Deep traps in high-purity semi-insulating 6H-SiC substrates: Thermally stimulated current spectroscopy

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Abstract. Thermally stimulated current spectroscopy (TSC) has been applied to characterize deep traps in high-purity semi-insulating 6H-SiC substrates. By using above bandgap to sub-bandgap light for illumination at 83 K and different applied biases, at least nine TSC traps in the temperature range of 80 to 400 K can be consistently observed. It is found that TSC peaks for $T < 130$ K are significantly affected by light and some peaks are strongly enhanced by the applied bias. Measured trap activation energies range from 0.15 eV to 0.76 eV. Theoretical fittings of selected traps give more accurate trap parameters. Based on literature results connected with deep traps in *conductive* 6H-SiC, the origin of these TSC traps is discussed.

Introduction

Unintentionally doped high-purity semi-insulating (HPSI) 6H-SiC has been grown by advanced physical vapor transport, which involves in-situ synthesis and growth of SiC [1]. In the HPSI 6H-SiC, background shallow impurities (such as N and B) can be reduced to such low levels (low or mid-10^{15} cm^{-3}) that the electronic transport is dominated by deep centers, which are related to intrinsic point defects. To control the material quality of HPSI 6H-SiC, it is important to understand the nature of these deep traps. In this paper, we investigate HPSI 6H-SiC using thermally stimulated current spectroscopy (TSC), which is known to be a very sensitive technique for studying point-defect and impurity related traps in various SI semiconductors [2-4].

TSC spectroscopy: theory and experiment

TSC spectroscopy involves filling electron traps (above the Fermi-level, E_F) or hole traps (below E_F) at a low temperature and measurement of the thermal emission of carriers from these traps upon warming. Typically, the traps are filled at ~80 K by illumination with near-bandgap light for several minutes, and then emptied by sweeping the temperature at a fixed rate, β (i.e., 0.3 K/s). The emission is thermally activated, so the emission rate, e_n or e_h (for electrons or holes), can be determined approximately from detailed-balance considerations, such as:

$$e_n = s_n N_C v_{th} \exp(-E_T/kT) \qquad (1)$$

where s_n is the capture cross section for the trap, N_C the effective conduction-band density of states, v_{th} the thermal velocity, and E_T the trap energy with respect to the conduction band. A given trap will begin to emit at a characteristic temperature, with the emission rate increasing rapidly according to Eq. (1). However, the emission probability will drop as the trap is depleted of electrons, so the thermally stimulated current I_{TSC} exhibits a peak. Thus, for an electron trap, peaked at T_m, the TSC will be given by [5]:

$$I_{TSC} = C V_b e m_n t_n N_T e_n \exp(-?e_n/b\, dT'), \qquad (2)$$

where e is the electronic charge, μ_n the electron mobility, τ_n the free-electron lifetime, N_T the trap density, V_b the bias voltage, and C a constant related to sample geometry. A fit of the integral equation (2) (or its analytical version [6]) to a TSC peak for a given trap will yield the following fitting parameters: $\mu_n\tau_nN_T$, σ_n, and E_T. However, E_T can be also approximately estimated from the peak temperature T_m, using equation (assuming a small σ) [5]:

$$E_T /kT_m = ln (T_m^4/b) \qquad (3)$$

The present study involves one HPSI 6H-SiC sample (7 x 7 mm^2 in size) with conductivity activation energy of 1.1 eV and 300-K resistivity of ~1 x 10^{11} Ω-cm. For current measurements, indium contacts were soldered onto the sample after degreasing using organic solvents. The sample was always cooled from 400 K to 83 K in the dark. The traps were filled at 83 K using light of 360-nm (above bandgap), 400-nm (near-bandgap), 475-nm (sub-bandgap), or white light produced by using a 15-W halogen lamp and appropriate band-pass filters. Photocurrent (PC) responses were recorded at 83 K during the 5 min sample illumination and for 30 sec with the light off. The TSC spectrum was then measured upon warming at β=0.1-0.4 K/s under V_b=10-80 V. Theoretical TSC data fittings were performed to obtain E_T and σ_n (or σ_p) for the main electron and hole traps.

