Deep Level Near E_C - 0.55 eV in Undoped 4H-SiC Substrates

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Abstract. A variety of 4H-SiC samples from undoped crystals grown by the physical vapor transport technique have been studied by temperature dependent Hall effect, optical and thermal admittance spectroscopy and thermally stimulated current. In most samples studied the activation energies were in the range 0.9 - 1.6 eV expected for commercial grade HPSI 4H-SiC. However, in several samples from developmental crystals a previously unreported deep level at E_C-0.55 ± 0.01 eV was observed. Thermal admittance spectroscopy detected one level with an energy of about 0.53 eV while optical admittance spectroscopy measurements resolved two levels at 0.56 and 0.64 eV. Thermally stimulated current measurements made to study compensated levels in the material detected several peaks at energies in the range 0.2 to 0.6 eV.

Introduction

The semi-insulating properties of high purity semi-insulating (HPSI) SiC are produced by compensation of residual shallow impurities by intrinsic deep levels with activation energies near the center of the band gap rather than by transition element impurities. The thermal activation energies of these intrinsic deep levels are in the range 0.9 to 1.5 eV.[1,2] A variety of intrinsic defects have been observed in this material by electron paramagnetic resonance (EPR), including vacancies, antisites and complex defects.[3-5] However, it has been very difficult to correlate electronic levels from Hall effect and resistivity measurements with the defects detected by EPR. We report here additional studies of temperature dependent Hall effect experiments on HPSI SiC, including the observation of a previously unreported level at E_C-0.55 ± 0.01 eV in addition to previously reported levels near E_C-1.0 eV. Both optical and thermal admittance spectroscopy (OAS and TAS) measurements confirm the 0.55 eV activation energy. Thermally stimulated currrent measurements suggest that compensated defects are similar to those in samples with higher activation energies.

Experimental Details

The HPSI 4H-SiC crystals in this study were grown at Cree, Inc. by the Physical Vapor Transport (PVT) process as part of a research and development contract. These research crystals were grown using high purity source material without intentional doping but do not necessarily represent commercial quality material. Most samples were oxidized at 1150°C for several hours followed by an etch to remove surface damage. Ohmic contracts for the van der Pauw samples used in temperature dependent Hall effect (TDH) and resistivity experiments were formed by alloying Ta/NiCr/W at 925°C for two minutes in forming gas. Schottky contacts for TAS and OAS were made by depositing unannealed indium tin oxide dot grid patterns. TSC experiments are described elsewhere in this conference.[6] For this experiment, indium solder was used for ohmic contacts and the samples did not recieve the oxidation step. TAS and TSC samples were taken from the same wafers as the TDH samples and as close together as possible.

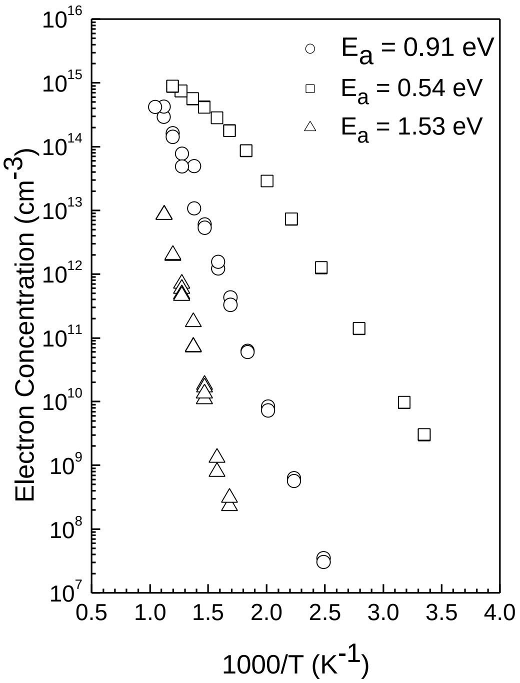

Fig. 1: Concentration versus inverse tempeature for HPSI 4H-SiC samples with different activation energies: A = 0.54, D = 0.91 and E = 1.53eV.

Results

Fig.1 shows the electron concentration versus inverse temperature results for three HPSI samples representing the range of activation energies observed in this study. These and all other samples studied that had measureable Hall voltages had n-type conduction. Activation energies in the range 0.9 to 1.6 eV are typical of high quality HPSI 4H-SiC and have been reported previously.[1,2] The 0.54 eV activation energy in Fig. 1 is unusual and is the focus of this study. This level was found in samples from three separate crystals. It should be noted here that while E_a is significantly lower than that observed is standard HPSI material, the 0.55 eV level is still deep enough to make the material semi-insulating with room temperature resistivities greater than 10^5 Ωcm. The activation energy and concentration of the defects present in the material, along with the compensating acceptor concentration, were determined by fitting the charge balance equation at each temperature point in a manner similar to that of Götz et al.[7] The number of conduction band minima, M_C, in the charge balance equation was taken to be 3 and the electron effective mass was assumed to be 0.390. A degeneracy factor, g, of 2 was assumed for donor type defects. In two of the three samples the best fit was obtained by assuming two deep levels. The fitting results are given in Table I. It should be noted that the accuracy of the energy for the deeper level is significantly less than the lower energy because of the lack of higher temperature data. The acceptor concentrations are similar to values determined from separate fits to the temperature dependence of the mobility and to those reported by Cree, Inc.[1]

Table I: Hall effect fitting results for 0.55 eV level samples, N_{di} = deep level concentration, E_{di} = deep level activation energy, N_a = total compensating acceptor concentration.

