Influence of Defects on the Splitting of the Acceptor Ground State in Silicon

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The distribution of strain fields from specified defects in otherwise pure silicon crystals is reflected in the resulting distribution of splittings E of the partially orbitally degenerate Γ_8 ground state of effective mass acceptors. The spectral density N(E) can be probed by resonant scattering of $h\nu = E$ ultrasonic [1] or $3.8\ kT \cong E$ thermal phonons [2]. The results of both methods (in the following: $\alpha(\nu)$ and $\kappa(T)$) are compared for Si(B) and Si(In) crystals containing definite amounts of C and O [Tab.1]. Monte Carlo calculations (M.C.) for point defects and for 60^0 dislocations in Si (isotropic approximation) have been made to obtain N(E) as well as $D_1(E)$, the latter being the mean coupling constant of a specified phonon (L,T1,T2,[100],[110],[111]) to splittings at E. This average coupling for all 9 types of phonons practically does not depend on E and therefore presumably also for the thermal phonons. Thus, though in both experiments $D_1^2(E)\cdot N(E)$ is measured the form of N(E) is preserved and D_1 can be estimated by integrating over the whole distribution normalizing with $n_a = \int N(E)dE$. The calculated distribution for point defects derives from Lorentzians and from Gaussians for dislocations. Fig.1 shows $D_1^2\cdot N(E)/n_a$ for Si(B) crystals with various concentrations of point defects from $\alpha(\nu)$. Analysis shows that only for the crystal with the highest concentration of point defects (S 80) $D_1^2\cdot N(E)/n_a$ can be fitted by the calculated "Lorentzian". The smaller the concentration the more "Gaussian" is mixed into N(E) merging into the quasi Gaussian residual distribution of unknown origin of the pure crystal S 87. S125 and S 54 of Fig.2

Fig. 1

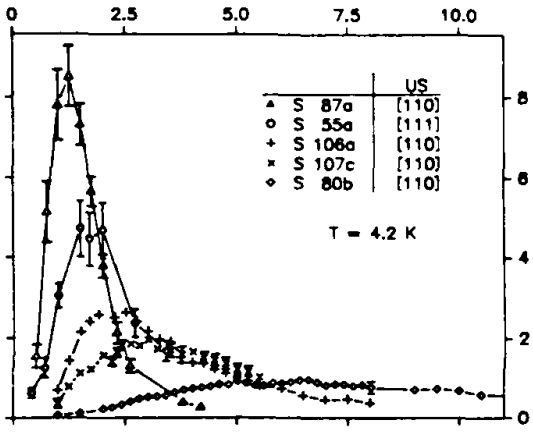

Fig. 2

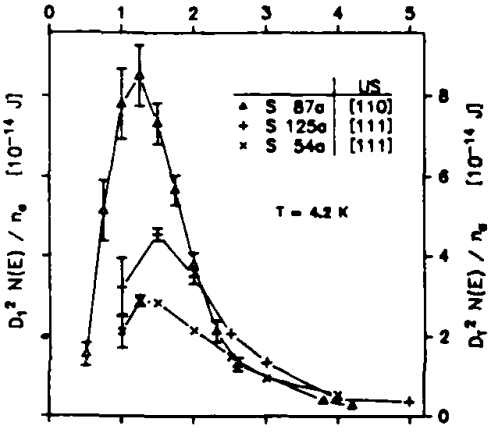

Fig.1. Splitting distribution of Si(B) with point defects

Fig.2. Splitting distribution of pure Si for different concentration of boron

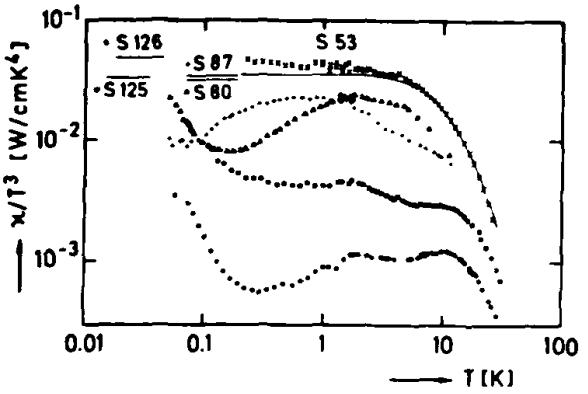

Fig.3. Thermal scattering in Si(B)

