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Analysis of Admittance Data: Comparison of a Parametric and a Nonparametric Method

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The thermal relaxation times are characteristic parameters of deep levels which can be calculated by the analysis of admittance data. The contributions of these characteristic parameters can be sharp or broadened. If sharp contributions are assumed the analysis procedure is called a parametric method. This procedure leads to a well-posed inverse problem but additionally the unknown number of discrete contributions must be determined. For broadened contributions a nonparametric method is used. This procedure leads to an ill-posed inverse problem but the number of contributions is determined automatically. Both kinds of analysis methods are compared with a Monte Carlo study on simulated admittance data. In addition, the parametric and nonparametric procedures are used to analyze experimental admittance data in order to obtain the deep levels and electrical properties of a semi-insulating GaAs Schottky diode. © 1999 Academic Press

Key Words: ill-posed problem; Tikhonov regularization; parametric method; nonparametric method; admittance spectroscopy.

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1. INTRODUCTION

Material parameters of Schottky diodes can be calculated from admittance data [1]. Characteristic parameters are the resistivity and the dielectric constant of the semiconductor material, the potential barrier of the metal-semiconductor interface, the energy of the band gap between the valence and the conduction band of the semiconductor, and the relaxation times of the energy levels within this band gap. The main topic of this article is the calculation of these relaxation times for deep levels.

From the view of solid state physics the contributions of the relaxation times should be sharp for single crystal material: All deep levels which originate from the same type of crystal defect have the same characteristic relaxation time. But for real crystals these

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contributions can be broadened due to the influence of a slightly varying local environment of the deep levels. This local influence leads to slightly different relaxation times. The reason for variations in the local environment can be twofold: Due to local interaction of different lattice defects and due to the influences introduced by the experimental method.

Local interactions depend strongly on the distance between the different kinds of point defects. Even in the case of a regular distribution the local distances will vary slightly. One reason for this is the different concentration for each type of defect. Therefore, the overlapping of a certain deep level with different energy levels results in different relaxation times. This overlapping effect is stronger if the surrounding defects have a small activation energy. In this case, the corresponding Bohr radius is of the order of the distances between the defects. In addition, a macroscopic strain exerted to the material could induce a further broadening of the relaxation times.

Experimental broadening of the contributions of deep level is caused by the influence of the applied measurement technique on the local environment. If the electric field induced by an applied bias voltage varies in the Schottky diode the defects will show different emission rates depending on their position in the Schottky junction according to the Poole–Frenkel effect [2]. Further broadening is introduced by the influence of the so-called Debye tail connecting the neutral with the depletion region of a diode. Defects in the Debye tail have different relaxation times [3].

As a matter of principle all deep levels are subjected to broadening effects, but in some cases they can be neglected and the corresponding levels can be characterized by sharp relaxation times. But if these effects are essential the deep levels must be characterized by a broad distribution of their relaxation times.

According to the sharp and broadened contributions there are two classes of data analysis methods—the parametric and the nonparametric method. With the parametric method discrete parameters for each relaxation time of a deep level are estimated from experimental data. This is the numerical approach of Macdonald [4]. In nonparametric methods a continuous distribution for the relaxation times of deep levels is estimated. Such a nonparametric method was presented in our previous article [1].

In this paper we compare these two different data analysis methods. By this comparison the reliability of their estimated results can be judged. This is not only restricted to the analysis of admittance data but can also give an useful insight for general data anlysis with parametric and nonparametric methods.

2. MODELS FOR THE ADMITTANCE OF A SCHOTTKY DIODE

The electric characteristics of a Schottky diode can be represented by an equivalent circuit consisting of resistances and capacitances. Figure 1 shows the equivalent circuit we introduced previously [1]. This circuit is especially adapted to high resistivity semiconductor materials because the semiconductor bulk is taken into account.

In our previous article the equivalent circuit is discussed in detail. A short motivation is as follows: The first part in the equivalent circuit (marked with Z_1) is due to the conductivity of the depletion region represented by the resistor R_{01} and due to the charge separating effect of this region represented by the capacitor C_{01}. The influence of the deep levels is represented by the series connections of resistors R_i and capacities C_i according to Losee [5]. The admittance of the first part is denoted by $Y_1(\omega)$. In the second part of the equivalent

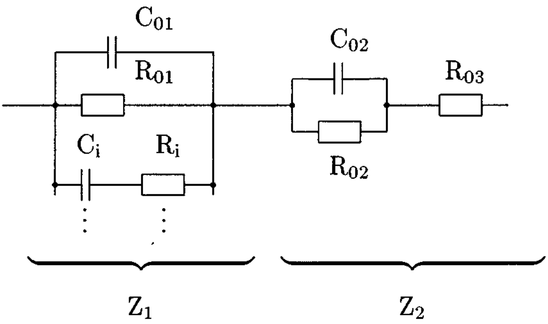


FIG. 1. Equivalent circuit of a Schottky diode. Z_1 is the impedance of the depletion region and Z_2 the impedance of the semiconductor material and the contact on the semiconductor.

circuit (marked with Z_2) the resistance R_{02} and capacitance C_{02} of the semiconductor bulk are taken into account. In addition, the resistor R_{03} stands for the ohmic back contact of the semiconductor. Both parts together yield the expression

$$Y(\omega) = \left(\frac{1}{Y_1(\omega)} + \frac{1}{G_{02} + i\omega C_{02}} + R_{03} \right)^{-1} \tag{1}$$

for the complex admittance of a Schottky diode in dependence on the frequency ω. In this expression the resistance R_{02} is replaced by its conductivity $G_{02} = R_{02}^{-1}$.

The product $R_i C_i = \tau_i$ leads to the thermal relaxation time of the corresponding deep level. This relaxation time has the well known dependence on the activation energy ΔE_i and the cross section σ_i of the deep level,

$$\tau_i^{-1} = \frac{1}{4} \left(\frac{3k_B}{m_e^*} \right)^{1/2} \left(\frac{2m_e^* k_B}{\pi \hbar^2} \right)^{3/2} \sigma_i T^2 e^{-\Delta E_i / k_B T}. \tag{2}$$

In the above equation k_B denotes the Boltzmann constant, $\hbar$ Planck's constant, m_e^* the effective mass of an electron in the crystal lattice of a semiconductor, and T the absolute temperature.

For the admittance $Y_1(\omega)$ of the first part, which contains the influence of the deep levels, two different approaches can be introduced. In the first approach the contributions of deep levels are supposed to be discrete. In this case the real- and imaginary parts of $Y_1(\omega)$ have the form [6]

$$\Re(Y_1(\omega)) = G_{01} + \sum_{i=1}^{n} \frac{\omega^2 \tau_i}{1 + \omega^2 \tau_i^2} h_i, \tag{3a}$$

$$\Im(Y_1(\omega)) = \omega C_{01} + \sum_{i=1}^{n} \frac{\omega}{1 + \omega^2 \tau_i^2} h_i, \tag{3b}$$

where the $\{h_i\}$ denote the discrete weights of the deep levels. Each deep level is parametrized by τ_i and h_i and therefore this approach is called *parametric*. Further, the resistance R_{01} is replaced by its conductivity $G_{01} = R_{01}^{-1}$.

