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Violation of the rate-window concept in the charge deep-level transient spectroscopy using second-order filtering

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Abstract

When applying the thermal-scan charge deep-level transient spectroscopy (Q-DLTS) utilizing second-order filtering to diamond- or GaAs-based Schottky-like diodes, we found correlated Q-DLTS signals which increased monotonically with temperature and did not depend on the rate window set at $t_1{}^{-1}$. In accordance with the hyperbolic kinetics of the transient current in diamond films, the related transient charge $Q(t)$ (integrated current), when correlated, is *invariant* for the rate window. Thermal activation energy of the transient current is easily deduced from the Q-DLTS experiment. Possible consequences for feedback-charge capacitance–voltage measurements, which may also be classified as second-order filtering in the time domain, are pointed out. One of them might be a sign reversal of the excess capacitance at short times of observation.

1. Introduction

It is a convenient way of using the capacitance deep-level transient spectroscopy (capacitance DLTS) developed by Lang [1, 2] when detecting deep energy levels (traps) in the band gap of semiconductors arranged to form either a Schottky- or a p–n junction. Yet if trying to extend the palette of materials explored in this way towards large-gap semi-insulating materials, severe issues connected mainly with the series resistance of the 'neutral' bulk of the semiconductor may arise. Focusing our attention on diamond, this is the reason why current [3] or charge DLTS (Q-DLTS) [4] versions were preferred.

Usually, a series of thermal-scan DLTS runs is performed at different rate windows set by the timing circuitry for obtaining corresponding peak positions on the temperature scale and finally constructing an Arrhenius plot yielding a thermally activated emission rate. When exploring defect properties of a variety of hetero-epitaxial diamond films on Si while using second-order filtering [5], we have been systematically confronted with monotonously increasing Q-DLTS signals without approaching a peak maximum at the highest temperature of the temperature interval used. Sampling the response in the sub-millisecond region, the signal resembling a low-temperature tail of a peak shifted with the rate window in the expected manner. Still, when going to delays amounting to tens of milliseconds, the spectra obtained from thermal DLTS scans at different rate windows started to merge one with another, becoming invariant to the rate window set. Being motivated by the work of Jauhiainen *et al* [6] comprising a thorough study of steady-state and transient currents, we arrived at a simple explanation for the failure of the rate-window concept after having adopted the nearly hyperbolic $j(t) \propto \text{const}/t$ kinetics. In addition, one should reconsider the eventual consequences of the result for the feedback capacitance method (FCM) [7, 8], keeping in mind the close connection between Q-DLTS and FCM.

2. Second-order filtering in Q-DLTS

The response of the junction under test to a double-bias step ΔU (of duration *pulse*) superimposed on the quiescent bias U_g is usually analysed in terms of an exponential decay of the quantity measured (capacitance or charge). Actually, there is rather a train of pulses arriving at a repetition period defined as *period*, to mediate exponential averaging. The decay is routinely characterized by the emission time constant

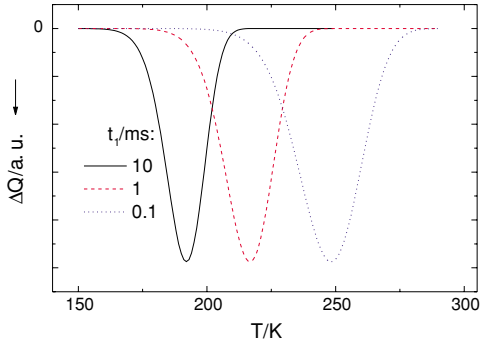

Figure 1. A set of simulated Q-DLTS spectra belonging to three different rate windows defined as t_1^{-1}. The correlated signal ΔQ is always a maximum when the time constant $\tau(T_{\max})$ is equal to t_1.

$\tau_e = \tau_0 \exp(\Delta E/kT)$, with τ_0 being the factor comprising the product of the capture cross section of the traps, thermal velocity of free carriers in the transport band and the density of the states in the latter. The quantity k is the Boltzmann's constant, T is the temperature and ΔE is the thermal activation energy of the charge transition. Restricting ourselves on discrete τ_0 and ΔE, the transient charge of the type $Q(t) =$ Q1 $Q_0[1 - \exp(-t/\tau)]$ processed by the three-channel correlator (second-order filter)

$$\Delta Q = Q(t_1) - \tfrac{3}{2}Q(2t_1) + \tfrac{1}{2}Q(4t_1) \qquad (1)$$

reveals a maximum at $\tau(T_{\max}) \cong t_1$, the delay t_1 being measured from the trailing edge of the pulse. For the height $\Delta Q_{\max} = \Delta Q(T_{\max})$ of the peak there is a simple relation $\Delta Q_{\max} \cong 0.17\ Q_0$, Q_0 being the total released charge. Making the delay t_1 appearing in the timing of all channels longer, the peak would appear at a lower temperature and vice versa. Find a thorough definition of a second-order DLTS filter in the fundamental work by Crowell and Alipanahi [9]. Note that the filter defined by equation (1) is capable of rejecting any constant or linear (with time) charge contribution contained in the input signal $Q(t)$. An example of simulated ΔQ versus T spectra corresponding to three different rate windows 0.1, 1 and 10 ms, respectively, is shown in figure 1. There is a remarkable shift of the whole peak along the temperature axis whenever t_1 has changed. The FWHM of the peak is a linear function of the temperature at the maximum temperature $T_{\max}$.