are pure crystals with high [B], where a dynamic B-B interaction had been found by hole burning [3]. Possibly an interaction shows up also in these curves, not so much in the form of N(E) but in a reduction of D_1. Analogous results in the form $\kappa(T)/T^3$ vs. T are shown for crystals with as sawn side faces in Fig.3. The extra scattering below 1K is due to the split levels, whereas the depression around 5K - going monotonously with [B]- is interpreted as due to Jahn-Teller resonance scattering [4]. Boundary scattering for the defect-free and undoped S 53c is found to be temperature dependent and about 20 % larger than the theoretical Casimir term. A check with chemically polished side faces and also with an extra dummy collar showed that there is only negligible change for the S 80 but that thermometer mounting and strains from side face damage may have a significant influence for S 87 with narrow distribution. For the S 53 with polished side faces $\kappa(T)/T^3$ increases by about 1.6 at 2 K to 3.4 at 60 mK. These facts make it difficult to analyse narrow distributions of small acceptor concentrations where the extra scattering is at low temperatures and weak. In crystals with high [B] (S 125,S 126) the scattering regime is much larger than expected from $\alpha(\nu)$. Again the S 80 can be fitted by the calculated distribution but with a maximum at 8.3 GHz instead of about 6.5 GHz as obtained from $\alpha(\nu)$. The experimental/theoretical average coupling constants are 1.22/1.2 eV and 1.94/2.22 eV for $\kappa(T)$ and $\alpha(\nu)$ respectively.

Table 1: Si(B) samples

sample	ρ[Ωcm]	concentrations [10^{21}m^{-3}] [B]	[O]	[C]	ν_{max} in GHz from $\alpha(\nu)$	$\kappa(T)$
S 53*	>2500.0	0.005	< 0.5	–		
S 54*	0.3	85.0			1.2	
S 55	1.6	9.0	< 2.0	75.0	1.7	
S 80	10.85	1.2	570.0	41.0	6.5	8.3
S 87*	2.5	5.4	< 2.0	< 5.0	1.2	4.6
S 106		5.0	<20.0	200.0	2.2	
S 107		1.8	<20.0	280.0	2.8	
S 125*	0.74	24.0			1.2	
S 126	0.3	85.0	200.0	<50.0		10.4

* Wacker chemitronic, waso quality

For Si(In) the deformation potential constants being about 0.6 of those of Si(B), one would expect the distributions and the phonon scattering to be correspondingly smaller.A possible In-In interaction should set in at a concentration about 8 times larger than for B be-

cause of the smaller Bohr radius. In Tab. 2 reliable figures for the concentration can be given only for samples S 52 and S 123 where temperature-dependent Hall measurements have been made [5]. The results of $\kappa(T)$ are normalized to the pure case to show the additional scattering [Fig.4]. The Jahn-Teller resonance at about 20 K increases monotonously with [In] whereas the scattering at low temperatures is due to the splitting distributions. For S 123 from $\alpha(\nu)$ we get E_{max} = 3.2 GHz as compared to ~5 GHz from $\kappa(T)$. Estimating the elastic strength A from the covalent radii gives A_{In}/A_C= 0.68 and taking into account the deformation potential constants one would obtain E_{max}=0.5 GHz from M.C. For the S 52 with high concentration of point defects a fit somewhat broader than "Lorentzian" gives E_{max} = 14.5 GHz, whereas from M.C. one would expect E_{max} < 9 GHz if the indicated figures for [In] and [O] are correct. The deformation potential constant from this analysis is 0.24eV as compared to the theoretical value 0.72 eV. Since [In] is rather high the reduction could be due to an In-In interaction in analogy to the case of boron.

Table 2: Si(In) samples

sample	ρ[Ωcm]	concentrations [$10^{21}m^{-3}$] [In]	[O]	[C]	ν_{max} in GHz from α(ν)	κ(T)
S 33	2.0		700.0			
S 52	0.1	500.0	800.0			14.5
S 123	1.29	100.0	<10.0	< 1.0	3.2	≈ 5
S 196	0.55					

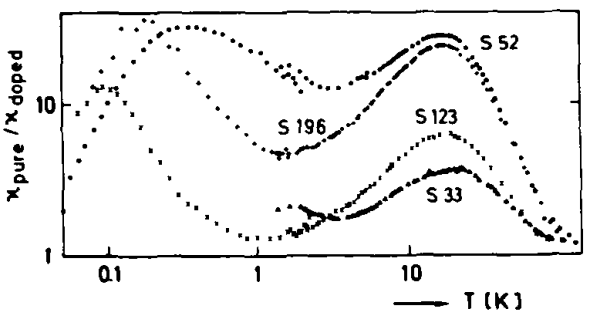

Fig.4. Thermal scattering in Si(In)

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2 A.M.de Goer, M.Locatelli and K.Laßmann, J. de phys. 42 C 6-235(81)
3 H.Zeile, U.Harten and K.Laßmann, Phys. Stat. Sol. (b) 111,213(82)
4 J.Maier and E.Sigmund, these Proceedings
5 S 52 obtained by J.S.Blakemore (sample 260 in PR B4 1873(71))
S 123 obtained by R.Helbig, Univ. Erlangen (sample Ru 237/1-1b)