# Complete set of deep traps in semi-insulating GaAs

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Reevaluation and recalculation of thermally stimulated current (TSC) data from semi-insulating (SI) GaAs, published by many different authors over a period of three decades were done by means of the new analytical method, simultaneous multiple peak analysis (SIMPA). The SIMPA procedure clearly resolved contributions from various overlapping TSC peaks and enabled the precise determination of signatures (activation energy, $E_a$ and capture cross section, $\sigma$) of all observed deep traps. The analyzed TSC spectra refer to SI GaAs samples that have been grown/treated in quite different ways (various growth techniques, growth under As or Ga rich conditions, different annealing procedures, irradiation with neutrons, $\gamma$ rays, etc.). Although the SIMPA procedure was applied to apparently quite different TSC spectra, in all cases excellent fits were achieved, with the unique set (or subset from it) of eleven different deep traps, the only difference being in relative and absolute concentrations of traps. Despite a broad variety of samples analyzed in this article, the set of deep traps obtained is the same as the one being previously seen in the narrow range of SI GaAs samples. This finding suggests that this set of traps is a finite and complete set of all defects with deep levels in SI GaAs. It was also concluded that these defects are primarily complexes containing simple native defects. © *2000 American Institute of Physics.* [S0021-8979(00)05820-5]

## I. INTRODUCTION

Semi-insulating (SI), undoped GaAs is an important material being used as a substrate for integrated circuits and field effect transistor technologies. The performance of those devices is essentially influenced by the quality of the substrate, which depends on the concentration of native defects, chemical impurities, and complexes having deep energy levels in band gap. Hence, it is very important to monitor, understand and control defects with deep levels in order to produce high quality substrates.

The EL2 level, main deep donor level situated in the middle of the forbidden energy gap, enables high resistance of the undoped GaAs crystals by compensation of residual shallow acceptors. Beside the omnipresent EL2 level there are other defects with deep levels in the undoped SI GaAs energy gap for which it was recently found that also play an important role in low-temperature transient phenomena like photosensitivity,[1–6] Hall mobility,[7] and EPR signals.[8,9] Furthermore, they affect temperature dependence of photoconductivity[2,10,11] and persistent photocurrents,[2,11] as well. Several of these levels show metastability-like behavior similar to that of EL2 level[3,12] indicating their possible microscopic connection with EL2. It has also been shown that most of these defects are electron traps.[13–15]

Characterization of deep traps means the determination of their main parameters, (''trap signature''), particularly activation energy, $E_a$, and capture cross section, $\sigma$, as well as determination of trap concentration, $N_T$, which has been an object of investigation of many different research groups, and the results up to 1992 have been analyzed and systematized in Ref. 16. As visible from this review, most reports give only limited and insufficient trap parameters, primarily $T_m$ (temperature at which particular peak has maximum) and $E_a$. The $\sigma$ as well as trap concentrations were rarely evaluated and in most cases only for a few dominant traps.[13,14,17,18]

Great discrepancies in reported main trap parameters are obvious; up to four orders of magnitude for $\sigma_n$, for example, Ref. 16. Reasons for such a large difference in reported data for supposedly the same peaks, as well as for the incompleteness of data for most deep traps in SI-GaAs are numerous, especially limitations of applied analytical methods and approximations,[16] and particularly the fact that all these methods are based on a single peak analysis. Since in practically all present SI GaAs materials a number of deep levels are present, the interference of various peaks is practically inevitable, particularly in cases when different traps have similar $E_a$.

Thermally stimulated current (TSC) spectroscopy is a well known and often used method for characterization of deep levels in SI materials,[1,2,10,12–16] especially since capacitance methods [like deep level transient spectroscopy (DLTS)] cannot be applied. The simplicity is an additional advantage of TSC, because it gives qualitative information on various deep levels in a single temperature run.

The interpretation of TSC spectra is complicated since measured peak positions are dependent on various parameters. Fasbender *et al.*[19] demonstrated the quantitative dependence of a TSC peak on the heating rate, capture cross section, kinetics order, and initial trap occupancy. The peak position can be significantly shifted by each of the above-

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mentioned parameters (up to several tens of Kelvin), so that an evaluation of activation energies exclusively from the peak temperature $T_m$ results in large uncertainties. Furthermore, the existence of different traps which release their charge carriers simultaneously may lead to an additional shift of apparent peak maximum. As the TSC spectrum is usually formed from the contributions of closely spaced levels, in single peak analysis it is necessary to perform so-called ''thermal cleaning procedure'' or some other procedure for the isolation of one peak from the spectrum. Errors in such treatments are just summed up and propagated through further analysis. When $E_a$ is known, the other important parameter, $\sigma$, can be estimated.[16] Since $\sigma$ varies exponentially with $E_a$, even small errors in $E_a$ greatly magnify errors in $\sigma$. There are some modified TSC measurement techniques like fractional thermally stimulated currents (FTSC)[19] which improved the reliability of TSC data interpretation, but measurement becomes cumbersome and significantly longer (10–50 times), while some problems still remain unresolved.

To improve the reliability of TSC spectra interpretation, while still retaining the simplicity of the measurement, a new analytical method, simultaneous multiple peak analysis (SIMPA) which comprises simultaneous fitting of whole measured TSC spectra was introduced recently.[20] The procedure clearly resolves contributions from various overlapping TSC peaks and minimizes total error which results in much more precise determination of parameters (signature) for each trap. Some key ideas of the SIMPA method are presented in Sec. II.