Now let us consider a power-law kinetics of the current decay in response to a bias step ΔU, i.e. we write

$$j(T,t) = K_0 t^{-\alpha} \exp\left(-\frac{E_0}{kT}\right) \qquad (2)$$

without specifying the physical meaning of the constant E_0 and admitting $\alpha \to 1$ [6]. Passing to Q-DLTS, the current is first integrated (current → charge → voltage conversion is performed electronically):

$$Q(t) = \int_{t_0}^{t} j(t)\,\mathrm{d}t = K_0\,[\ln(t) - \ln(t_0)] \exp\left(-\frac{E_0}{kT}\right). \qquad (3)$$

Here we have avoided integrating the current from $t_0 = 0$, postulating that the initial kinetics is not hyperbolic. Then introducing $K(T)$ equal to $K_0 \exp(-E_0/kT)$ and putting equation (3) into equation (1), we arrive at a strikingly simple result:

$$\Delta Q = -K(T)\frac{\ln 2}{2}. \qquad (4)$$

Evidently the signal proportional to ΔQ is *invariant* to the parameter t_1 that normally defines the rate window. In other words, having an almost hyperbolic transient current, the signal corresponds to a 'transient conductivity' thermally activated by E_0. The resulting ΔQ–T plot represents a signal rising super-linearly (exponentially) with temperature. The negative sign is consistent with that of the DLTS peak corresponding to $Q(t) = Q_0[1 - \exp(-t/\tau)]$ or to the current $j(t) = \mathrm{d}Q/\mathrm{d}t = Q_0\tau^{-1}\exp(-t/\tau)(Q_0 > 0)$. One can easily check that this negative sign holds for charge power-law time dependencies with $\alpha < 1$, a reversal of the sign takes place if we deal with a super-linear kinetics ($\alpha > 1$). It may be evident that the sign of the measured charge DLTS response can be altered by either changing the polarity of the pulse ΔU and/or by the hardware implementation of the filter.

3. Results and discussion

Since the leading idea of the present work was derived from the work by Jauhiainen *et al* [6] concentrating on the electrical characterization of the hetero-epitaxial diamond layers on Si, the result provided by equation (4) was tested primarily on Al/diamond/p-Si diodes. Boron doped p-type Si wafers (0.8–1.2 Ω cm) were used as substrates, the Al dots on top of the structures had an area of 1.96×10^{-3} cm^2. Two groups of diamond-based devices, both relying upon diamond layers prepared by the hot-filament technique, were examined by the Q-DLTS:

i. Al/diamond/p-Si heterostructures annealed in vacuum at 800 °C for 30 min, labelled as D_a diodes,
ii. Al/diamond/p-Si heterostructures exposed to a hydrogen discharge at 150 °C for 30 min, D_h.

In addition, Ag/n-GaAs Schottky diodes fabricated by vacuum deposition of Ag on heavily doped ($N_d \approx 3 \times 10^{17}$ cm^{-3}) n-type GaAs initially exposed to the same hydrogen plasma treatment, were tested in the temperature region of 90–450 K.

Representative Q-DLTS plots, belonging to different rate windows t_1^{-1}, of the group D_a diodes are reproduced in figure 2. Selecting the rate window within the region of milliseconds, the individual ΔQ–T spectra tend to merge with one another (the high-temperature tail of the signal), in contrast to the behaviour of the regular DLTS peak positioned around $T_{\max} \approx 200$ K, shifting in the manner expected for exponential kinetics. The total $U_g + \Delta U$ bias of −5 V during the pulse is expected to establish an accumulation of holes at the Al/diamond interface. The group D_h of diamond-based diodes shows a broad Q-DLTS peak at relatively low temperatures (figure 3), with a superimposed feature reminding of a derivative $\mathrm{d}(\Delta Q)/\mathrm{d}T$ of the peak at ≈200 K from figure 2 detected in D_a-type devices, nevertheless the merging monotonic tails are again present above ≈400 K.

The third example of the rate-window-independent signal in figure 4 stems from one of the Ag/n-GaAs Schottky diodes.

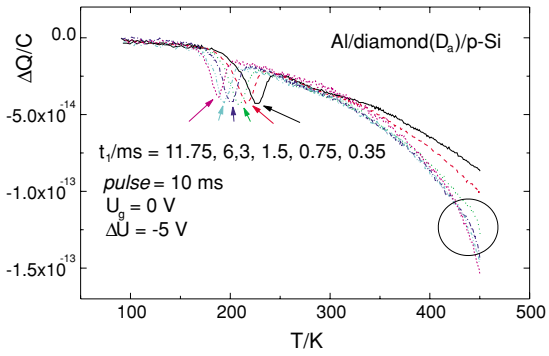

Figure 2. Q-DLTS temperature scans of an Al/diamond(D_a)/p-Si diode. Note the signal tails merging into another at longer times of observation above the temperature range where a regular peak coming from an exponential response is detected.

