

# Defect characterization by differential capacitance spectroscopy without the Arrhenius plot

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Jian V. Li<sup>a</sup> 

## AFFILIATIONS

Department of Aeronautics and Astronautics, National Cheng Kung University, Tainan 701, Taiwan

<sup>a</sup>Author to whom correspondence should be addressed: [jianvli@ncku.edu.tw](mailto:jianvli@ncku.edu.tw)

## ABSTRACT

A new method of Arrhenius transformation and matching is developed in this study based on the rate-temperature duality of the admittance spectroscopy measurement to extract the activation energy  $E_a$  and the attempt-to-escape frequency  $v_0$  of a defect in GaAsN from differential capacitance spectroscopy without the Arrhenius plot and without identifying the  $f\partial C/\partial f$  spectra peaks. The method consists of a set of variations that transform the iso-rate scan and/or the isothermal scan to a virtual space—activation energy, attempt-to-escape frequency, temperature, or rate. The transformed scans must be matched prior to extracting  $E_a$  and  $v_0$  local to a fixed point in the two-dimensional temperature-rate experimental space.

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Carrier emission from defects<sup>1,2</sup> in semiconductor materials is a thermally activated process.<sup>3</sup> The admittance spectroscopy (AS)<sup>4,5</sup> finds defects by identifying a peak in the frequency differential capacitance  $f\partial C/\partial f$  spectra at a certain temperature and frequency  $f_{peak}$ ; the latter is related to the carrier emission/capture rate<sup>1</sup> by  $f_{peak} = v/2\pi$ . According to the Arrhenius equation,

$$v = v_0 \exp(-E_a/k_B T), \quad (1)$$

where  $E_a$  is the activation energy of the defect,  $v_0$  is the attempt-to-escape frequency,  $k_B$  is Boltzmann's constant, and  $T$  is temperature. The measurements of  $E_a$  and  $v_0$  are essential to the characterization of defects, and such measurements have traditionally relied on the classic Arrhenius plot line-fitting (APL) method.<sup>1</sup> Over a range of temperatures,  $E_a$  is extracted from the slope and  $v_0$  is extracted from the y-intercept by line-fitting the Arrhenius plot that is composed of the peak frequencies of the  $f\partial C/\partial f$  spectra.

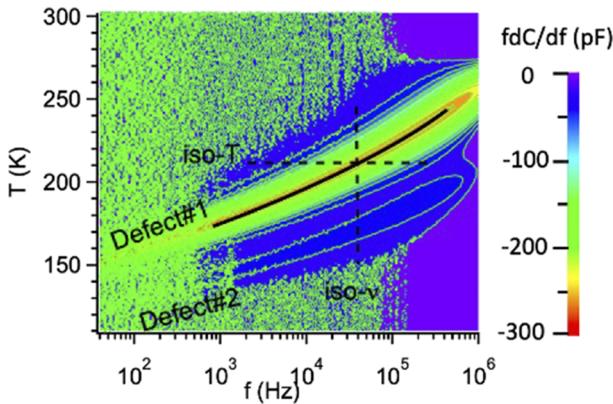
The APL method requires accurate identification of the peak positions in the  $f\partial C/\partial f$  spectra and cannot extract  $E_a$  and  $v_0$  local to a temperature point, which contain valuable information of a non-Arrhenius process.<sup>6,7</sup> Recently, I developed the Arrhenius transformation and matching (ATM) method to extract  $E_a$  and  $v_0$  without identifying the peaks and therefore bypassing

the Arrhenius plot from deep-level transient spectroscopy<sup>8</sup> and capacitance-frequency<sup>9</sup> measurement (a rare form of AS). In this work, I systematically present the ATM method for extracting  $E_a$  and  $v_0$  from the differential capacitance  $f\partial C/\partial f$  spectra (the standard<sup>5</sup> form of AS).

The admittance measurement was performed with a Keysight 4294A impedance analyzer from 100 Hz to 1 MHz with 35 mV<sub>rms</sub> AC modulation voltage. The sample was a  $1 \times 1 \text{ mm}^2$  GaAs<sub>0.988</sub>N<sub>0.012</sub> asymmetrical PN<sup>+</sup> junction (p-doping =  $1.38 \times 10^{17} \text{ cm}^{-3}$ ) solar cell<sup>10</sup> grown by metal-organic chemical vapor deposition. The temperature of the sample was stabilized between 12 and 450 K in a Janis closed-cycle He-cooled cryostat.