In this article we are presenting results of SIMPA fitting of previously measured and published TSC spectra obtained from different SI GaAs samples, distinguished by quite different growth and post-growth treatments, different annealings and irradiation with neutrons and $\gamma$ rays. TSC curves of many different research groups,[13,14,17,22–41] reported over the time period of three decades, were digitally scanned from the original papers and subsequently subjected to SIMPA fitting. Although measured TSC spectra appear very different (due to different trap concentrations and different parameters of measurements, particularly heating rate) they all can be excellently fitted with the finite set of not more than eleven different deep trap parameters. Hence, no additional traps were observed whatsoever in comparison with the TSC and SIMPA results obtained from a much narrower set of SI GaAs samples.[21] These findings indicate that the number of deep traps (and respective defects) in SI GaAs seems to be finite and limited, which is opposite to previous reviews[42,43] where, probably due to the imprecisions in determination of trap ''signatures'' the presence of a much larger total number of different deep levels in SI GaAs was suggested.

## II. ANALYSIS

### A. Data acquisition

Data taken for the reevaluation in this work were obtained from papers published by more than twenty different authors/groups over a period of three decades. First, respective TSC curves were enlarged to approximately the same size to ensure comparable resolution. Subsequently, spectra were subjected to digital scanning using Calcomp Drawing Board III (model 34120) with resolution of 2540 lpi, so prepared data files were then ready for the SIMPA fitting procedure.

### B. Analysis of TSC spectra by the SIMPA method

All TSC spectra were subjected to the new analytical method—SIMPA.[20] This method is based on the description of TSC spectrum as a sum of TSC peaks belonging to specific deep levels, and dark current, $I_{\mathrm{dark}}$. Temperature dependent fitting function, $I_{\mathrm{SIMPA}}(T)$, comprising the sum of all features of the TSC spectrum was built as

$$I_{\mathrm{SIMPA}}(T)=\sum_{i=1}^{m} I^{i}_{\mathrm{TSC}}(T)+I_{\mathrm{dark}}(T), \tag{1}$$

where $I^{i}_{\mathrm{TSC}}(T)$ represents single $i$th TSC peak, $m$ is the total number of deep traps taken in calculations, and $I_{\mathrm{dark}}(T)=C\exp[-E_{\mathrm{EL2}}/kT]$. $C$ is a constant, $E_{\mathrm{EL2}}$ is donor (EL2) activation energy and $k$ is Boltzmann's constant.

In the ''first order kinetics'' approximation, single TSC peak, resulting from an electron trap can be described as[20]

$$I^{i}_{\mathrm{TSC}}(T)=K_G\mu_n N_{\mathrm{Ti}}\tau_n D_{t,i}T^2 \times\exp\left[-\frac{E_{a,i}}{kT}-\frac{kD_t}{\beta E_{a,i}}T^4 e^{-E_{a,i}/kT} \times\left(1-4\frac{kT}{E_{a,i}}+20\frac{k^2T^2}{E^2_{a,i}}\right)\right]. \tag{2}$$

$K_G$ denotes geometrical factor expressed as $K_G=eAE$, where $e$ is an electron charge, $A$ is the area of electrode, and $E$ is applied electric field. $N_{\mathrm{Ti}}$ is a carrier density of the filled $i$th deep traps at the beginning of the temperature ramp. $\mu_n$ and $\tau_n$ denote electron mobility and free lifetime, respectively. $E_{a,i}$ is $i$th trap activation energy and $\beta$ denotes heating rate. $D_{t,i}$ is the trap dependent coefficient which includes electron capture cross section ($\sigma_{n,i}$) and it is defined as:[20] $D_{t,i}=3.0\times10^{21}(m^*/m_0)\sigma_{n,i}$, with $m_0$ and $m^*$ representing electron rest and effective mass, respectively. $\sigma_{n,i}$ is practically $T$ independent for most of the deep traps in SI GaAs.[44] The function defined with Eq. (1) was used as the fitting function, with $E_{a,i}, D_{t,i}(\sigma_{n,i})$, as well as the product $K_G\mu_n N_T\tau_n$ taken as unknowns. Whenever $\beta$ was not specified in the original data, it was taken as another unknown (fitting parameter), otherwise the proper reproduction of $\beta$ by fitting was taken as an additional check of the validity of the fitting procedure. Analogous formulas are valid for hole traps as well. If the photocurrent temperature dependence was available, as well as geometrical constants, relative and absolute concentrations of respective deep traps could be evaluated.[20,45]

### C. Survey of reported deep trap parameters in SI GaAs

Table I presents a survey of deep trap signatures obtained by different authors from their TSC measurements and analysis. Our recent results, which represent average val-

TABLE I. Survey of TSC deep trap studies of SI GaAs. For each trap peak maximum temperature, $T_m$/K (first value), activation energy, $E_a$/eV (second value), and capture cross section, $\sigma\times10^{-17}$/cm$^2$ (third value) are shown for each trap.

