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Improved interface state density function in metal-semiconductor junctions by deep-level transient spectroscopy

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Deep-level transient spectroscopy (DLTS) measurements have been made to obtain the activation energy and capture cross section in Schottky diodes. Previous theories for interface state density (ISD) functions, which are derived for metal-semiconductor junctions, made approximations that were inappropriate. This paper derives improvements to the previous analysis and calculates ISD using the measured DLTS data. As for examples, Schottky diodes of Si, GaAs, and $\text{Al}_x\text{Ga}_{1-x}\text{As}$ have been investigated with both methods. It has been found that the previously used method overestimated both the peak maximum position and peak height of the ISD.

I. INTRODUCTION

The interface state density (ISD) is one of the most important parameters in the study of metal-semiconductor junctions or Schottky diodes. Recently, several papers¹⁻⁵ have appeared on the subject outlining the usefulness of the deep-level transient spectroscopy (DLTS) data in the investigation of ISD in compound semiconductors, such as GaAs, $\text{Al}_x\text{Ga}_{1-x}\text{As}$, etc. No doubt, by performing either capacitance or current spectroscopy one can obtain accurate signatures of the active defect centers. However, the techniques used for the analysis of the experimental data still need improvement.

To alleviate this problem, Zhang *et al.*⁶ have proposed a simple theory illustrating a calculation of the ISD in $\text{Al}_x\text{Ga}_{1-x}\text{As}$. In their work, they emphasized the DLTS data obtained from isothermal capacitance transient spectroscopy (ICTS). The purpose of the present paper is to point out that in the Zhang *et al.*⁶ theory the expressions for ISD (N_{ss}) and the position of energy maximum (E_{max}) are not justified due to an approximation they made in evaluating the integrals involved in their theory. We show in this investigation that when those integrals are properly evaluated, one gets quite different final expressions for N_{ss} and E_{max} , which lead to different results for the distribution plots.

II. THEORY AND CORRECTION

Calculation of the distribution function can be achieved via the charge density function Q_{ss} . A change in the charge density in ISD due to emission during sampling time t_1-t_2 may be written as

$$\Delta Q_{ss}(t_2, t_1) = q \int_{E_F(t_1)}^{E_F(t_2)} N_{ss}(E) S(\tau, E) dE, \quad (1)$$

where τ is the emission time constant and $S(\tau, E)$ the spectral function. The two functions can be expressed as

$$\begin{aligned} \tau &= [g/(\sigma_n v_{th} N_c)] \exp[(E_c - E)/kT] \\ &= A \exp[(E_c - E)/kT], \end{aligned} \quad (2)$$

where

$$A = g/(\sigma_n v_{th} N_c)$$

and

$$S(\tau, E) = \exp[-t_1/\tau] - \exp[-t_2/\tau], \quad (3)$$

where σ_n is the emission cross section, v_{th} the thermal velocity, N_c the effective density of states in the conduction band edge, g the degeneracy factor, E_c the conduction band energy, and k the Boltzmann factor. It can be shown that

$$\Delta C(t_2, t_1) = \frac{C(t_1)^2}{N_d \epsilon} \int_{E_F(t_1)}^{E_F(t_2)} N_{ss}(E) S(\tau, E) dE, \quad (4)$$

where ΔC is the DLTS signal corresponding to the sampling time t_1 and t_2 , N_d the trap density, and ϵ the dielectric constant. According to the mean value theorem, if $p(x)$ is a slowly varying function in x and $g(x)$ a sharply peaked function, one can write

$$\int p(x) g(x) dx = p_{max} \int g(x) dx, \quad (5)$$

where p_{max} is the value of $p(x)$ at the peak of $g(x)$. Therefore, for our case, we can write

$$\Delta C(t_2, t_1) = \frac{C(t_1)^2}{N_d \epsilon} N_{ss}(E_{max}) \int_{E_F(t_2)}^{E_F(t_1)} S(\tau, E) dE, \quad (6)$$

which gives

$$N_{ss}(E_{max}) = \left(\frac{\Delta C(t_1, t_2) N_d \epsilon}{C(t_1)^2} \right) \left(\int S(\tau, E) \right)^{-1} dE. \quad (7)$$

An evaluation of the integral can be carried out by switching the variable from E to τ

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TABLE I. Sample data. Note that the data presented in this table are obtained from the Arrhenius plots of the measured DLTS. These data are then subsequently used in the theory outlined in the text to generate the ISD plots as illustrated in Figs. 4–6.