The contributions of the deep levels are supposed to be continuous in the nonparametric approach. That is, the relaxation times τ are subjected to a continuous distribution $h(\tau)$.

The sums in Eqs. (3a) and (3b) must be written in the continuous limit as integrals. In this case $Y_1(\omega)$ has the form

$$\Re(Y_1(\omega)) = G_{01} + \int_{\tau_{\min}}^{\tau_{\max}} \frac{\omega^2\tau}{1+\omega^2\tau^2}\tau h(\tau)\, d(\ln\tau), \tag{4a}$$

$$\Im(Y_1(\omega)) = \omega C_{01} + \int_{\tau_{\min}}^{\tau_{\max}} \frac{\omega}{1+\omega^2\tau^2}\tau h(\tau)\, d(\ln\tau). \tag{4b}$$

The additional factor τ in both integrals appears because of the logarithmic scale for the integration variable $d\tau = \tau\, d(\ln\tau)$. The notation $\ln\tau$ means exactly $\ln(\tau/\tau_0)$ with $\tau_0 = 1$ s in order to get a dimensionless argument for the logarithm. This approach is called *non-parametric* because the contributions of the deep levels are given by an arbitrary continuous distribution $h(\tau)$. For discrete contributions of the relaxation times the distribution $h(\tau)$ is expected to show sharp peaks. A characteristic relaxation time of this distribution can be estimated by the average

$$\tau_i = \frac{\int_{\mathrm{peak_i}} \tau^2 h(\tau)\, d(\ln\tau)}{\int_{\mathrm{peak_i}} \tau h(\tau)\, d(\ln\tau)} \tag{5}$$

and the corresponding weight by

$$h_i = \int_{\mathrm{peak_i}} \tau h(\tau)\, d(\ln\tau). \tag{6}$$

An interesting point is the temperature dependence of the additional parameters C_{01}, G_{01}, C_{02}, G_{02}, and R_{03}. The parameters C_{01}, C_{02}, and R_{03} are expected to be nearly independent of the temperature whereas the two remaining parameters should have a characteristic temperature dependence according to [7]

$$G_{01} \sim T^2 e^{-eV_0/k_BT}, \tag{7a}$$

$$G_{02} \sim T^2 e^{-E_g/2k_BT}. \tag{7b}$$

V_0 is the potential of the barrier at the metal-semiconductor interface and e the elementary charge. E_g is the energy of the band gap between the valence and the conduction band.

Within the nonparametric approach the contributions of the deep levels are assumed to be given by a continuous distribution $h(\tau)$. Estimating this distribution function $h(\tau)$ numerically as outlined in the next section one has, however, to discretize the integrals in (4a), (4b), obtaining, e.g.,

$$\Re(Y_1(\omega)) = G_{01} + \sum_i \frac{\omega^2\tau_i}{1+\omega^2\tau_i^2}\tau_i h(\tau_i) w_i, \tag{8a}$$

$$\Im(Y_1(\omega)) = \omega C_{01} + \sum_i \frac{\omega}{1+\omega^2\tau_i^2}\tau_i h(\tau_i) w_i, \tag{8b}$$

where the $\{w_i\}$ are weights due to the discretization and the $\{\tau_i\}$ are fixed points with constant spacing within the range $\tau_{\min}$, $\tau_{\max}$ of the distribution.

Thus, there seems no great difference between the two approaches; the models for the functions $\Re(Y_1(\omega))$ and $\Im(Y_1(\omega))$, given in (3a), (3b) for the parametric and in (8a), (8b) for the nonparametric approach look very similar. There is, though, the difference that in the parametric approach the positions of the contributions τ_i belong to the unknowns, which have to be estimated, whereas in the nonparametric approach they are taken to be fixed. But this is not of great relevance. If we would use in both approaches the least squares estimator, we had only to choose the appropriate minimization routine for the determination of the estimates, either a nonlinear or a linear one. The main point is that the two models for the measurable quantities differ in the number of unknown parameters and therefore in the mathematical properties of the map between unknowns and data. One has only a few parameters in the parametric approach, a lot and in principle an infinite number of unknowns in the nonparametric approach. The number of unknowns, however, has a strong influence on the reliability of the estimation. This can be easily seen, if one writes the relation between data and unknowns $\{h(\tau_i)\}$ in (8a), (8b) as

$$Y_j = \sum_i K_{ji} h(\tau_i), \quad j = 1, \ldots, N, \qquad Y_j = \Re(Y_1(\omega_j)), \Im(Y_1(\omega_j)), \quad \text{resp.} \tag{9}$$

The kernel functions in (4a), (4b) taken as operators in a function space have a spectrum of singular values which converges to zero. Their discrete version, combined into the matrix K in (9), is therefore ill conditioned. This is most drastically seen in the underdetermined situation: The more the number of unknowns exceeds the number of data points, the more zeros are in the spectrum of the singular values of the matrix K. Furthermore, the worse the condition of the matrix is, the larger in turn the confidence regions of the estimated values become.

The condition of the matrix is thus of utmost importance for the estimation and for the decision which type of estimator one has to use. In the parametric case one assumes that the matrix is not ill conditioned; one may use the least squares estimator. In the nonparametric case the ill-conditioning of the matrix is obvious; the least squares estimator turns out to be not consistent. One has to use another estimator, e.g., the estimator provided by some regularization procedure. In such estimators one has to introduce a prior knowledge in order to replace the information which is destroyed by the ill-conditioning of the matrix [8].

Thus the Eqs. (3a), (3b) and (4a), (4b) constitute different mathematical models for the measurable quantities $\Re(Y_1(\omega))$ and $\Im(Y_1(\omega))$ and the inference of the unknown parameters resp. of the unknown function from a finite set of data needs different estimators.

The assumptions about the experimental errors of the data also play a crucial role in the estimation. They influence the mathematical expression of the estimator and in turn the estimates and their confidence regions [9]. A precise formulation of the error model and a careful determination of the uncertainty regions of the estimates are indispensable in order to have a measure for the reliability of the estimation. An ill-conditioning of the map between unknowns and data is immediately revealed by studying the size of the confidence regions. Using the least squares estimator in the ill-conditioned case, e.g., leads to huge uncertainty regions for the estimates, because the size of these regions are inverse proportional to the singular values.

3. METHODS OF DATA ANALYSIS

In the data analysis the additional model parameters C_{01}, G_{01}, C_{02}, G_{02}, and R_{03} and the contributions of the deep levels are estimated from measured admittance data. The method of this analysis depends on the approach used to model the deep levels.