Sample	N_{d1} (cm^{-3})	E_{d1} (eV)	N_{d2} (cm^{-3})	E_{d2} (eV)	N_a (cm^{-3})
A	1.01E15	0.541	8.77E14	0.72	5.04E14
B	3.09E15	0.555			3.39E14
C	1.09E15	0.564	1.35E15	0.80	4.29E14
Ave E		0.553		0.76	

TAS and OAS measurements were made to confirm the presence of a level at 0.55 eV. Figure 2 show a TAS spectra for a sample wafer A. Fits to the Arrhenius plot of the peak frequency to inverse temperature gave an activation energy of 0.551 eV, in very close agreement with the TDH results. OAS measurements were made on the same same sample and results are shown in Fig. 3. Peak fitting of the spectra indicated four peaks, two strong peaks at 0.55 and 0.64 eV that merge to make the dominant spectral feature around 0.6 eV, and two on the high energy shoulder at 0.76 and 0.83 eV. These could be hexagonal and cubic lattice site levels for the 0.55 eV level and the deeper level at 0.72 seen in TDH. However, the deeper OAS levels, at nearly the same energy, were also observed in sample B.

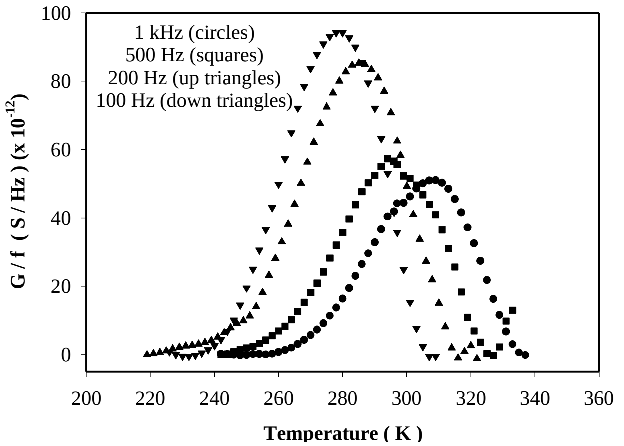

Fig. 2: Thermal Admittance Spectroscopy results for HPSI 4H-SiC sample A.

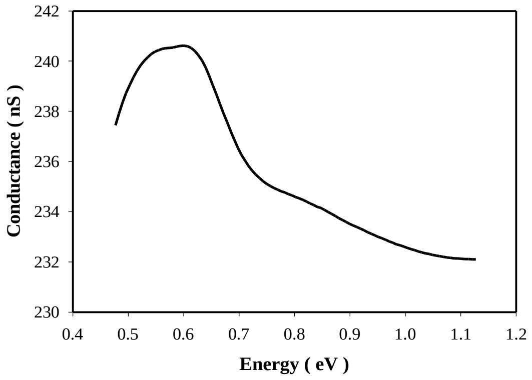

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Fig. 3: Optical Admittance Spectroscopy for sample A.

TSC experiments were performed on samples from wafers A, B, D and E. The dark current was recorded as the samples cooled and an activation energy for the conductance was extracted. Activation enegies of 1.4 and 1.04 eV were measured for samples E and D respectively, which argee well with the 1.53 eV and 0.91 eV TDH values. The TSC activation energy for samples A and B, however, were both 0.26 eV. This energy has been observed in several semi-insulating SiC samples with activation energies from 0.9 to 1.6 eV and is presently assumed to be related to activation from surface defects. The TSC scans themselves gave similar defect levels for most of the samples studied here. The results are presented in Table II where peaks at similar temperatures are associated together for different samples. The energies are calculated from the peak temperature using $E_T/kT_m = \ln(T_m^4/\beta)$ where T_m is the peak tempeature and β is the heating rate. Sample F was an additional sample with E_a = 0.93 eV from TDH. The identification of these peaks with specific defects have not been accomplished yet but the similarity of peaks present in the 0.55 eV TDH samples with those xxxxxxxxx. This experiment can not determine which half of the band gap the defect level is located in so we cannot positively correlate peak f (0.53 eV) with the TDH level but it is a definite possibility.

Discussion

The n-type conduction of these samples confirms that the 0.55 eV level observed in TDH measurements is located with respect to the conduction band. However, it cannot be determined if this level is donor or acceptor like, since a

Table II: TSC peaks identified in semi-insulating HPSI 4H-SiC samples.

Sample	a	b	c	d	e	f	g
	(0.20 eV)	(0.25 eV)	(0.30 eV)	(0.34 eV)	(0.37 eV)	(0.53 eV)	
A	-	140K	160K	180K	195K	260K	280K
B	115K	140K	160K	180K	195K	255K	-
D	-	-	-	175K	190K	260K	310K
E	-	135K	160K	-	200K	265K	355K

F	115K	140K	160K	-	195K	260K	320K

compensated very deep acceptor could neutralize by thermally emitting electrons to the conduction band. The fact that the TSC peaks are very similar for 0.55 eV samples and those with deeper activation energies suggests that the compensated levels in the two types of samples are the same. This in turn suggests that the 0.55 eV level might be present in all or most HPSI samples but is compensated by deeper levels. Concentrations in the 10^{15} cm^{-3} range for this defect fall within the range of shallow impurity levels so it could play a major role in the compensation mechanism that results in the semi-insulating properties of standard HPSI material. Annealing studies are underway and will be reported at a later date.

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