Samples	Method	Lab code	Level	E_A (eV)	σ_∞ (cm^2)	N_s (cm^{-3})	N_T (cm^{-3})
Si	Bulk	NBS2	A	0.54	5.4×10^{-15}	0.30×10^{16}	0.03×10^{16}
GaAs	MBE	GAS1	EL2	0.76	2.0	1.07	0.30
$\text{Al}_x\text{Ga}_{1-x}\text{As}$ ($x = 0.385$)	MBE	GAL4	A	0.39	0.16	2.20	3.30

$$\begin{aligned}
 \int S(\tau, E) dE &= \int_{E_F(t_2)}^{E_F(t_1)} S(\tau, E) \left(\frac{dE}{d\tau} \right) d\tau \\
 &= kT \int_{x(t_2)}^{x(t_1)} S(x) x^{-1} dx \\
 &= kT \int_{x(t_2)}^{x(t_1)} [\exp(-t_1 x) \\
 &\quad - \exp(-t_2 x)] x^{-1} dx, \quad (8)
 \end{aligned}$$

where $x = 1/\tau$. Now expanding the two exponential terms as power series before integrating and writing the time constant for maximum energy as,

$$\tau(E_{\max}) = \frac{t_2 - t_1}{\ln(t_2/t_1)}, \quad (9)$$

we obtain for the integral

$$\begin{aligned}
 \int S(\tau, E) dE &= kT \left(\frac{\ln(t_2/t_1)(t_2 - t_1)}{(t_2 - t_1)} \right. \\
 &\quad - \frac{\ln^2(t_2/t_1)(t_2^2 - t_1^2)}{4(t_2 - t_1)^2} \\
 &\quad + \frac{\ln^3(t_2/t_1)(t_2^3 - t_1^3)}{18(t_2 - t_1)^3} \\
 &\quad \left. - \frac{\ln^4(t_2/t_1)(t_2^4 - t_1^4)}{96(t_2 - t_1)^4} + \dots \right). \quad (10)
 \end{aligned}$$

Up until now we made no approximation except that we chose the time constant at E_{\max} . The higher order terms were dropped in the Zhang *et al.* paper.⁶ It turns out that these terms are not insignificant and may be retained by selecting $t_2 = R t_1$ for the higher order terms. Thus, we find

$$\begin{aligned}
 \int S(\tau, E) dE &= kT \left(\ln R - \frac{\ln^2 R}{4(R-1)^2} (R^2 - 1) \right. \\
 &\quad + \frac{\ln^3 R}{18(R-1)^3} (R^3 - 1) \\
 &\quad \left. - \frac{\ln^4 R}{96(R-1)^4} (R^4 - 1) + \dots \right) \quad (11)
 \end{aligned}$$

or

$$\int S(\tau, E) dE = kT I(R), \quad (12)$$

where $I(R)$ represents the expression in the square bracket in Eq. (11). It then easily follows that

$$N_{ss}(E_{\max}) = \frac{\Delta C(t_2, t_1) N_d \epsilon}{C(t_1)^2 kT I(R)} \quad (13)$$

with

$$E_{\max} = E_c - kT \ln[\sigma_n(E_{\max}) v_{th} N_c (t_2 - t_1) / I(R)]. \quad (14)$$

III. ANALYSIS AND RESULTS

In order to investigate the distribution function N_{ss} we have considered several Schottky diodes as illustrated in Table I. A detailed description of the sample preparation and history are described elsewhere.⁷⁻⁸ Experimental measurements were done on a fully automated ICTS system. All isothermal capacitance transients spectra (ICTS) were captured at 1 MHz frequency in the temperature range 100–300 K at 2 K intervals. We applied several bias and pulse voltage combinations in the respective plots. The heart of our measurement system consists of HP4280A C-meter, LS-DRC91C temperature controller, HP8112A pulser, and Z248 computer with HP7475A plotter.

Data analysis was done using modulating function (MF) waveform analysis as discussed in our earlier paper.⁹ This technique is rapid, accurate, and requires no presupposition of trial parameters. With the MF technique one can now obtain an effective activation energy. Briefly, one can formulate an integral equation with MF $\phi(t)$

$$\begin{aligned}
 \int_{T_s}^{T_e} \dot{C}(t, T) \phi(t) dt &= (-1)^n \sum_i A_i / \tau_i \\
 &\quad \times \int_{T_s}^{T_e} e^{-t/\tau_i} \phi(t) dt, \quad (15)
 \end{aligned}$$

where T_e is the end-time and T_s the start-time of the transient. To obtain A_i , the amplitude function, the required condition to satisfy is