3.1. *Parametric Method*

In the parametric approach the discrepancy

$$D_Y = \sum_{i=1}^{m} \frac{1}{\eta_{1,i}^2} \left[\Re\left(Y_i^\eta\right) - \Re(Y(\omega_i))\right]^2 + \sum_{i=1}^{m} \frac{1}{\eta_{2,i}^2} \left[\Im\left(Y_i^\eta\right) - \Im(Y(\omega_i))\right]^2 \tag{10}$$

of the measured admittance data Y_i^η and the calculated ones $Y(\omega_i)$ is minimized with respect to the additional model parameters and with respect to the parameters of the discrete contributions of the deep levels given by τ_i and h_i. The admittance data $Y(\omega_i)$ are calculated by Eq. (1) with the discrete approach in Eqs. (3a) and (3b). The value m is the number of measured data and $\eta_{1,i}$ and $\eta_{2,i}$ are the experimental errors. These experimental errors are supposed to be relatively constant and Gaussian distributed. This means that $\eta_{1,i} \sim \Re(Y_i^\eta)$ and $\eta_{2,i} \sim \Im(Y_i^\eta)$.

The discrepancy D_Y in Eq. (10) depends on the number n of discrete contributions of the deep levels. This number n is unknown and must additionally be determined. It must be large enough in order to take all relevant contributions into account but it must also be small enough in order to avoid additional and incorrect contributions. These additional contributions would reduce the discrepancy D_Y only by adapting the noise on the admittance data but would not lead to reasonable contributions of deep levels.

A possible method for the determination of the number of discrete contributions is the application of a statistical test. A test consists of a rule that makes a decision to accept or reject a hypothesis on the basis of measured data.

The hypothesis is in our case that the number of discrete contributions is equal to n. The hypothesis is accepted if

$$\frac{|D_Y(n+1) - D_Y(n)|}{D_Y(n)} < \alpha \tag{11}$$

and rejected otherwise. $D_Y(n)$ denotes the discrepancy in Eq. (10) in dependence on the number n of discrete contributions. The term on the left hand side of the inequality (11) measures the relative decrease of the discrepancy if n is increased to $n+1$. α is an upper limit for this decrease.

This relative decrease is significant if it is larger than α. Then, the hypothesis is rejected. If the relative decrease is smaller than α it is taken to be insignificant and the hypothesis is accepted. With this test the number n is increased gradually until the above inequality is fulfilled. We have chosen $\alpha = 10^{-2}$. This value of α is small enough in order to take significant contributions of deep levels into account and it is large enough to prevent n from pretending too many additional contributions. It should be mentioned that the choice of α depends on the investigated problem.

3.2. *Nonparametric Method*

In the nonparametric approach a continuous distribution of the relaxation times τ must be calculated from measured data Y_i^η. This case was discussed extensively in our previous article [1]. The calculation leads to a so-called ill-posed inverse problem [10]. Even a small noise on experimental admittance data has a large influence on the continuous distribution. Therefore, special methods are needed to calculate a continuous distribution from experimental data. Such methods are called regularization methods [11]. In Tikhonov's regularization method the functional

$$V(\lambda) = \sum_{i=1}^{m} \frac{1}{\eta_{1,i}^2} \left[\Re\left(Y_i^\eta\right) - \Re(Y(\omega_i))\right]^2 + \sum_{i=1}^{m} \frac{1}{\eta_{2,i}^2} \left[\Im\left(Y_i^\eta\right) - \Im(Y(\omega_i))\right]^2 + \lambda \int_{\tau_{\min}}^{\tau_{\max}} [\tau h(\tau)]^2 \, d(\ln \tau) \qquad (12)$$

is minimized with respect to the additional model parameters C_{01}, G_{01}, C_{02}, G_{02}, and R_{03} and with respect to the function $\tau h(\tau)$. This functional consists of three terms. The first and the second term are the discrepancy of the measured data comparable to Eq. (10) of the parametric method. The difference is that the values for the admittance are calculated according to Eqs. (4a) and (4b) instead of Eqs. (3a) and (3b). These two terms force the calculated values to be compatible with the experimental ones. The third term is the so-called regularization functional with the regularization parameter λ. This term leads to a stable estimate of the function $\tau h(\tau)$ without large irregular fluctuations. The regularization parameter which controls the stability is determined with the self-consistent (SC) method [12].

In the nonparametric method the number of contributions is calculated automatically by the number of peaks in the continuous distribution. Discrete deep level contributions can be easily calculated from the continuous distribution by Eqs. (5) and (6).

Although the parametric and nonparametric methods are in principle different there is a similarity between these methods. Besides the minimization of a discrepancy $D_Y(n)$ or of a functional $V(\lambda)$, both methods include an additional criterion for the estimation of their solution. In the parametric method this criterion concerns directly the number of discrete contributions, whereas in the nonparametric method the criterion for the determination of λ deals with the degree of stability for the function $\tau h(\tau)$.

4. RESULTS FOR SIMULATED DATA

In this section the parametric and nonparameteric method for the analysis of admittance data are compared with a Monte Carlo study. The comparison is carried out for three different cases of deep level contributions:

(1) only discrete contributions,
(2) only continuous contributions, and
(3) discrete and continuous contributions simultaneously.

In a preliminary step a set of hypothetical model parameters

$$\begin{aligned} C_{01} &= 1.0 \cdot 10^{-10}\,\mathrm{F}, \\ G_{01} &= 1.0 \cdot 10^{-8}\,\Omega^{-1}, \\ C_{02} &= 1.0 \cdot 10^{-11}\,\mathrm{F}, \\ G_{02} &= 1.0 \cdot 10^{-6}\,\Omega^{-1}, \end{aligned}$$

and

$$R_{03} = 1.0\ \mathrm{k}\Omega$$

and hypothetical discrete and continuous relaxation time contributions are used to generate samples of admittance data for each of the three cases addressed above according to Eq. (1). For this purpose, 200 values for the angular frequency ω were chosen from a logarithmic scaled interval $[1\ \mathrm{s}^{-1}, 10^7\ \mathrm{s}^{-1}]$. The experimental error was simulated by adding a Gaussian random number corresponding to a relatively constant error of 1%, which is comparable to the noise in experimental data. In the Monte Carlo study for each case 1000 samples of admittance data are simulated. The samples differ only in the realization of the Gaussian random number.

For the 1000 samples the parametric and the nonparametric analysis method is applied. The results calculated from each sample are averaged over the results of the total number of samples. Thus, representative solutions can be calculated. With the parametric method averaged values of the parameters C_{01}, G_{01}, C_{02}, G_{02}, R_{03}, the number of discrete contributions n, and averaged values of the discrete contributions τ_i and h_i are estimated in the Monte Carlo study.

With the nonparametric method the averaged values of the model parameters C_{01}, G_{01}, C_{02}, G_{02}, R_{03} are estimated and the average of a continuous distribution of the deep levels is calculated. From this continuous distribution averaged discrete values for the relaxation times τ_i and the corresponding weights h_i are estimated with Eqs. (5) and (6).