| $T_i$/Reference | $T_0$ | $T_1$ | $T_{2a}$ | $T_{2b}$ | $T_3$ | $T_4$ | $T_{4a}$ | $T_5$ | $T_6$ | $T_7$ | $T_8$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 13 $T_m$/K | | 105 | | 124 | 141 | 156 | | 191 | 212 | 250 | |
| $E_a$/eV | | 0.18 | | 0.21 | 0.24 | 0.28 | | 0.35 | 0.46 | 0.53 | |
| $\sigma\times10^{-17}$/cm$^2$ | | | | 0.09 | 0.1 | | | 10 | | | |
| 14 | | 95 | 111 | 126 | 141 | 156 | | 191 | 212 | 250 | |
| | | 0.15 | 0.19 | 0.22 | 0.25 | 0.28 | | 0.35 | 0.46 | 0.53 | |
| | | 0.05 | | 0.07 | 0.08 | | | | 30 | | |
| 22 | | 96 | 114 | 130 | 145 | 153 | 185 | 206 | 223 | 242 | 256 |
| | | 0.18 | 0.225 | | 0.275 | | | 0.42 | 0.46 | | |
| | | 200 | 0.07 | | 800 | | | $10^4$ | | | |
| 23 | | | | | | | | | | | |
| | | 0.18 | 0.22 | 380 | 0.27 | | 0.36 | 0.42 | | | |
| | | 150 | 1500 | | | $6\times10^4$ | $2\times10^4$ | | | | |
| 24 | 85 | 102 | 113 | 125 | 135 | | 170 | 195 | 225 | | |
| | 0.16 | 0.19 | 0.21 | | | | | | | | |
| 25 | | 92.4 | 115 | | 139 | | 177 | 203 | 215 | 235 | |
| | | 0.15 | | | 0.31 | | 0.34 | 0.51 | | | |
| 26–28 | | 97 | 114 | 125 | 140 | 151 | | 189 | 210 | 233 | 250 |
| | | 0.17 | 0.21 | 0.23 | 0.27 | 0.29 | | 0.40 | 0.44 | 0.50 | 0.54 |
| | 1.8 | 3.6 | | | 1900 | | | $1\times10^4$ | $2\times10^4$ | | |
| 29 | 76 | | 111 | | 145 | 160 | 178 | | 220 | | |
| 30 | 83 | 92 | | 124 | 141 | 161 | | 192 | 238 | | |
| | 0.22 | 0.24 | | 0.33 | 0.35 | 0.39 | | 0.42 | 0.50 | | |
| 32 | | 87 | 115 | 125 | 135 | 145 | | 185 | 210 | | |
| | | 0.21 | 0.26 | 0.29 | 0.31 | | | 0.38 | 0.58 | | |
| 33 | | 97 | | 125 | 145 | 155 | | 192 | 220 | | |
| | | 0.13 | | 0.21 | 0.26 | 0.28 | | 0.37 | 0.44 | | |
| 34 | | | 110 | | 135 | 150 | | 190 | 210 | 235 | |
| | | | 0.20 | | 0.25 | | | 0.38 | 0.43 | | |
| 35 | | 95 | | 120 | 135 | 150 | | 190 | 210 | | |
| | | | | | | 0.36 | | | | | |
| 36 | 85 | | | | | | | 210 | 235 | | |
| 37 | 85 | 100 | | 130 | | | 180 | 200 | 230 | | |
| 38 | | 104 | | | | | | 202 | 235 | | |
| | | 0.167 | | | | | | 0.37 | 0.442 | | |
| 39 | | | 115 | | 140 | 155 | | 190 | 215 | 240 | |
| 40 | | 95 | | 125 | 145 | | | 200 | 220 | 235 | |
| | | 0.16 | | 0.23 | 0.34 | | | 0.40 | 0.42 | 0.40 | |
| 41 | | 100 | | | 137 | | | 207 | 228 | | 260 |
| 21 | 88 | 101 | 115 | 126 | 144 | 157 | 179 | 199 | 222 | 248 | 267 |
| | 0.15 | 0.158 | 0.202 | 0.229 | 0.271 | 0.281 | 0.325 | 0.439 | 0.478 | 0.519 | 0.578 |
| | 3.2 | 0.25 | 2.7 | 2.8 | 4.9 | 1.2 | 1.0 | 900 | 38 | 11 | 50 |

ues obtained from a set of close to 100 SI GaAs liquid encapsulated Czochralski (LEC) samples, via SIMPA analysis are also presented.[21] For each trap $T_m$ (K), $E_a$ (eV), and $\sigma$ (cm$^2$) are shown whenever calculated in original papers. Most of the data were obtained from undoped SI GaAs samples based on the analysis of TSC measurements. Some data were obtained from measurements on SI GaAs:O and SI GaAs:Cr as well as on nearly SI GaAs. One data set, obtained from the analysis of photoinduced transient spectroscopy (PITS) measurements, was also shown for the comparison. Table I also includes data obtained from samples grown either in As- or Ga-rich conditions and/or treated by quite different annealing procedures. Several reports show results of measurements done on samples treated by neutrons or $\gamma$ rays.