Figure 1 shows the  $f\partial C/\partial f$  contour plot in the temperature-rate plane with two defects. This work focuses on defect 1 only, which has a larger  $f\partial C/\partial f$ . The APL method uses the locus of the peaks in the  $T-v$  space (the black solid line in Fig. 1) to construct the Arrhenius plot (data not shown). Then,  $E_a = 335 \pm 1 \text{ meV}$  and  $\log_{10}(v_0) = 13.4 \pm 0.1 \text{ s}^{-1}$  are extracted from the plot by line-fitting between 160 and 240 K.

By rearranging the Arrhenius equation [Eq. (1)], one can obtain the various Arrhenius transformations between the spaces of the two experimentally controllable parameters ( $T$  and  $v$ ) and the two parameters to be extracted ( $E_a$  and  $v_0$ ) as follows:



**FIG. 1.** The contour plot of  $fdC/df$  in the  $T$ - $\nu$  plane. The isothermal and iso-rate scans at any ( $T_{fix}$ ,  $\nu_{fix}$ ) point (examples in dashed lines) may be visualized as “slicing” through the  $fdC/df$  surface in the 2D  $T$ - $\nu$  space. This contour plot is constructed from 220 pre-transformation  $fdC/df$  vs  $f$  spectra with a temperature step size of 1.0 K and 301 frequency points in each spectrum.

$T$ - $E_a$  transformation:

$$E_{a,T} = k_B T \ln(\nu_0 / \nu_{fix}), \quad (2)$$

$\nu$ - $E_a$  transformation:

$$E_{a,\nu} = k_B T_{fix} \ln(\nu_0 / \nu), \quad (3)$$

$T$ - $\nu_0$  transformation:

$$\nu_{0,T} = \nu_{fix} \exp(E_a / k_B T), \quad (4)$$

$\nu$ - $\nu_0$  transformation:

$$\nu_{0,\nu} = \nu \exp(E_a / k_B T_{fix}), \quad (5)$$

$T$ - $\nu$  transformation:

$$\nu_T = \nu_{fix} \times \exp[E_a / k_B \times (T^{-1} - T_{fix}^{-1})], \quad (6)$$

$\nu$ - $T$  transformation:

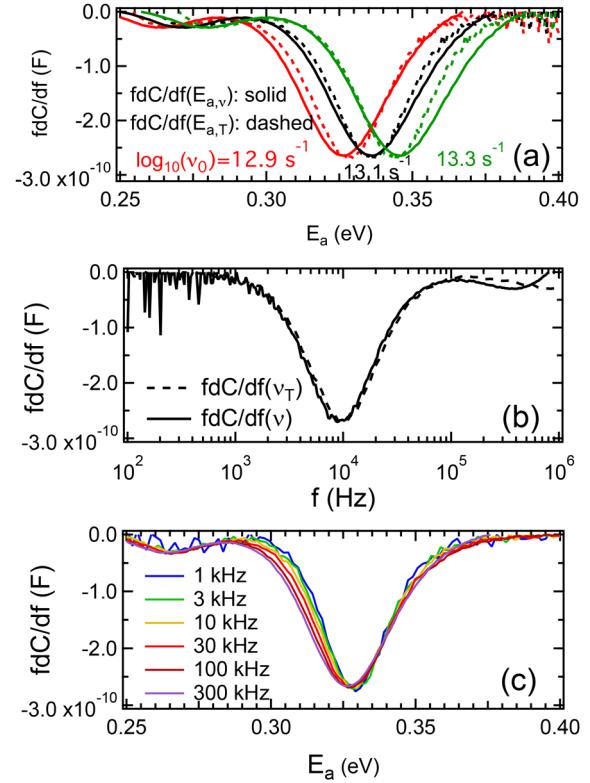
$$T_\nu = T_{fix} \times [\ln(\nu_0) - \ln(\nu)] / [\ln(\nu_0) - \ln(\nu_{fix})], \quad (7)$$

where  $\nu_{fix}$  and  $T_{fix}$  are from a fixed point in the  $T$ - $\nu$  space and all other parameters on the LHS of the equations are transformed parameters.