(1) Discrete contributions. Figure 2 shows the simulated admittance data and the three hypothetical discrete contributions with

$$\begin{aligned} \tau_1 &= 10^{-5}\ \mathrm{s}, \qquad h_1 = 0.2\ \mathrm{s}\,\Omega^{-1}, \\ \tau_2 &= 10^{-4}\ \mathrm{s}, \qquad h_2 = 0.3\ \mathrm{s}\,\Omega^{-1}, \end{aligned}$$

and

$$\tau_3 = 10^{-3}\ \mathrm{s}, \qquad h_3 = 0.6\ \mathrm{s}\,\Omega^{-1}.$$

With the parametric method the correct amount of $n = 3$ discrete contributions was determined in 92% of the 1000 simulated samples. In 8% of all simulated samples a wrong amount of $n = 4$ contributions was determined using the test procedure described in the previous section. The corresponding estimated contributions are depicted in Fig. 3. The results calculated with the parametric method show only very small deviations from the originally given values for the correct number $n = 3$. For the results estimated with $n = 4$ larger deviations are indicated by the error bars.

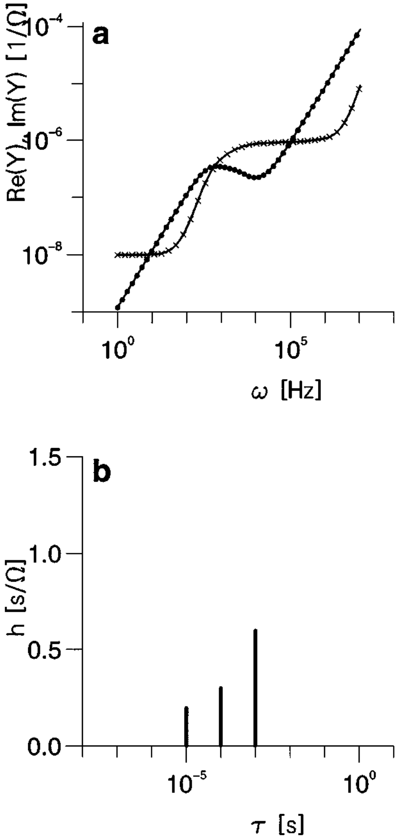


FIG. 2. (a) Simulated admittance data, ×, $\Re(Y)$; ●, $\Im(Y)$; and (b) the hypothetical discrete contributions of deep levels used for a Monte Carlo simulation.

In Fig. 4 the continuous distribution estimated with the nonparametric method is shown. The averaged estimated deep level parameters and the averaged estimated additional model parameters C_{01}, G_{01}, C_{02}, G_{02}, and R_{03} are shown in Tables I and II. The deep level contributions are nearly as accurate as the ones calculated with the parametric method. The results for the additional parameters agree very well with the hypothetical values for both analysis methods.

The disadvantage of the parametric method is that additional deep level contributions can be pretended which are not present in the data. Thus, the determination of the number of contributions is a crucial point in the parametric method, because additionally pretended

TABLE I
Estimated Parameters of the Parametric and the Nonparametric Method for Discrete Deep Level Contributions

	Parametric ($n = 3$)	Parametric ($n = 4$)	Nonparametric
C_{01} [10^{-10} F]	0.99 ± 0.10	0.97 ± 0.12	0.95 ± 0.07
G_{01} [10^{-8} Ω^{-1}]	1.0 ± 0.001	0.999 ± 0.002	0.999 ± 0.002
C_{02} [10^{-11} F]	1.0 ± 0.01	1.0 ± 0.01	1.006 ± 0.008
G_{02} [10^{-6} Ω^{-1}]	1.001 ± 0.009	1.0 ± 0.01	1.01 ± 0.005
R_{03} [kΩ]	1.0 ± 0.005	1.0 ± 0.005	0.995 ± 0.009

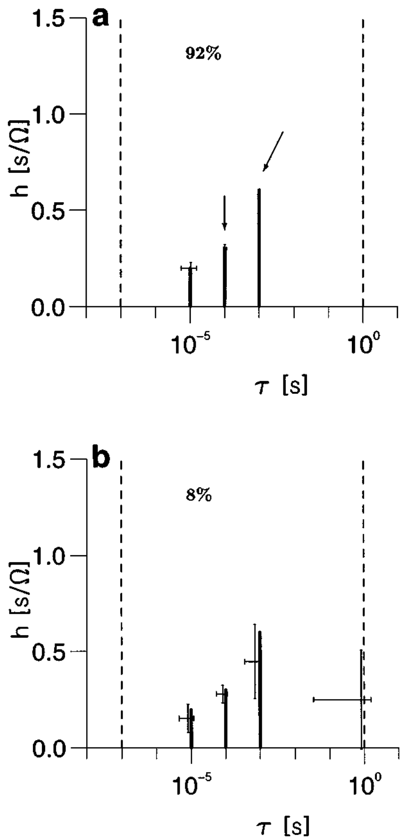


FIG. 3. Estimated discrete contributions in the Monte Carlo simulation. (a) $n = 3$ contributions (92%) and (b) $n = 4$ contributions (8%). The vertical lines mark the hypothetical discrete values and the error bars characterize the estimated ones. The arrow point at error bars which are too small to be seen. The left and right dashed lines mark the borders where the solution is unique.

contributions can worsen the results of the relevant contributions. In contrast to this, with the nonparametric method the correct number of deep level contributions was always determined.

A disadvantage of the nonparametric method can appear if contributions are so close together that the regularization procedure can only resolve one broader peak. The parametric method could better deal with this situation in the case when the number of discrete contributions is known.

TABLE II

Estimated Deep Level Contributions of the Parametric and the Nonparametric Method for Discrete Deep Level Contributions

Parametric ($n = 3$)		Parametric ($n = 4$)		Nonparametric	
τ_i [s]	h_i [10^{-9} s/Ω]	τ_i [s]	h_i [10^{-9} s/Ω]	τ_i [s]	h_i [10^{-9} s/Ω]
$(1.0 \pm 0.5) \cdot 10^{-5}$	0.2 ± 0.03	$(8.2 \pm 3.7) \cdot 10^{-6}$	0.15 ± 0.07	$(1.02 \pm 0.2) \cdot 10^{-5}$	0.15 ± 0.02
$(1.01 \pm 0.09) \cdot 10^{-4}$	0.3 ± 0.02	$(8.2 \pm 2.9) \cdot 10^{-5}$	0.28 ± 0.05	$(0.97 \pm 0.4) \cdot 10^{-4}$	0.33 ± 0.02
$(1.0 \pm 0.01) \cdot 10^{-3}$	0.6 ± 0.008	$(7.2 \pm 2.6) \cdot 10^{-4}$	0.45 ± 0.2	$(1.0 \pm 0.01) \cdot 10^{-3}$	0.62 ± 0.07
		$(8.2 \pm 0.8) \cdot 10^{-1}$	0.25 ± 0.26		

