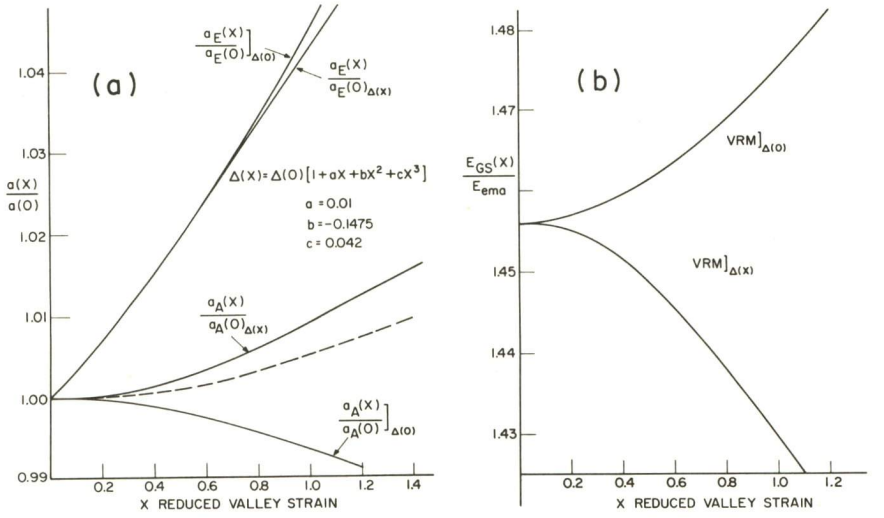

Fig. 3 Bohr radii $a_A(x)$ and $a_E(x)$ and energy $E_{GS}(x)$ vs. x for Si:P

slightly smaller for the $\Delta(0)$ case and slightly larger for the $\Delta(x)$ case. The latter result is in qualitative agreement with the Bohr radius (dashed line) required to explain the donor piezohyperfine interaction. Figure (3b) shows the ground state energy $E_{GS}(x)$ for the two cases $\Delta(0)$ and $\Delta(x)$. Contrary to the Wilson-Feher results[2] $E_{GS}(x)$ for the $\Delta(x)$ case decreases in magnitude in agreement with the increase in $\alpha_D(x)/\alpha_D(0)$ for $x_{100}>x_{100}^{min}$. In summary the donor $\alpha_D(x)/\alpha_D(0)$ and piezohyperfine data agree qualitatively when self-consistent changes in $a_A(x)$, $a_E(x)$, $\Delta(x)$ and $E_{GS}(x)$ are considered.

Another interesting aspect of the results is the surprisingly small N_D-dependence of $\alpha_D(x)/\alpha_D(0)$ from $6\times10^{16}/cm^3$, where isolated donors dominate, to $1.9\times10^{18}/cm^3$ where clusters are expected to dominate in their contribution to $\varepsilon(N_D)-\varepsilon_h$. In the low temperature limit only x_{100}^{min} seems to change with increasing N_D.

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1) H. Fritzsche: Phys. Rev. 125 (1962) 1552; ibid 125 (1962) 1560.
2) D. K. Wilson and G. Feher: Phys. Rev. 124 (1961) 1068.
3) E. B. Hale and T. G. Castner: Phys. Rev. B1 (1970) 4763.
4) R. A. Faulkner: Phys. Rev. 184 (1969) 713.
5) M. Cardona, W. Paul, and H. Brooks: Proc. Int. Conf. on Solid St. Phys. in Elect. and Telecomm., Brussels(1958); J. Phys. Chem. Solids 8 (1959) 204.
6) H. S. Tan and T. G. Castner: Phys. Rev. B, to be published.
7) D. L. Dexter: Proc. of 13th Int. Semicond. Conf., Rome(1976) 1137.
8) T. G. Castner: Phys. Rev. B21 (1980) 3523.
9) I. Balslev: Phys. Rev. 143 (1966) 636.