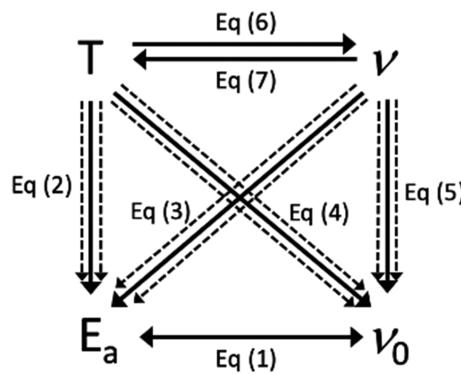
Consider the two independent scans indicated by the dashed lines in Fig. 1: (i) the iso-rate scan  $fdC/df(T)$  with fixed  $\nu_{fix}$  and (ii) the isothermal scan  $fdC/df(v)$  with fixed  $T_{fix}$ . One can use Eq. (2) to turn  $fdC/df(T)$  into a virtual scan  $fdC/df(E_{a,T})$ , accomplishing a  $T$ - $E_a$  transformation in the  $E_a$  space. Similarly, one can use Eq. (3) to transform  $fdC/df(v)$  into a virtual scan  $fdC/df(E_{a,v})$ . The  $T$ - $E_a$  and  $\nu$ - $E_a$  transformations share the same  $\nu_0$ , which adjusts simultaneously the curvatures of  $fdC/df(E_{a,T})$  and  $fdC/df(E_{a,v})$ . Both experimental scans,  $fdC/df(v)$  and  $fdC/df(T)$ , are based on the same thermally activated process that determines the carrier exchange rate. Therefore, the necessary and sufficient condition for two corresponding virtual scans  $fdC/df(E_{a,v})$  and  $fdC/df(E_{a,T})$  to concur is to

use the  $\nu_0$  in the  $T$ - $E_a$  and  $\nu$ - $E_a$  transformations from the thermal activation process from which these scans were physically obtained. Once  $\nu_0$  is determined,  $E_a$  can then be calculated through Eq. (1) at  $(T_{fix}, \nu_{fix})$ . Alternatively,  $E_a$  can be read from the common peak shared by  $fdC/df(E_{a,v})$  and  $fdC/df(E_{a,T})$ . Figure 2(a) is an example of applying this procedure to extract  $\log_{10}(\nu_0) = 13.1 \text{ s}^{-1}$  and calculate  $E_a = 338 \text{ meV}$  local to  $T_{fix} = 197 \text{ K}$ . These results agree well with what the APL method produces. In the exaggerated cases of  $\log_{10}(\nu_0) = 12.9 \text{ s}^{-1}$  and  $13.3 \text{ s}^{-1}$ , the matching is poor. Similarly, one can use Eqs. (4) and (5) to transform  $T/\nu$  to  $\nu_0$  space, obtain the best fit value of  $E_a$  by matching the virtual scans, and calculate  $\nu_0$  from Eq. (1). While the fixed point  $(\nu_{fix}, T_{fix})$  can be any arbitrary point in the  $T$ - $\nu$  plane in principle, the points near the solid line in Fig. 1 are the more convenient choices because the curvatures match at the peak of two  $fdC/df$  spectra and the near-peak data are less noisy.

Alternatively, one can use Eq. (6) to perform a  $T$ - $\nu$  transformation and generate a virtual scan  $fdC/df(\nu_T)$  from an experimental iso-rate scan  $fdC/df(T)$ , which is matched to the experimental isothermal scan  $fdC/df(v)$ ; to obtain the best fit value of  $E_a$ ; and to calculate  $\nu_0$ . Figure 2(b) is an example of applying the



**FIG. 2.** (a) The virtual scan  $fdC/df(E_{a,v})$  (solid) and iso-rate scan  $fdC/df(E_{a,T})$  (dashed) are transformed from the isothermal ( $T_{fix} = 197 \text{ K}$ ) and iso-rate ( $\nu_{fix} = 10 \text{ kHz}$ ) scans using Eqs. (2) and (3). A match (black) is obtained with  $\log_{10}(\nu_0) = 13.1 \text{ s}^{-1}$ . Green and red curves show exaggerated poor matching. (b) The virtual scan  $fdC/df(v)$  (dashed) is transformed from the experimental iso-rate ( $\nu_{fix} = 10 \text{ kHz}$ ) scan  $fdC/df(v)$  (solid) to extract  $E_a = 338 \text{ meV}$ . (c) Several iso-rate  $fdC/df(T)$  scans are transformed to the  $E_a$  space using Eq. (2) with  $\log_{10}(\nu_0) = 13.1 \text{ s}^{-1}$ . The resultant  $fdC/df(E_{a,T})$  spectra collapse together.