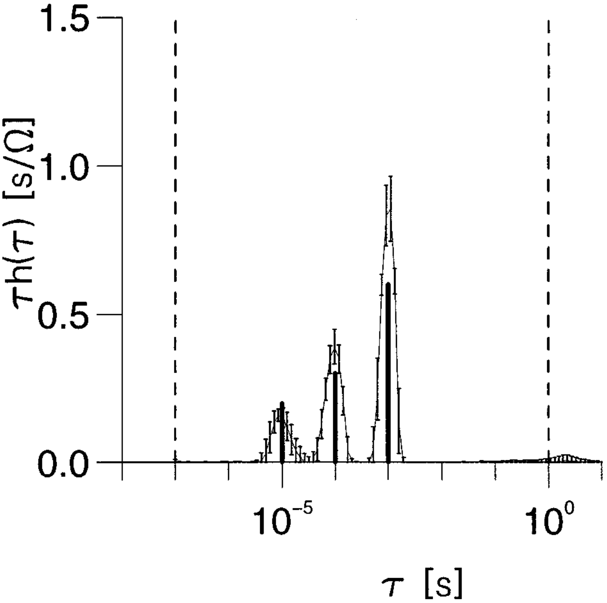


FIG. 4. The distribution $\tau h(\tau)$ estimated with the regularization procedure in the Monte Corlo simulation. The vertical lines mark the hypothetical discrete values and the error bars characterize the estimated values of the distribution. The left and right dashed lines mark the borders where the solution is unique.

(2) Continuous contribution. Figure 5 shows the simulated admittance data and the hypothetical continuous distribution for the relaxation times. This distribution was chosen to be gaussian on a logarithmic scale with mean value $5 \cdot 10^{-2}$ and variance 2.0. With the parametric method the number of different relaxation time contributions was determined to $n = 4$ (32%), 5 (66.5%), and 6 (1.5%). The corresponding estimated discrete contributions using the parametric method are depicted in Fig. 6. Although the estimated discrete contributions are located near the continuous hypothetical distribution, their continuous character cannot be assessed with the estimated results of the parametric method.

The continuous distribution estimated with the nonparametric method is shown in Fig. 7. The nonparametric method yields a very accurate estimation of hypothetical distribution. The averaged estimated model parameters are shown in Tables IIIa and IIIb. As in the previous case these additional model parameters are estimated very well for both analysis methods.

TABLE IIIa

Estimated Parameters of the Parametric Method for a Continuous Deep Level Contribution

	Parametric ($n = 4$)	Parametric ($n = 5$)	Parametric ($n = 6$)
C_{01} [10^{-10} F]	1.0 ± 0.002	1.0 ± 0.01	0.995 ± 0.004
G_{01} [10^{-8} Ω^{-1}]	1.0 ± 0.002	0.999 ± 0.008	0.982 ± 0.02
C_{02} [10^{-11} F]	0.999 ± 0.001	1.0 ± 0.002	1.0 ± 0.001
G_{02} [10^{-6} Ω^{-1}]	0.999 ± 0.001	1.0 ± 0.003	1.0 ± 0.002
R_{03} [kΩ]	1.0 ± 0.004	1.0 ± 0.004	1.001 ± 0.005

TABLE IIIb

Estimated Parameters of the Nonparametric Method for a Continuous Deep Level Contribution

	Nonparametric
C_{01} [10^{-10} F]	0.99 ± 0.01
G_{01} [10^{-8} Ω^{-1}]	1.0 ± 0.002
C_{02} [10^{-11} F]	1.0 ± 0.002
G_{02} [10^{-6} Ω^{-1}]	1.0 ± 0.002
R_{03} [kΩ]	0.997 ± 0.008

(3) Discrete and continuous contributions simultaneously. Figure 8 shows the simulated admittance data and the hypothetical discrete and continuous deep level contributions. The discrete contributions are taken from the first case and the continuous one is taken from the second case.The number of estimated discrete contributions is $n = 5$ (92.5%), 6 (3.1%), 7 (4.1%), and 8 (0.3%) using the parametric method in the Monte Carlo simulation. The corresponding estimated discrete contributions are depicted in Fig. 9.

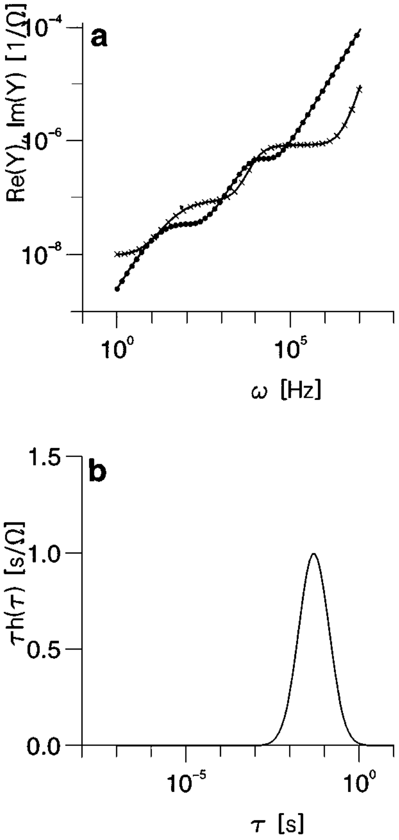


FIG. 5. (a) Simulated admittance data, ×, $\Re(Y)$; ●, $\Im(Y)$; and (b) the hypothetical continuous distribution $\tau h(\tau)$ of relaxation times used for a Monte Carlo study.

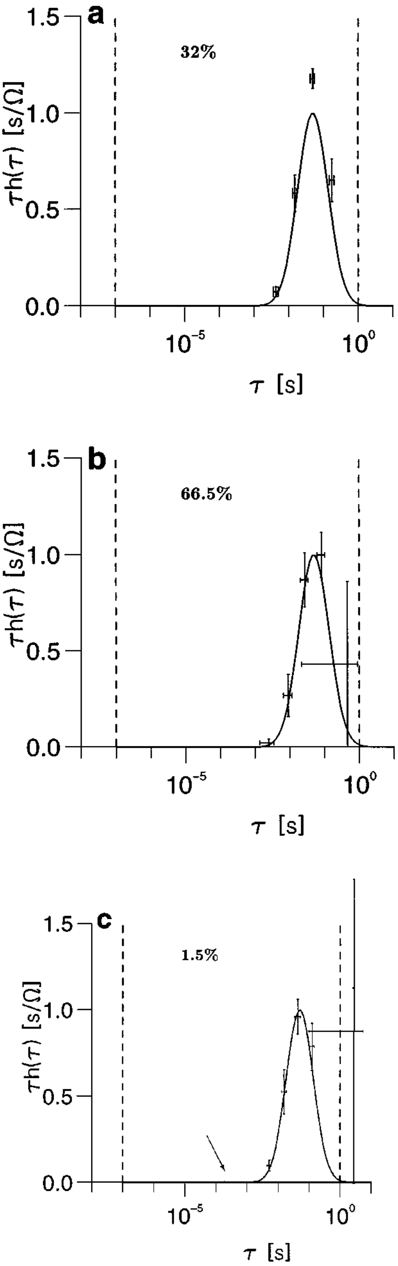


FIG. 6. Estimated discrete contributions in the Monte Carlo study. (a) $n = 4$ (32%), (b) $n = 5$ (66.5%), and (c) $n = 6$ (1.5%) contributions. The curve marks the hypothetical continuous distribution and the error bars characterize the estimated discrete values. The arrow points at an error bar which is too small to be seen. The left and right dashed lines mark the borders where the solution is unique.