## III. RESULTS AND DISCUSSION

All reports in Table I which were based on classical analytical approaches of TSC spectra gave incomplete data sets. Since these procedures use some variation of the single peak approach, they could have been applied only to well defined and prominent TSC peaks. Hence small peaks and shoulders, even if clearly visible in the TSC spectra, could not have been analyzed. Therefore, some data consisted of only $T_m$'s, most reports contained peak maxima temperatures and activation energies, while $\sigma$'s were estimated in just a few papers. Furthermore, many of the reported parameters differ from author to author even when the simplest visual inspection of TSC spectra suggests the same peak. Even in reported $E_a$'s, the scattering is considerable but for $\sigma$'s it becomes drastic. For example, for trap $T_3$ the variation in the estimates of $\sigma$ amounts to four orders of magnitude. The origin of such great discrepancies is rooted in limits of single peak analysis, and it was elaborated in details in Refs. 16 and 20.

In this work TSC spectra from references indicated in Table I were recalculated and reevaluated by the SIMPA procedure.[20] Since all curves have been prepared in a consis-

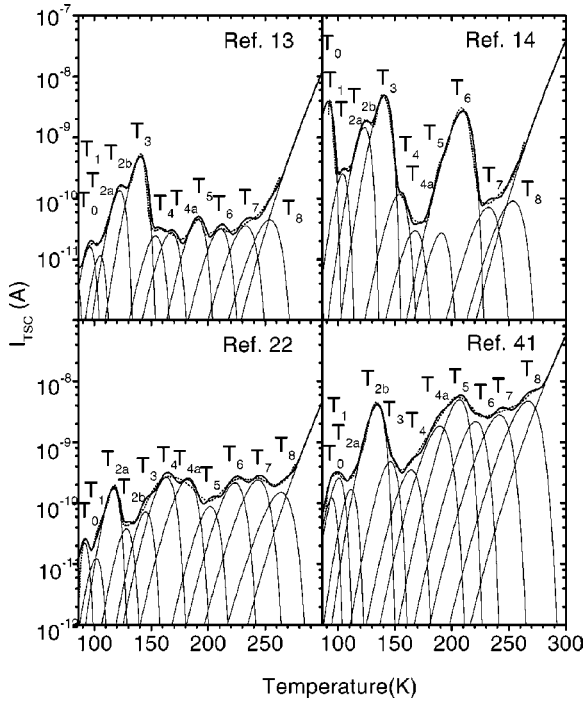


FIG. 1. TSC experimental curves and their SIMPA fits. Thick dotted lines denote scanned, previously published TSC measurements (references indicated in figure). Thick solid lines represent the best fits obtained by SIMPA method, while thin solid lines denote components (particular TSC peaks).

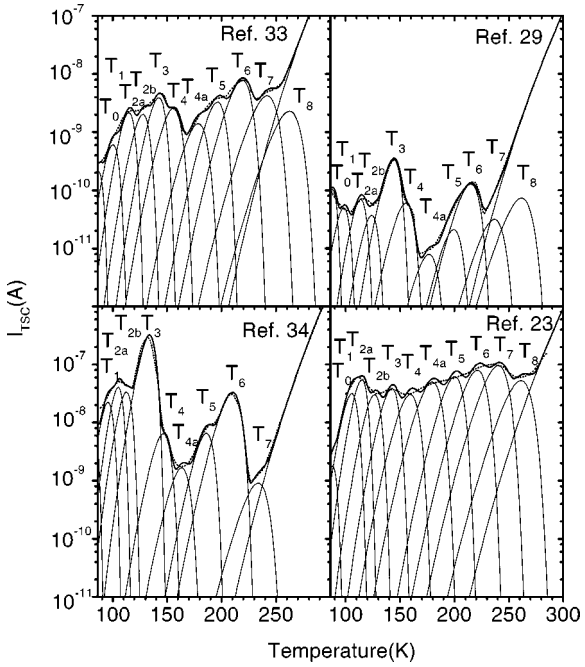


FIG. 3. TSC experimental curves and their SIMPA fits. Thick dotted lines denote scanned, previously published TSC measurements (references indicated in figure). Thick solid lines represent the best fits obtained by SIMPA method, while thin solid lines denote components (particularly TSC peaks).

tent way the possible scanning errors, as much as they are small, are comparable for all curves. Figures 1–6 present the best SIMPA fits of all digitally scanned curves. Thick dotted lines denote scanned (measured) TSC spectra. Thick solid lines present the best fits of the whole TSC spectra, while thin solid lines represent particular TSC peaks (components) including dark currents (nearly straight lines). In all cases the SIMPA simulation, in contrast to the analysis in original pa-

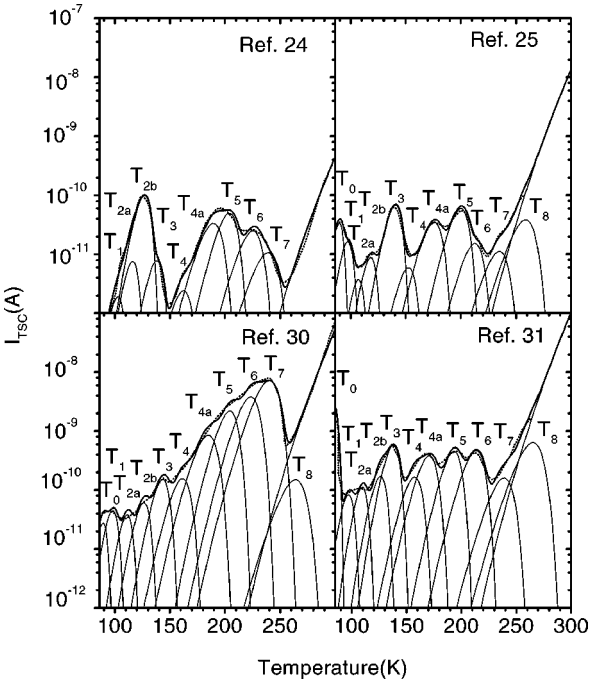


FIG. 2. TSC experimental curves and their SIMPA fits. Thick dotted lines denote scanned, previously published TSC measurements (references indicated in figure). Thick solid lines represent the best fits obtained by SIMPA method, while thin solid lines denote components (particularly TSC peaks).