Results and discussion

Typical 83-K PC responses and TSC spectra, measured using different illumination wavelengths with V_b=40 V, are shown in Fig.1 (a) and (b), respectively. From Fig. 1 (a), we find that each PC response consists of an initial transient (related to the trap-filling process), a saturation region (with trap emission and capture processes equalized), and a decay (related to thermal emission of carriers from shallow traps at T=83 K). From Fig. 1 (b), we see that: i) at least nine traps can be observed, producing TSC features at 90 K, 105 K, 115 K, 155 K, 175 K, 205 K, 265 K, 305 K, and 355 K; and ii) unlike the traps peaked at T>130 K, the TSC signal for the two traps peaked at 90 K and 105 K increases dramatically when using 400-nm and 360-nm light illumination. This observation provides indirect evidence that these are shallow electron traps, since electrons can be easily excited from valence band to the traps by the light. Interestingly, illumination with white light causes the lowest TSC signals for the two traps, showing multi-chromatic light-induced de-trapping.

Low temperature TSC peaks, measured under illumination with either wavelength, show strong effects due to applied bias. Figure 2 shows typical TSC spectra measured using 360-nm light and V_b=10-80 V. For TSC measurements, the sample was immediately warmed following illumination, so the decay of PC (as shown in Fig. 1(a)) produces the initial TSC signals at T<90 K. In contrast to traps at 115 K, 155 K, 265 K, 305 K, and 355 K, which show an intensity proportional to bias, the

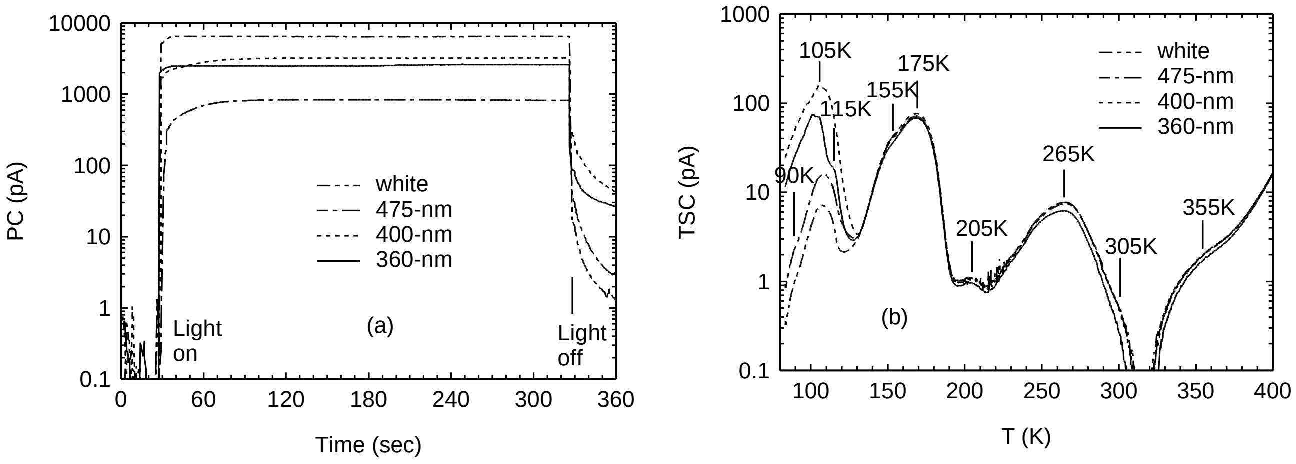

Fig. 1 (a) PC responses at 83 K and (b) TSC spectra, measured with V_b=40 V using different wavelengths.