The solution estimated with the nonparametric method is shown in Fig. 10. The results for the additional model parameters C_{01}, G_{01}, C_{02}, G_{02}, and R_{03} are nearly the same as in the two cases before. For this reason, they are not shown separately.

The results for the deep level contributions are comparable with the results in the previous case. For $n = 5$ and $n = 8$ determined contributions large deviations are observed for the

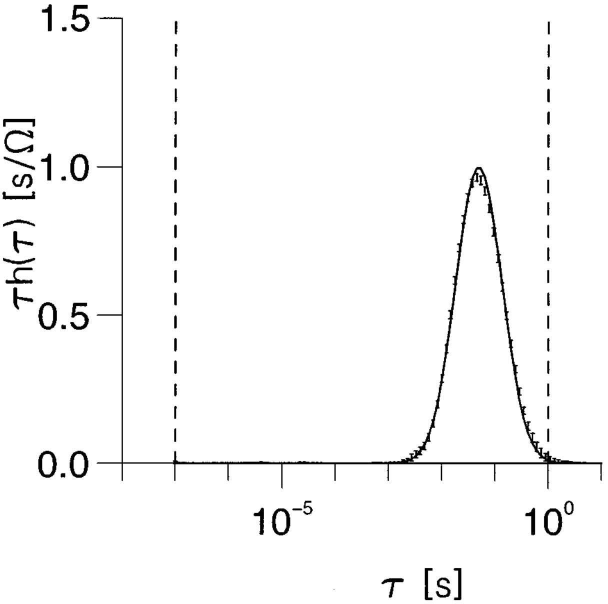


FIG. 7. The distribution $\tau h(\tau)$ estimated with the regularization procedure in the Monte Carlo simulation. The full line characterizes the hypothetical distribution and the error bars the estimated values of the distribution. The left and right dashed lines mark the borders where the solution is unique.

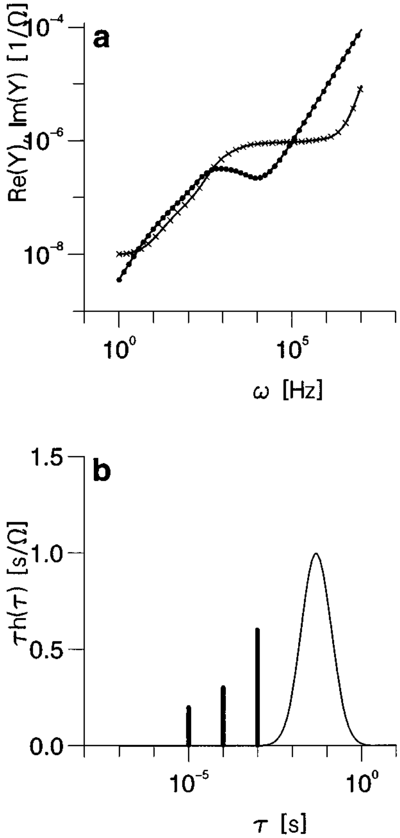


FIG. 8. (a) Simulated admittance data, ×, $\Re(Y)$; ●, $\Im(Y)$; and (b) the hypothetical discrete and continuous contributions of deep levels used for a Monte Carlo simulation.

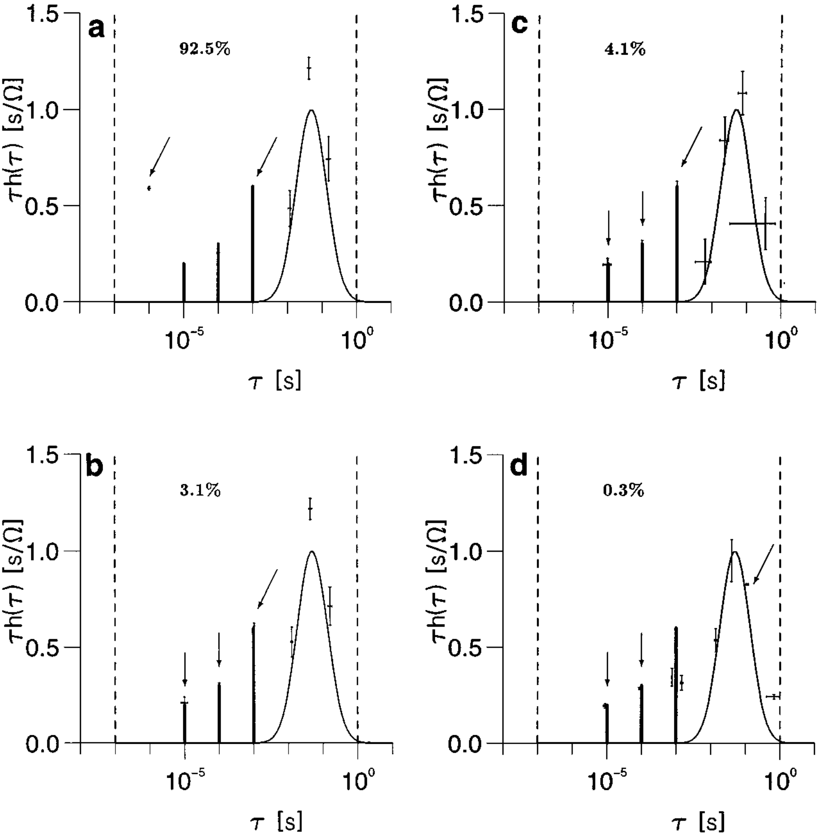


FIG. 9. Estimated discrete contributions in the Monte Carlo study. (a) $n = 5$ (92.5%), (b) $n = 6$ (3.1%), (c) $n = 7$ (4.1%), and (d) $n = 8$ contributions (0.3%). The curve shows the hypothetical continuous distribution and the vertical lines mark the hypothetical discrete contributions. The error bars characterize the estimated values. The arrows point at error bars which are too small to be seen. The left and right dashed lines mark the borders where the solution is unique.

results estimated with the parametric method. Even the three discrete contributions are not resolved correctly in this case. For $n = 6$ and $n = 7$ at least the discrete contributions are well estimated, which happens only in 7.2% of all simulated data. But as in the previous case of completely continuous contributions the continuous part is only poorly characterized.

In contrast to these results the solution is well estimated with the nonparametric method. The continuous part of the whole hypothetical contribution is estimated very accurately and the estimations of the weights of the discrete part are nearly the same as in the first case of pure discrete contributions.