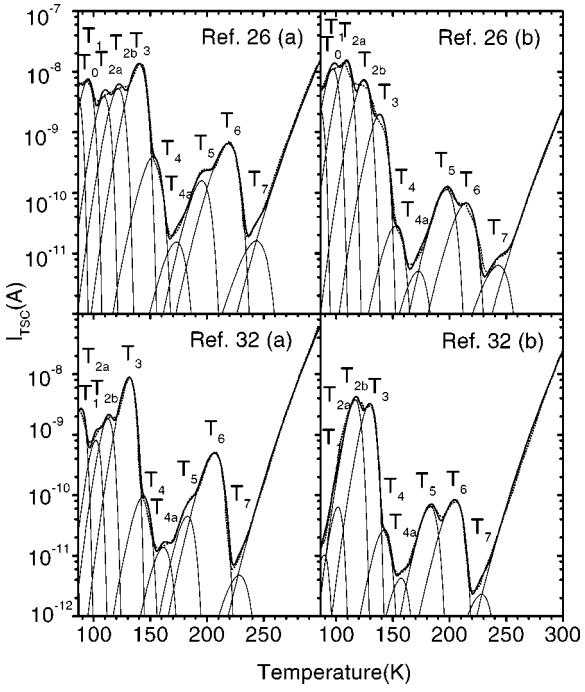


FIG. 4. TSC experimental curves and their SIMPA fits. Thick dotted lines denote scanned, previously published TSC measurements (references indicated in figure). Thick solid lines represent the best fits obtained by SIMPA method, while thin solid lines denote components (particularly TSC peaks).

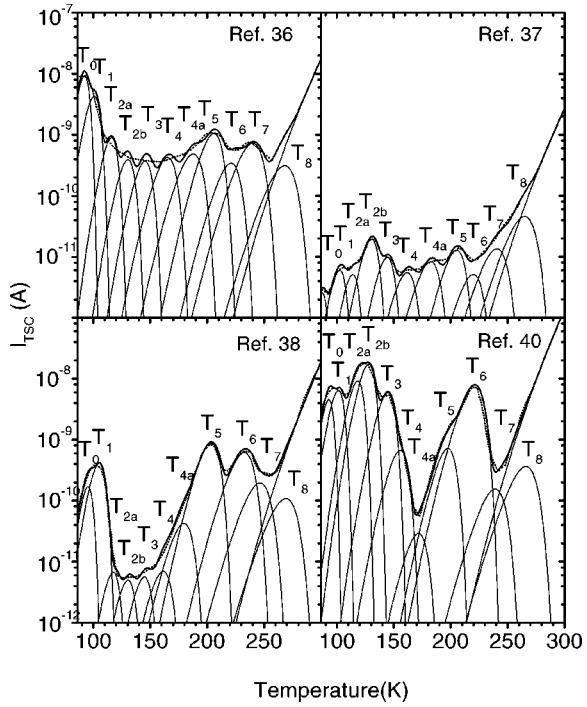


FIG. 5. TSC experimental curves and their SIMPA fits. Thick dotted lines denote scanned, previously published TSC measurements (references indicated in figure). Thick solid lines represent the best fits obtained by SIMPA method, while thin solid lines denote components (particularly TSC peaks).

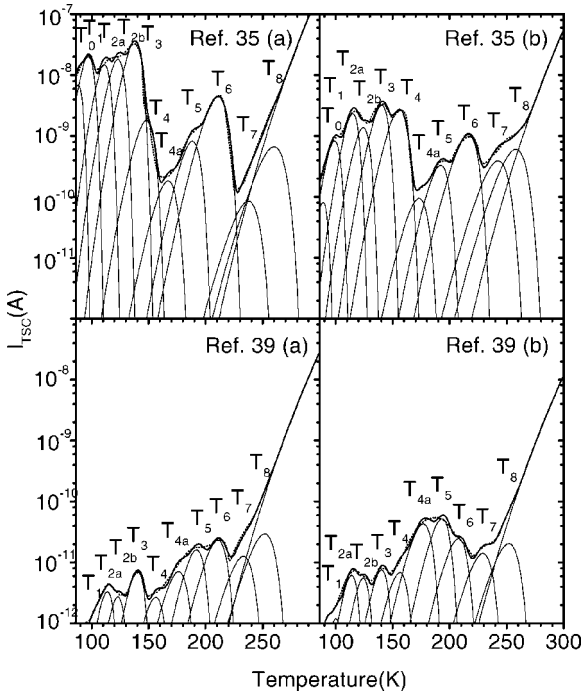


FIG. 6. TSC experimental curves and their SIMPA fits. Thick dotted lines denote scanned, previously published TSC measurements (references indicated in figure). Thick solid lines represent the best fits obtained by SIMPA method, while thin solid lines denote components (particularly TSC peaks).

pers (Table I), gave the complete signature for all observed deep traps.