$$\dot{C} + \alpha_1 \ddot{C} + \dots + \alpha_m C^{(m+1)} = 0, \quad (16)$$

with the α_m coefficients written to satisfy the condition

$$\tau^{(m)} - \alpha_1 \tau^{(m-1)} + \dots + (-1)^m \tau = 0. \quad (17)$$

The MF derivatives are then normalized to zero at the two transient times

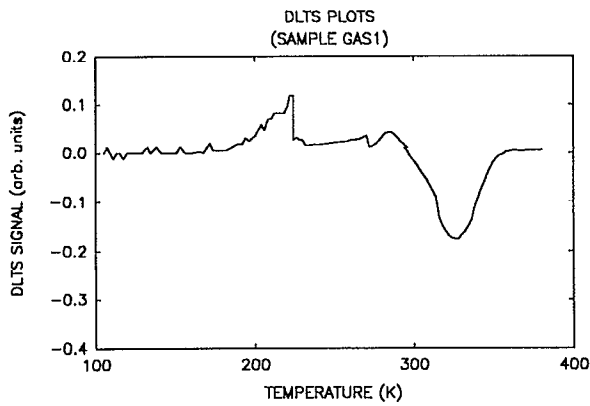


FIG. 1. DLTS signal plot for GaAs (Si-implanted), (sample GAS1), diodes. Pulse bias voltage $-3-0$ V was applied.

$$[\phi^{(m)}(t)]_{T_s} = [\phi^{(m)}(t)]_{T_e} = 0. \quad (18)$$

These equations now lead to

$$\int_{T_s}^{T_e} \dot{C} \phi(t) dt + \alpha_1 \int_{T_s}^{T_e} \ddot{C} \phi(t) dt + \dots + \alpha_n \int_{T_s}^{T_e} C^{(m+1)} \phi(t) dt = 0. \quad (19)$$

Using partial integration, Eq. (19) can be reduced from C -differential to $\phi(t)$ -differential

$$\int_{T_s}^{T_e} C \phi(t) dt - \alpha_1 \int_{T_s}^{T_e} \dot{C} \phi(t) dt + \dots + (-1)^m \alpha_m \int_{T_s}^{T_e} C^{(m+1)} \phi(t) dt = 0. \quad (20)$$

If one considers MF's of the form UV, the product derivative rule gives

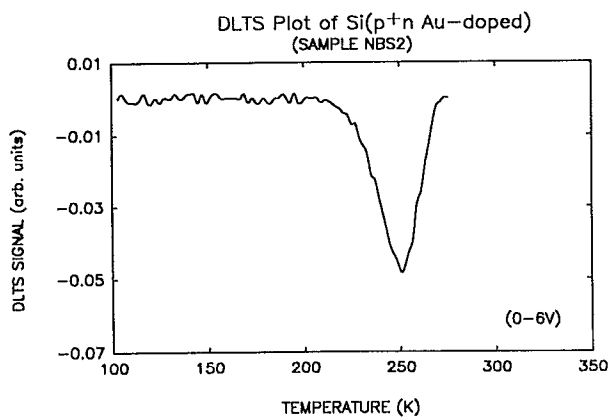


FIG. 2. DLTS signal plot for Si (Au-doped), (sample NBS2), diodes. Pulse bias voltage $-6-0$ V was applied.

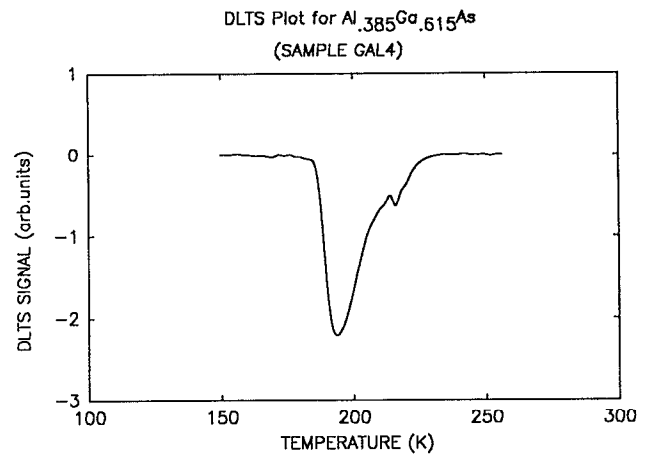


FIG. 3. DLTS signal plot for $Al_{0.385}Ga_{0.615}As$ (sample GAL4) diodes. Pulse bias voltage $-2-0$ V was applied.