5. RESULTS FOR MEASURED DATA

The admittance of a GaAs Schottky diode was measured for several temperatures in dependence on the frequency ω. The measurement details are pointed out extensively in the previous articles [1, 13]. Here the measured admittance data were used to focus on the differences of the parametric and nonparametric approach for their analysis.

As an example Fig. 11 shows the admittance data measured for a temperature of 6°C, the estimated discrete contributions using the parametric method, and the estimated continuous

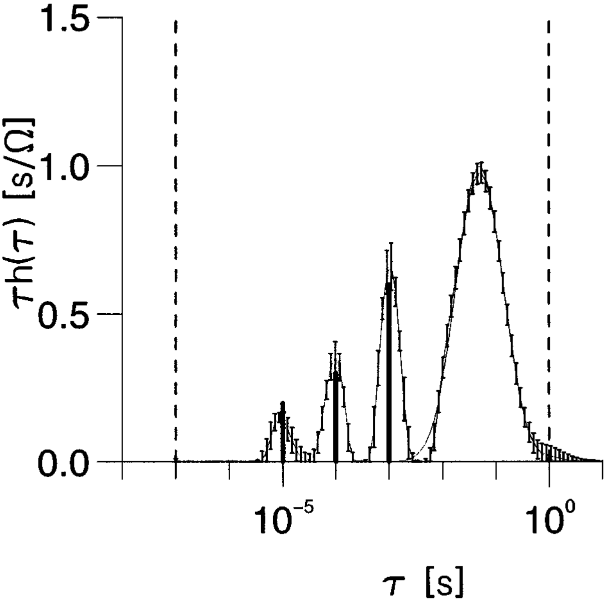


FIG. 10. The distribution $\tau h(\tau)$ estimated with the regularization procedure in the Monte Carlo simulation. The vertical lines mark the hypothetical values for the discrete contributions and the error bars characterize the estimated values of the continuous distribution. The left and right dashed lines mark the borders where the solution is unique.

distribution using the nonparametric method. The parametric method produced seven discrete contributions and the nonparametric method a continuous distribution with four broad peaks. The comparison leads to the problem of judging the accuracy of the results of each method. If a continuous distribution is assumed then the parametric analysis could not resolve the peaks below $\tau = 10^{-4}$ s. Furthermore, the broad distribution between $\tau = 10^{-4}$ s and $\tau = 10^{-1}$ s is represented by a set of four discrete relaxation times. If on the contrary, sharp relaxation times are assumed then the nonparametric method could not resolve this discrete structure correctly.

To distinguish between the results of the different methods the analysis was performed for different temperatures to obtain the Arrhenius plots (Fig. 12) for the relaxation times of the levels. In order to calculate the activation energies and cross sections the points in the Arrhenius plot must be related to straight lines. The following seven deep levels were determined with the parametric method:

(1) $\Delta E_1 = (0.87 \pm 0.03)$ eV, $\sigma_1 = (7.0 \pm 9.6) \cdot 10^{-11}$ cm^2
(2) $\Delta E_2 = (0.76 \pm 0.04)$ eV, $\sigma_2 = (4.3 \pm 6.2) \cdot 10^{-12}$ cm^2
(3) $\Delta E_3 = (0.76 \pm 0.04)$ eV, $\sigma_3 = (1.3 \pm 2.0) \cdot 10^{-11}$ cm^2
(4) $\Delta E_4 = (0.77 \pm 0.05)$ eV, $\sigma_4 = (6.9 \pm 12.2) \cdot 10^{-11}$ cm^2
(5) $\Delta E_5 = (0.77 \pm 0.05)$ eV, $\sigma_5 = (3.0 \pm 5.7) \cdot 10^{-10}$ cm^2
(6) $\Delta E_6 = (0.74 \pm 0.04)$ eV, $\sigma_6 = (3.1 \pm 4.8) \cdot 10^{-10}$ cm^2
(7) $\Delta E_7 = (0.62 \pm 0.09)$ eV, $\sigma_7 = (3.1 \pm 9.9) \cdot 10^{-11}$ cm^2.

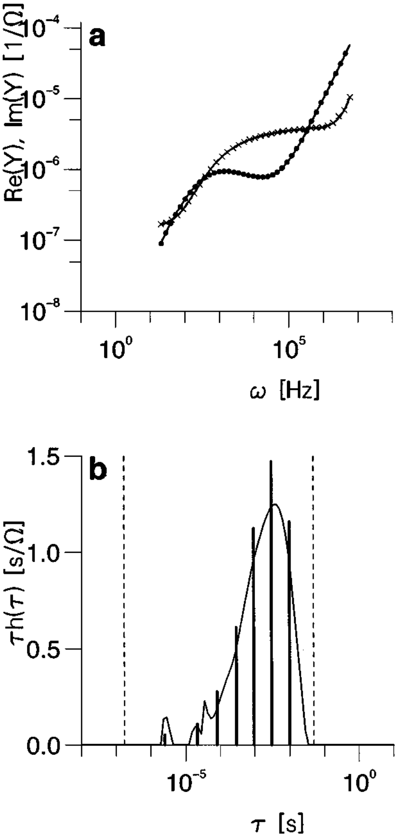


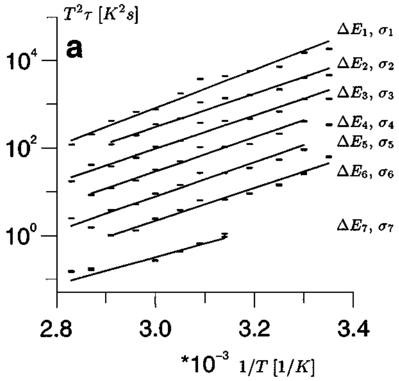
FIG. 11. (a) Measured admittance data for a temperature of 60°C. ×, $\Re(Y)$; ●, $\Im(Y)$. (b) The curve is the continuous distribution estimated with the nonparametric method and the vertical lines represent the discrete contributions estimated with the parametric method. For clarity the corresponding error bars are not shown. The left and right dashed lines mark the borders where the solution is unique.

The following four deep levels were determined with the nonparametric method:

$$\begin{aligned}
&(1)\ \Delta E_1 = (0.72 \pm 0.03)\,\text{eV}, &\sigma_1 = (7.96 \pm 9.29) \cdot 10^{-13}\,\text{cm}^2\\
&(2)\ \Delta E_2 = (0.65 \pm 0.02)\,\text{eV}, &\sigma_2 = (8.86 \pm 5.67) \cdot 10^{-12}\,\text{cm}^2\\
&(3)\ \Delta E_3 = (0.63 \pm 0.02)\,\text{eV}, &\sigma_3 = (6.27 \pm 5.24) \cdot 10^{-12}\,\text{cm}^2\\
&(4)\ \Delta E_4 = (0.50 \pm 0.04)\,\text{eV}, &\sigma_4 = (6.49 \pm 9.11) \cdot 10^{-11}\,\text{cm}^2.
\end{aligned}$$

The calculated deep levels are compared with results from literature in our previous article [1]. In that article the reason for the large deviations of the estimated cross section is discussed as well.