Figure 1 presents SIMPA fits of TSC curves in Refs. 13, 14, 22, and 41 which were all published in the mid-1970's, and refer to SI GaAs:O and SI GaAs:Cr samples. In Ref. 41 original TSC spectrum was shown in arbitrary units and it was multiplied here with factor $10^{-10}$ so that it could be comparable with the other TSC curves. It can be noticed that all scanned curves are excellently fitted, using the same set of peaks obtained recently from LEC undoped SI GaAs samples.[21] In all four cases complete deep trap set $(T_0 - T_8)$ was needed in fitting. If any traps have been omitted or exchanged with some new peak, it would result in worsened fits. In Ref. 22, the heating rate was 0.4 K/s, while in Ref. 41 it was reported to be 0.66 K/s and this value for $\beta$ indeed gave the best fits. In Refs. 13 and 14 the $\beta$ was not reported and it was determined from the best fit to be $\beta = 0.12$ K/s, in both cases.

Figure 2 presents results of SIMPA fitting of scanned TSC curves from Refs. 24, 25, 30, and 31. Samples in Refs. 24 and 25 were SI GaAs cut from melt-grown Cr compensated ingots, while in the other two references samples were undoped LEC SI GaAs. Again very good fits were obtained using the same set of all eleven deep traps except the spectrum from Ref. 24 where $T_0$ and $T_8$ had negligible concentrations. In Refs. 24 and 25 heating rates were declared (0.5 and 0.2 K/s, respectively), while for the other two curves in both cases the same value of 0.4 K/s came out from the best fit. It can be noticed that TSC curves from Refs. 24 and 25, having more prominent peaks, are better fitted than the other two spectra. This happened because in later curves neighboring peaks were of similar intensities and overlap of emitted charge carriers is stronger. For these as well as for all other samples presented in Figs. 2–6, the simulation of activation energy of the $I_{dark}$ at and around RT gave values in the 0.73–0.78 eV range, which are consistent with the activation energy of EL2 level ($E_{EL2} = 0.75 \pm 0.03$ eV).[44]

Figure 3 shows the best SIMPA fitting results of TSC curves from Refs. 29, 33, and 34 and PITS curve from Ref. 23. In Refs. 23, 29, and 34 samples were cut from undoped SI LEC GaAs wafers, while measurements in Ref. 33 were done on Cr doped SI GaAs samples. Generally, good fits were obtained. However, the curve from Ref. 23, being practically flat, was fitted with the most uncertainty since there were no dominant peaks. The heating rate was indicated only in Ref. 33 (0.35 K/s), while in Refs. 23, 29, and 34 the best fits were obtained with 0.3 K/s; 0.35 and 0.06 K/s, respectively.

Figure 4 depicts fitting results for TSC curves from Ref. 26 (a and b curves), where the first curve is obtained on As-rich undoped LEC SI GaAs, while the second one is measured on Ga-rich undoped LEC SI GaAs. The other two curves (a and b) originate from Ref. 32, both obtained on the same undoped LEC SI GaAs sample, but after different annealing procedures. Curve 32a) represents TSC before annealing, while curve 32b) presents measurements after annealing at 700 °C. In all cases excellent fits were achieved, again with the same set of deep traps. Trap $T_8$ was completely absent in all TSC spectra of this group. For all four curves heating rates were known, being 0.2 K/s (Ref. 26, curves a and b) and 0.03 K/s (Ref. 32 curves a and b), and they were well reproduced in fits.

TABLE II. Calculated signatures of eleven deep traps obtained from experimental TSC spectra of many different authors. Data show the best fits using SIMPA characterization method. Average values and respective standard deviations of $E_{a,i}$ and $\sigma_{n,i}$ obtained in this work are given in the second and third column. The analogous results from Ref. 21 are presented in the other two columns.