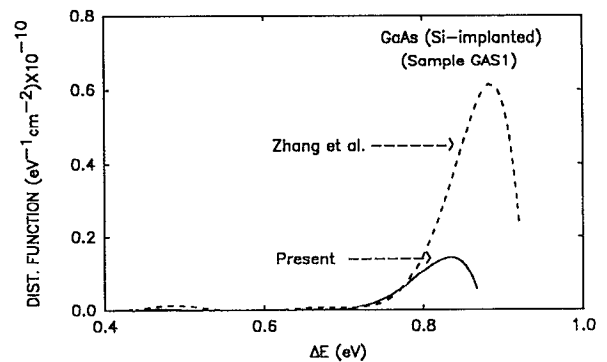


FIG. 4. Distribution function plots for sample GAS1.

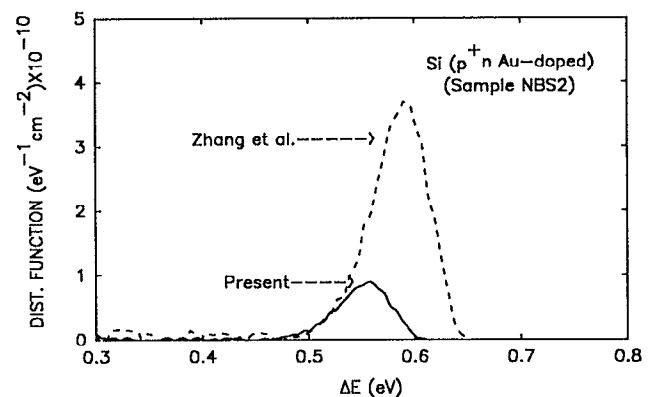


FIG. 5. Distribution function plots for sample NBS2.

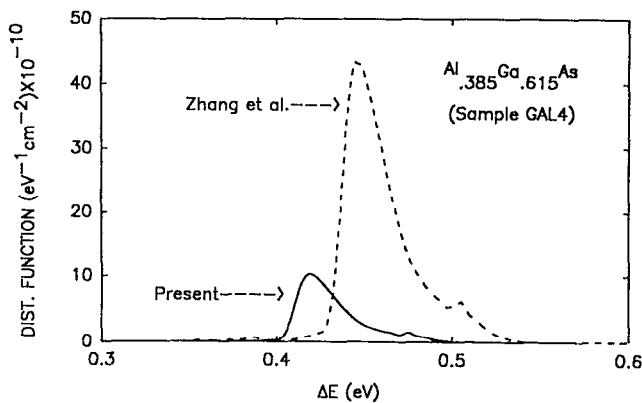


FIG. 6. Distribution function plots for sample GAL4.

$$\phi^{(m)}(t) = \sum (j)^m U^{(m-j)} V^{(j)} \quad (21)$$

To test the convergency, one can select several different types of functions; all should give the same results if the analysis is correctly done within the limits of computational errors.

In this particular investigation, we have selected a power function of the type, which is known to work well in our earlier paper,⁸

$$\phi(t) = (t - T_s)^{P_1} (T_e - t)^{P_2} \quad (22)$$

The m th derivatives of the two product functions are then

$$U^{(m)} = [P_1! / (P_1 - m)!] (t - T_s)^{P_1 - m}, \quad (23)$$

and

$$V^{(m)} = (-1)^m [P_2! / (P_2 - m)!] (T_e - t)^{P_2 - m}, \quad (24)$$

which can be substituted in Eq. (21). The values of A_i and τ_i were thus obtained from the measurement of ICTS at each value of the temperature. The measured plots of the DLTS signal for three samples, NBS2, GAS1, and GAL4, are shown in Figs. 1–3, respectively. In all these samples, we have concentrated mainly on the predominant deep levels, for example EL2 level in GAS1, etc.

IV. CONCLUSIONS

We show our calculated results in Figs. 4–6 for the three samples. From Table I we note the values of activation energy E_A , emission cross-section σ_∞ and trap density

TABLE II. Four terms of the rate function in Eq. (12). Relative importance of the four terms in Eq. (12) are shown for several values of the rate window parameter R .

R	First	Second	Third	Fourth
5	1.60	3.84	0.4408	0.1664
7	1.95	7.53	0.6442	0.2732
10	2.30	14.55	0.9263	0.4442

TABLE III. Shift parameters. This table illustrates the percentage difference of the peak maximum positions and peak heights of the ISD when the present method is compared with that of Zhang *et al.*⁶

Samples	ΔE_{\max} (%)	$\Delta (N_{ss})_{\max}$ (%)
Si	5.39	368
GaAs	5.26	275
$Al_xGa_{1-x}As$ ($x = 0.385$)	6.68	281

^aSee Ref. 6.