**FIG. 3.** A diagram summarizing the variations of the ATM method. The transformations between  $T$ ,  $v$ ,  $E_a$ , and  $v_0$ , which are based on the Arrhenius equation indicated by the double-ended arrow, are represented by single-ended arrows with the corresponding equations labeled next to them.

above-mentioned procedure to extract  $E_a = 338$  meV and calculate  $\log_{10}(v_0) = 13.1\text{ s}^{-1}$  from Eq. (1). A symmetrical variation of the ATM method<sup>11</sup> based on the temperature-rate duality<sup>12</sup> uses Eq. (7) to perform the  $v-T$  transformation and generate a virtual scan  $f\text{d}C/\text{d}f(T_v)$  from an experimental isothermal scan  $f\text{d}C/\text{d}f(v)$ , which is matched to the experimental isothermal scan  $f\text{d}C/\text{d}f(T)$  to obtain the best fit value of  $v_0$  and calculate  $E_a$ .

In practical situations, only one kind of scan, either iso-rate or isothermal, may be preferred as the other may be unavailable or sparsely distributed in the  $T-v$  space. In this case, one can use one of Eqs. (2)–(5) to transform all scans of that particular kind (iso-rate or isothermal) to either the  $E_a$  or the  $v_0$  virtual space. Figure 2(c) is an example of how all the iso-rate  $f\text{d}C/\text{d}f(T)$  scans taken at several temperatures are transformed to the  $E_a$  space using only Eq. (2). All resultant virtual scans  $f\text{d}C/\text{d}f(E_{a,T})$  collapse together, indicative of an optimal fitting condition for extracting  $\log_{10}(v_0) = 13.1\text{ s}^{-1}$  used in Eq. (2). Since  $T_{fix}$  is not defined in this case,  $E_a$  cannot be calculated from Eq. (1). Instead,  $E_a = 328$  meV is read directly from the shared peak of all  $f\text{d}C/\text{d}f(E_{a,T})$  spectra.

Figure 3 is a summary of all the variations of the ATM method. The three types of transformation and matching between  $T$ ,  $v$ ,  $E_a$ , and  $v_0$  are represented by arrows with the corresponding equations labeled next to them. (i) As in the example in Fig. 2(a), transformation involving two single-ended solid arrows [Eqs. (2)–(5)] are required to match one isothermal to one iso-rate scan in the  $E_a/v_0$  virtual space. (ii) Only one transformation involving one of the two single-ended solid arrows between  $T$  and  $v$  [Eqs. (6) and (7)] is

needed to match the virtual scan to another experimental scan, as shown in Fig. 2(b). (iii) The dashed arrows pointing from  $T/v$  to  $E_a/v_0$  indicate that one of these four transformations [Eqs. (2)–(5)] can be used to transform and collapse multiple spectra of the same kind, as shown in Fig. 2(c). After the best fit value of either  $E_a$  or  $v_0$  is determined from one of the three scenarios mentioned above, the other parameter is calculated from Eq. (1) at  $(T_{fix}, v_{fix})$  as indicated by the double-ended arrow or simply read from the common peak shared by the virtual scans.

In conclusion, the ATM method from the differential capacitance spectroscopy is demonstrated to extract  $E_a$  and  $v_0$  without using the Arrhenius plot and without identifying the peaks in the  $f\text{d}C/\text{d}f$  spectra. This method extends Arrhenius equations to transform the experimental isothermal and iso-rate scans to the activation energy, attempt-to-escape frequency, temperature, or rate virtual space and extracts  $E_a$  and  $v_0$  at any temperature point by matching the curvatures of the virtual scans and the experimental scans.

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## DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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