| Trap | $E_{a,i}$ /EV (This work) | $\sigma_{n,i}$ /cm$^2$ (This work) | $E_{a,i}$ /eV (Ref. 21) | $\sigma_{n,i}$ /cm$^2$ (Ref. 21) |
|---|---|---|---|---|
| $T_0$ | $0.155\pm0.006$ | $(3.4\pm0.8)\times10^{-17}$ | $0.152\pm0.004$ | $(3.2\pm0.3)\times10^{-17}$ |
| $T_1$ | $0.154\pm0.004$ | $(1.9\pm0.4)\times10^{-18}$ | $0.158\pm0.004$ | $(2.5\pm0.4)\times10^{-18}$ |
| $T_{2a}$ | $0.199\pm0.005$ | $(1.9\pm0.8)\times10^{-17}$ | $0.202\pm0.004$ | $(2.7\pm0.4)\times10^{-17}$ |
| $T_{2b}$ | $0.224\pm0.006$ | $(1.6\pm0.6)\times10^{-17}$ | $0.229\pm0.006$ | $(2.8\pm0.8)\times10^{-17}$ |
| $T_3$ | $0.271\pm0.006$ | $(5.3\pm1.4)\times10^{-17}$ | $0.271\pm0.004$ | $(4.9\pm0.5)\times10^{-17}$ |
| $T_4$ | $0.278\pm0.006$ | $(0.7\pm0.2)\times10^{-17}$ | $0.281\pm0.005$ | $(1.2\pm0.6)\times10^{-17}$ |
| $T_{4a}$ | $0.319\pm0.008$ | $(0.7\pm0.3)\times10^{-17}$ | $0.325\pm0.008$ | $(1.0\pm0.2)\times10^{-17}$ |
| $T_5$ | $0.441\pm0.005$ | $(0.9\pm0.3)\times10^{-15}$ | $0.439\pm0.006$ | $(0.9\pm0.1)\times10^{-15}$ |
| $T_6$ | $0.479\pm0.007$ | $(4.5\pm0.8)\times10^{-16}$ | $0.478\pm0.007$ | $(3.8\pm0.8)\times10^{-16}$ |
| $T_7$ | $0.513\pm0.006$ | $(1.8\pm0.8)\times10^{-16}$ | $0.519\pm0.006$ | $(1.1\pm0.4)\times10^{-16}$ |
| $T_8$ | $0.583\pm0.005$ | $(3.9\pm1.1)\times10^{-16}$ | $0.578\pm0.004$ | $(5.0\pm1.5)\times10^{-16}$ |
| EL2 | $0.76\pm0.3$ | | $0.75\pm0.02$ | |

In all four simulated curves depicted in Fig. 5, all eleven deep traps were present. In Refs. 36–38 undoped SI LEC GaAs was studied. The sample from Ref. 37 was subjected to $\gamma$ ray irradiation with a dose of $1.5\times10^{15}$ ph/cm$^2$. In Ref. 40 studied material was high resistive GaAs. In none of Refs. 36, 37, 38, and 40, the heating rate was declared. The best fits were obtained with 0.66, 0.63, 0.5, and 0.25 K/s, respectively, which are all very reasonable values for $\beta$.

Finally, Fig. 6 presents SIMPA fitting of TSC spectra scanned from Refs. 35 (two curves) and 39 (two curves). In both papers LEC SI GaAs was studied. Curve (a) from Ref. 35 was obtained on unirradiated sample and it was also reproduced in Refs. 46 and 47, while TSC spectrum 35(b) was obtained on sample irradiated by fast neutrons of $2\times10^{15}$ cm$^{-2}$ fluence. In both cases excellent fits were obtained again with the same set of all eleven different deep traps. The first (a) of TSC curves from Ref. 39 was measured on SI GaAs specimen grown in As-rich conditions, while the other one was obtained on sample grown in Ga-rich conditions. Trap $T_0$ was absent from both later spectra. The last two curves are characterized with the lowest intensities of TSC peaks of all studied spectra. Heating rates, not declared in Refs. 35 and 39, were obtained to be 0.2 K/s for both spectra in Ref. 35 and 0.1 K/s for both curves in Ref. 39.

Here it is important to say that none of the eleven deep traps used in simulations was not constructed artificially or taken without strong experimental support—each of these traps was clearly observed as a well resolved or even dominant peak in at least one and usually in a number of analyzed TSC spectra.

Obtained values for activation energies and capture cross sections (trap signatures) were statistically analyzed. Results are presented in the Table II (first two columns). Note the very small scattering of $E_a$ values (1.5%–3%), and reasonably small scattering in $\sigma$ values (typically 20%–30%). The uniqueness of fits was within confidence limits defined earlier by analysis of SIMPA simulations.[20] These results are compared with values obtained from the analysis of TSC spectra, obtained on undoped SI GaAs samples grown by only one technique and within a limited time period[20,21] (the last two columns of Table II).

Several points should be emphasized in this comparison:

(1) Results of this work cover samples of different origin, produced in the period of the last three decades. Samples include not only LEC undoped SI GaAs, but also doped samples: SI GaAs:O (Refs. 14, 22, and 41); SI GaAs:Cr (Refs. 13, 22, 24, 25, and 41), while in Ref. 22 SI GaAs:Cr was also codoped with copper.

(2) Samples from this work also cover a wider span of different growth and post-growth treatments, in particular: (a) Growth in As or Ga rich conditions (Refs. 26–28, 39, and 45); (b) various annealing procedures of As grown samples (Ref. 32); (c) various irradiations [with neutrons (Ref. 35) and $\gamma$ rays (Ref. 37)].

All these findings emphasize the fact that different growth and post-growth processes and treatment do not introduce new traps (defects) in SI GaAs, influencing only relative concentrations of deep traps which were all detected in a much narrower range of SI GaAs samples.[21]

(i) Therefore, it appears that these eleven deep traps represent the complete set of all defects having deep levels present in undoped (or Cr or O doped) SI GaAs, including material which is subsequently modified by annealing or irradiation. The only caution is that some of these eleven deep traps might also be a composite of two peaks having very close signature values within uncertainties inherent to SIMPA procedure,[20] which are relatively small.