The number of deep levels determined with the parametric and with the nonparametric method is quite different. But several deep levels estimated with the parametric method have nearly the same activation energy and similar cross sections. Therefore, it seems to be possible that the discrete levels (2)–(6) are due to an originally continuous contribution. With the nonparametric method a continuous contribution is calculated with an average activation energy of 0.72 eV. The levels (2)–(6) calculated with the parametric method would agree with this activation energy within their estimated error range. The results of the Monte Carlo



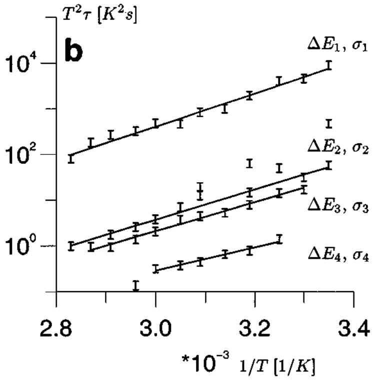


FIG. 12. Arrhenius-plots of the relaxation times obtained from measured admittance data. (a) The contributions are estimated with the parametric method and (b) with the nonparametric method.

simulations in the previous section have also shown this effect, that the parametric method yields several discrete contributions for an originally continuous contribution.

Additionally, the model parameters are estimated with the parametric and the nonparamtric method in dependence on the temperature (Figs. 13 and 14). Both analysis methods yield nearly the same model parameters but the values estimated for the capacity C_{01} with the parametric and the nonparametric method are not quite identical. Table IV shows the average values for the nearly temperature independent parameters C_{01}, C_{02}, and R_{03},

TABLE IV
Estimated Parameters of the Parametric and the Nonparametric Method for Measured Admittance Data

	Parametric	Nonparametric
C_{01} [10^{-10} F]	0.75 ± 0.4	0.79 ± 0.01
C_{02} [10^{-11} F]	1.1 ± 0.01	1.1 ± 0.01
R_{03} [kΩ]	2.0 ± 0.05	1.99 ± 0.06
V_0 [V]	0.822 ± 0.009	0.814 ± 0.006
E_g [eV]	1.44 ± 0.02	1.43 ± 0.01

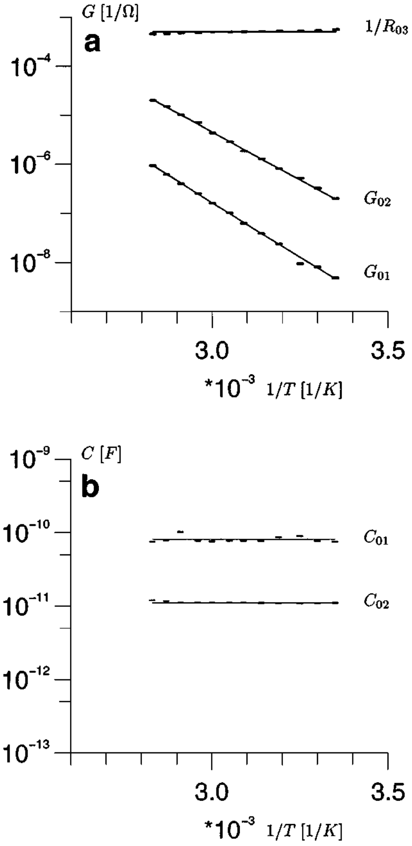


FIG. 13. The parameters obtained from the measured admittance data in dependence on $1/T$ estimated with the parametric method. (a) The conductivities G_{01}, G_{02}, and $1/R_{03}$. (b) The capacities C_{01} and C_{02}.

for the potential barrier V_0, and for the energy of the band gap E_g. The parameters V_0 and E_g were fitted on the temperature dependent values of G_{01} and G_{02} using the relationships of Eqs. (7a) and (7b).

The reliability of the estimated values of the both capacities C_{01} and C_{02}, the resistance R_{03}, and the values for the potential barrier V_0 and the band gap E_g are discussed extensively in our previous article [1].

6. CONCLUSIONS

For the analysis of measured admittance data of a Schottky diode two different methods are compared: A parametric and a nonparametric method. The parametric method assumes discrete deep level contributions whereas with the nonparametric method continuous contributions are supposed.

The comparison shows a great disadvantage of the parametric method to the nonparametric method. The parametric analysis is only suited for discrete contributions and cannot estimate continuous ones at all. A Monte Carlo study on simulated admittance data has shown that the parametric method is not able to estimate reliable results if a part of the deep level contribution is continuous. Even for completely discrete deep level contributions

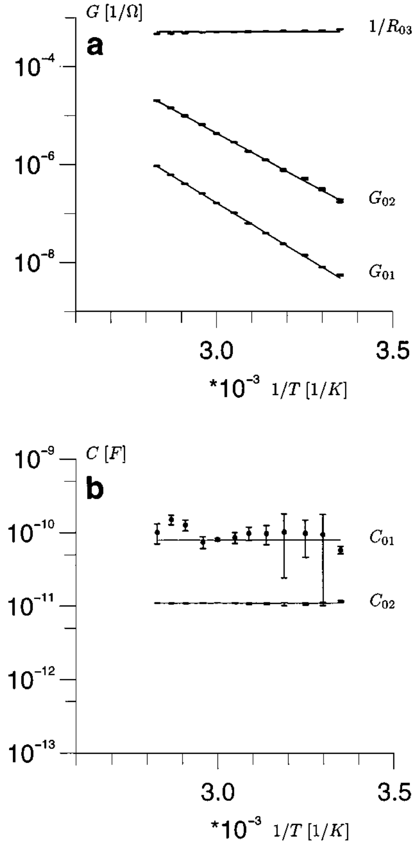


FIG. 14. The parameters obtained from the measured admittance data in dependence on $1/T$ estimated with the nonparametric method. (a) The conductivities G_{01}, G_{02}, and $1/R_{03}$. (b) The capacities C_{01} and C_{02}.

the results of the parametric method depend essentially on the number of contributions which must be determined separately. Only if this number is determined correctly the corresponding results are in a good agreement with the physical properties of the examined material.

On the contrary, the nonparametric method is suited for the estimation of discrete contributions as well as for continuous distributions of deep levels. In this sense nonparametric methods are superior to parametric ones. But it should be mentioned that the nonparametric method has the disadvantage that originally discrete contributions are estimated as slightly broadened peaks in the continuous distribution. The broadening for this continuous distribution is among other influences caused by the noise of the experimental data. Consequently, discrete peaks which are very close together could not be estimated as separate peaks but only as a single broadened one. We think that this disadvantage is compensated by the advantage that the number of discrete contributions is obtained automatically from the number of peaks in the estimated continuous distribution.

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