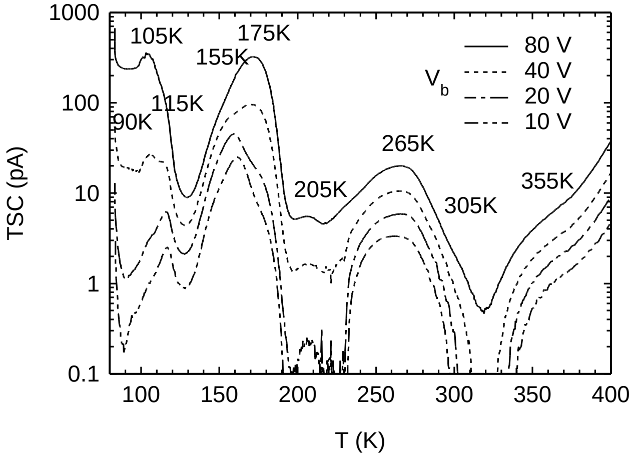

Fig. 2 TSC spectra measured as a function of V_b.

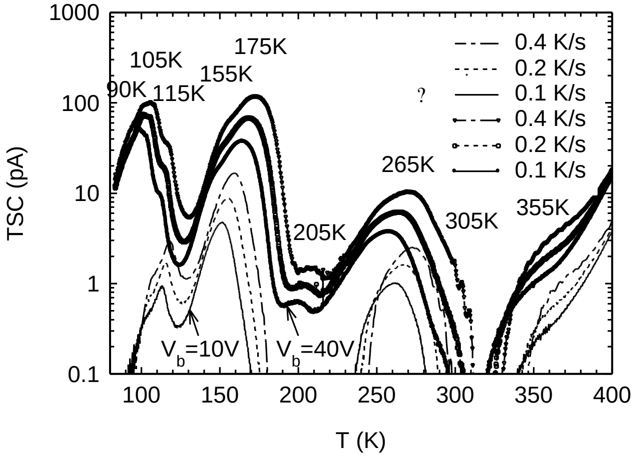

Fig. 3 TSC spectra measured as a function of β.

traps at 90 K, 105 K, 175 K, and 205 K show a significant intensity enhancement with increasing bias. Due to the large enhancement at V_b=80 V, the traps at 115 K and 155 K become shoulders on the peaks at 105 K and 175 K and are less observable. We consider two possible reasons for the super-linear enhancement: i) modification of the effective electron lifetime due to separation of electrons and holes under high bias or strong electric field; or ii) electron injection caused by non-ohmic contacts. Actually, 83-K PC, measured using 360-nm light, shows a super-linear relationship with applied bias, too (not shown here). Based on the understanding of the effects, we tentatively assign traps at 90 K, 105 K, 175 K, and 205 K to be electron traps, and traps at 115 K and 155 K to be hole traps. A significant bias-enhanced trap at ~175 K has also been observed in HPSI 4H-SiC, when using white light illumination [7].

To obtain more accurate trap parameters (E_T and σ) for the main traps at T<300 K, theoretical fits were performed on TSC spectra measured over a range of β, using different light illuminations and biases. The fits assume an effective mass m^*_e= 0.4 m_0 for electrons and m^*_h=1 m_0 for holes. Typical TSC spectra for β=0.1-0.4 K/s, measured using 360-nm light with V_b=10 and 40 V, are presented in Fig. 3. Fitting results were obtained from twenty-four TSC spectra measured using three heating rates, four illumination conditions, and two biases, and they give consistent values of E_T and σ, as follows: 0.14 eV and (4-18) x 10^{-21} cm^2 for the electron trap at 105 K; 0.24 eV and (3-11) x 10^{-17} cm^2 for the hole trap at 115 K; 0.26 eV and (5-12) x 10^{-20} cm^2 for the hole trap at 155 K; 0.28 eV and (6-19) x 10^{-20} cm^2 for the electron trap at 175 K; 0.51 eV and (1.5-5) x 10^{-18} cm^2 for the hole trap at 250 K; and 0.56 eV and (2-6) x 10^{-18} cm^{-2} for the hole trap at 265 K. Typical fitting results for the 10-V and 40-V spectra, measured with β=0.2 K/s as shown in Fig. 3, are presented in Fig. 4 (a) and (b), respectively. We clearly see a significant enhancement of the 105-K and 175-K traps with increasing bias. We estimate E_T as: ~0.15 eV for the electron trap at 90 K; ~0.40 eV for the electron trap at 205 K; ~0.63 eV for the trap at 305 K; and ~0.76 eV for the trap at 355 K.