(ii) All the above-mentioned different deep traps were observed in experimental TSC spectra of many different authors, some of them frequently, some more rarely. However, they were often interpreted as different traps, described by different set of parameters (Table I) and hence differently labeled. None of the previous reports claim more than eleven different deep traps in undoped SI GaAs at once. In some reports different authors observed a majority of the above-mentioned deep traps in the same TSC spectrum. For instance, in Refs. 12, 17, 26–28, ten deep traps were observed (in their notation declared as $T_6^*-T_0$), and in Refs. 20 and 21, eleven deep traps named from $T_0$ to $T_8$. In Refs. 13 and 14 maximally eight levels were observed (assigned as $a-h$), while in Ref. 30, in the same temperature range, authors

TABLE III. Proposed structural origin (defect) for particular deep trap ($T_i$).

| Reference/$T_i$ | References 17, 26, and 27 | Reference 28 | References 35, 46, and 47 | Other References |
|---|---|---|---|---|
| $T_0$ | | | | EL11 49 |
| $T_1$ | $V_{As}$; $Ga_{As}$ | | Cu related | $V_{As}$ 45 |
| $T_{2a}$ | $Ga_{As}^{--}$ | | | |
| $T_{2b}$ | | | | |
| $T_3$ | $V_{Ga}$ | $As_{Ga}+V_{As}$ | | $V_{As}+As_i$ 50 |
| $T_4$ | | | $As_{Ga}+V_{As}$ compl. | $V_{As}+As_i$ compl. 45 |
| $T_{4a}$ | | | | Cu related 51 |
| $T_5$ | $Ga_{As}+V_{Ga}$; $V_{As}$ | $V_{As}$ compl. | | $V_{As}+As_i$ compl. 45 C 52 |
| $T_6$ | $As_{Ga}^{++}$ compl. | $As_{Ga}$ compl. | | Fe, Cu, 52 and 53 O or C 33 |
| $T_7$ | | | $Cu_{Ga}+V_{As}$; or $Ga_{As}+V_{Ga}$ | |
| $T_8$ | | | | |

declared seven traps named from *d* to *j*. In Ref. 48 six deep traps were observed in TSC measurements, while in TEES[48] measurements ten different levels were reported (named from T1 to T10). In this article all of these defects (all traps having deep levels experimentally observed by various authors) were sorted out and systemized in a unique and self-consistent way.

(iii) After all deep traps are unambiguously identified with well established signatures, the remaining job of positively identifying their microscopic structure becomes better defined and hence easier. The survey of the proposed defects configurations is given in Table III. Obviously, the structure at the atomic level of most of the above deep levels has not yet been positively determined. The main suspects are native defects like $As_{Ga}$, $Ga_{As}$, $V_{As}$, $V_{Ga}$, $As_i$, and their complexes, as well as complexes with some of the unavoidable contaminants like Cu and Fe. The fact that any of the post-growth treatments or the variety of growing conditions doping with Cr and O did not expand the number of TSC observable defects gives support to the notion that these defects are indeed primarily complexes of simple lattice defects.

## IV. SUMMARY AND CONCLUSIONS

In this work practically all available published TSC data, regarding SI GaAs reported by many different authors over a time span of three decades were reevaluated and reinterpreted using the new analytical method (SIMPA). (SIMPA) enables clear separation of contributions from various overlapping TSC peaks and precise determination of signatures (activation energy, $E_a$, and capture cross section, $\sigma$) of all observed deep traps, and hence their complete systematization and cataloguing. Data were obtained by digital scanning of all available reported TSC curves measured on SI GaAs.

The SIMPA method was applied to TSC spectra, reported from a great variety of SI GaAs samples, undoped and Cr or O doped, produced over a very long period of time, by various manufacturers and/or laboratories which include: samples grown by various methods; growth under As or Ga-rich conditions; thermal treatment at various temperatures and by different annealing procedures, as well as irradiation with neutrons or $\gamma$ rays.

Although the SIMPA procedure was applied to apparently very different TSC spectra, done on various SI GaAs samples, in all cases excellent fits were achieved with the same, unique set (or subset from it) of only eleven different deep traps.

These deep traps, together with their signatures are:

$$T_0(0.155\,\text{eV},3.4\times10^{-17}\,\text{cm}^2),$$

$$T_1(0.154\,\text{eV},1.9\times10^{-18}\,\text{cm}^2),$$

$$T_{2a}(0.199\,\text{eV},1.9\times10^{-17}\,\text{cm}^2),$$

$$T_{2b}(0.224\,\text{eV},1.6\times10^{-17}\,\text{cm}^2),$$

$$T_3(0.271\,\text{eV},5.3\times10^{-17}\,\text{cm}^2),$$

$$T_4(0.281\,\text{eV},1.2\times10^{-17}\,\text{cm}^2),$$

$$T_{4a}(0.319\,\text{eV},0.7\times10^{-17}\,\text{cm}^2),$$

$$T_5(0.441\,\text{eV},0.9\times10^{-15}\,\text{cm}^2),$$

$$T_6(0.479\,\text{eV},4.5\times10^{-16}\,\text{cm}^2),$$

$$T_7(0.513\,\text{eV},1.8\times10^{-16}\,\text{cm}^2),$$

and

$$T_8(0.583\,\text{eV},5.0\times10^{-16}\,\text{cm}^2).$$

It appears that this set of eleven traps is a finite and complete set of all defects with deep levels in SI GaAs and that any of the different growth and post-growth processes as well as various irradiations do not introduce new traps (defects) in SI GaAs, but only influences their relative concentrations.

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