N_T . These values are seemingly in good agreement with the values reported earlier from similar measurements.^{10–17} We have included here the results of C - V profiling data also for the carrier concentration N_s . These numbers fall in the range 10^{15} – $10^{16}/\text{cm}^3$, in accord with the known results of these materials. However, the distribution function plots N_{ss} , as presented in Figs. 4–6, indicate that the Zhang *et al.*⁶ equations obviously overestimate the peak maximum positions and peak heights shifting them to higher values.

In an effort to attach some numerical significance to these results, we consider various error values and experimental parameters. In an investigation of the present type, experimental data are usually taken with a rate window setting of $R < 10$. In most cases, it is preset between 5 and 7. Since any further reduction of Eqs. (10) or (12) does not seem possible, at this time we will proceed numerically. For the calculation of N_{ss} , it is sufficient to keep the first three or four terms. With any AT desk-top computer this can be easily achieved. This is what was done in the present investigation, where the DLTS data were processed with a rate window of $R = 7$. For this case then the magnitude of the rate function turns out to be $I(R) = 5.55$, instead of being 1.95 as in the previous work.⁶ These calculations are shown in Table II for several values of R . The accuracy and sensitivity achievable in the present analysis are defined mainly by the limits in the measurement of temperature and transients, i.e., $\Delta T = \pm 0.01$ K and $\Delta C = \pm 0.001$ pF. These result in an accuracy for the activation energy of $\Delta E_A = \pm 0.01$ eV and DLTS signal of $\Delta(\Delta C/C) = \pm 0.001$. Subject to these factors, we have further checked the percentage of shifts between the present and the previous method for the peak maximum positions and peak heights of the calculated ISD plots. These numbers are illustrated in Table III. On the average, however, we find that both E_{\max} and $(N_{ss})_{\max}$ are overestimated, respectively, by about 5.77% and 308% in the Zhang *et al.* paper.⁶

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¹S. Dhar, K. S. Seo, and P. K. Bhattacharya, *J. Appl. Phys.* **58**, 4216 (1985).

²J. H. Zhao, J. C. Lee, Z. Q. Fang, T. E. Schlesinger, and A. G. Milnes, *J. Appl. Phys.* **61**, 1063 (1987).

- ³A. A. Lebedev and W. Ecke, *Sov. Phys. Semicond.* **20**, 1134 (1986).
⁴M. Katayama, A. Usami, and T. Wada, *J. Appl. Phys.* **62**, 528 (1987).
⁵L. Y. Leu and S. R. Forrest, *J. Appl. Phys.* **64**, 5030 (1988).
⁶H. Zhang, Y. Ayogi, S. Iwai, and S. Namba, *Appl. Phys. Lett.* **50**, 341, (1987).
⁷W. R. Thurber, R. A. Forman, and W. A. Philips, *J. Appl. Phys.* **53**, 7397 (1982).
⁸J. E. Bisbee and N. C. Halder, *Phys. Status Solidi A* **119**, 1085 (1990).
⁹N. C. Halder and A. A. Teate, *J. Phys. C: Cond. Mat.* **2**, 10359 (1991).
¹⁰Y. Tokumaru and H. Okushi, *J. Appl. Phys.* **19**, 2441 (1980).
¹¹D. V. Lang, H. G. Grimmeiss, E. Meijer, and M. Jarus, *Phys. Rev. B* **22**, 3917 (1980).
¹²P. K. Bhattacharya, J. K. Rhee, and S. J. T. Owen, *J. Appl. Phys.* **52**, 7224 (1981).
¹³A. Kitagawa, A. Usami, and T. Wada, *J. Appl. Phys.* **63**, 414 (1988).
¹⁴G. M. Martin, A. Mitonneau, and A. Mircea, *Electron. Lett.* **13**, 191 (1977).
¹⁵M. Kaminska, *Proceedings of the Seventh General Conference of Condensed Matter, Division of European Physical Society (Physics Scripta) T* **19**, 551 (1987).
¹⁶T. F. Kuech, D. J. Wolford, R. Potemski, J. A. Bradley, and J. K. Kelleher, *Appl. Phys. Lett.* **51**, 505 (1987).
¹⁷G. N. Maracus, W. D. Laidig, and H. R. Wittman, *J. Vac. Sci. Technol. B* **2**, 599 (1984).