Deep traps in as-grown and electron-irradiated n- and p-type 6H-SiC samples have been extensively studied by deep level transient spectroscopy (see a review [8] and recent work [9-11]). Based on literature results involving deep traps in *conductive* 6H- SiC, the impurity and point-defect nature of the observed TSC traps will be tentatively assigned as follows: the 90-K and 105-K traps, with E_T=~0.15 and 0.14 eV, are due to N (a major residual donor in 6H-SiC) and probably due to Ti (a common contaminant in SiC) [8,11]; the 115-K trap, with E_T=0.24 eV is due to Al [8]; the 155-K trap, with E_T=0.26 eV, is due to major residual acceptor B in a hexagonal site [9]; the 175-K trap, with E_T=0.28 eV, is due to ED2; and the 205-K trap, with E_T=~0.40 eV, is due to E_1/E_2 [10]. The 250-K trap, with E_T=0.50 eV, may be due to i-center (hole trap) [8] or E_i (electron trap) [10]. The 265-K trap, with E_T=0.56 eV could be related to the D-center (a B related complex) [8]. The 305-K trap, with E_T=~0.63 eV, could be due to the Z_1/Z_2 center [8,10]. The 355-K trap, with E_T=~0.76 eV,

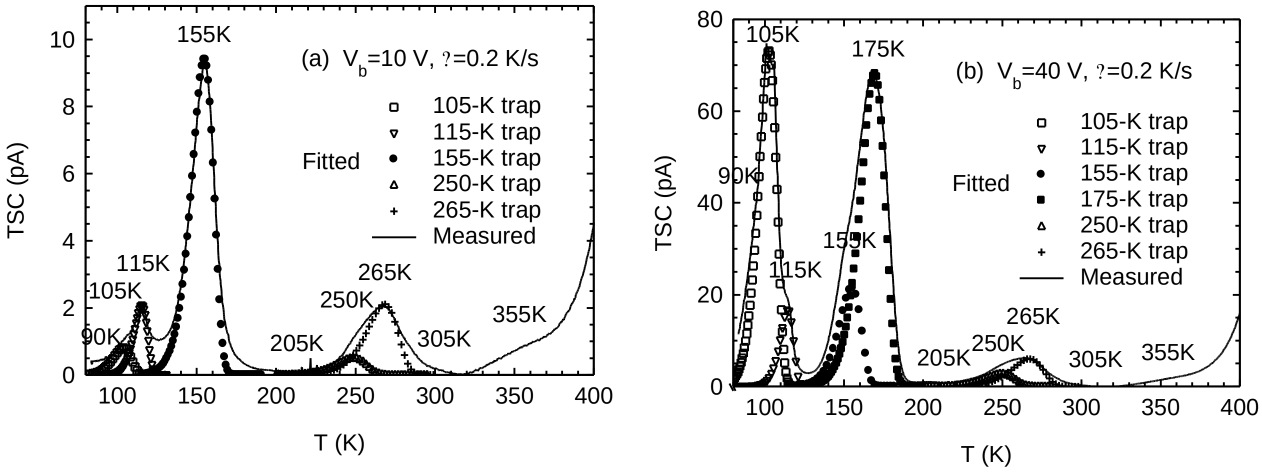

Fig. 4 Measured and fitted TSC spectra at (a) V_b=10 V and (b) V_b= 40 V, using 360-nm light illumination.

could be due to vanadium or a point-defect, since this center was strongly increased after 1-MeV electron-irradiation in a 6H-SiC layer grown by CVD on either standard or porous substrates [11].

In summary, at least nine deep traps in an HPSI 6H-SiC sample have been characterized by TSC spectroscopy. Theoretical fittings of selected TSC traps at T<300 K, measured using different heating rates, illumination conditions, and applied biases, give consistent trap parameters. Based on literature results connected with impurity and point-defect related deep traps in *conductive* 6H-SiC, the possible origins of these traps have been discussed.

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