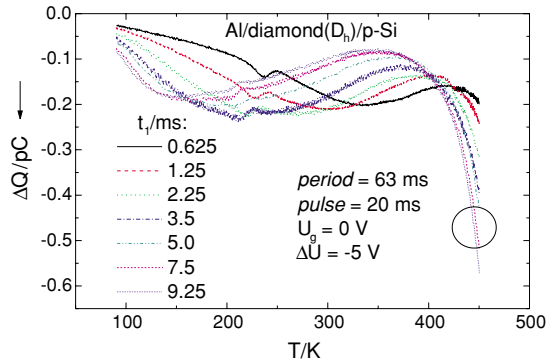

Figure 3. Q-DLTS response of the group D_h diodes shows a broad spectrum of relaxation times at low temperatures and monotonously rising tails at ultimate temperatures of the scans. Merging of the tails is localized by the circle.

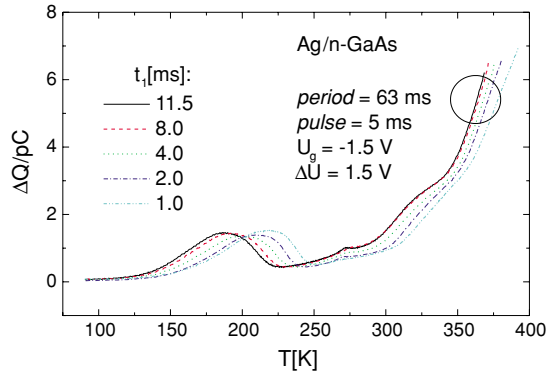

Figure 4. The tendency of the distinct Q-DLTS signals from an Ag/n-GaAs Schottky diode to merge at elevated temperatures is evident for $t_1 > 4$ ms. The peak that dominates the response at low temperatures is assigned to a bulk trap (0.3 eV) in GaAs.

This is not the first observation of the tail in GaAs-based structures, plasma oxides on GaAs showed similar behaviour [11]. Apart from the weak fine structure of the Q-DLTS response, the tail dominates the spectrum above ≈250 K with almost identical Q-DLTS spectra for $t_1 = 8$ ms and 11.5 ms. The standard Q-DLTS peak of a bulk GaAs trapping level, which occasionally also emerges around 200 K, shows the expected standard shift along the temperature scale for all the rate windows employed. The satellite peak at about 315 K, superimposed on the signal tail, might be of a similar origin while the minute feature positioned between the two GaAs-related peaks is due to the melting of residual ice crystals. The ultimate pressure achieved in the cryostat while using a mechanical pump was not low enough to prevent freezing out of residual water vapour.

Relevant FCM [7] capacitance versus voltage experimental data from a broad interval of temperatures is not yet available, so we restrict our considerations on the expected distortion of such measurements in the case of quasi-hyperbolic current transients. Referring to previous work [8], the correlator samples in the FCM mode first the baseline via activating channel one after a delay t_1 with respect to the *leading* edge of the pulse, just before the pulse-trailing edge. The remaining two channels sample the transient charges at t_2 and $3t_2$, respectively, after the *trailing* edge of the pulse. Such an algorithm may also be viewed as second-order filtering [8]. Then the FCM (differential) *excess* capacitance due to charge relaxation is defined as

$$\Delta C = \frac{\Delta Q_C}{\Delta U} = \frac{Q(t_1) - \frac{3}{2}Q(t_2) + \frac{1}{2}Q(3t_2)}{\Delta U}. \qquad (5)$$

Normally (if leakage current is absent), we can set $Q(t_1)$ to zero and combining equations (3) and (5) we obtain

$$\Delta C = \frac{K(T)}{\Delta U}\left[\ln\left(\frac{t_0}{t_2}\right) + \frac{\ln 3}{3}\right]. \qquad (6)$$

Since $t_0 \ll t_2$ and $K(T)/\Delta U > 0$, the excess capacitance splits into two components exhibiting conflicting features:

- the observation-time-dependent contribution (of negative sign),
- the constant contribution of reversed (positive) sign.

In analogy with the polarity of the Q-DLTS signal ΔQ the correct sign for the correlated charge ΔQ_C is negative, i.e. one should multiply the capacity dispersion obtained from equation (5) by -1, to comply with the standard definition of real differential capacitance. Then, if adopting equation (6) and passing to shorter times of observation ($t_2 \to t_0$), the overall real excess capacitance may go down to zero or even to negative values. The related magnitude $K(T)\ln 3/3$ of the charge of the constant component is comparable to the amplitude of the Q-DLTS signal—equation (4) and, therefore, cannot be neglected. To our knowledge there are no relevant data for the time-domain capacitance available.

4. Conclusions

The basic features of the anomalous Q-DLTS response due to hyperbolic transient-current kinetics were exemplified experimentally. The results of the analysis apply to higher-order filtering, the correlated transient charge being invariant to the rate window set. Moreover, a prediction of the compensation or even the reversal of the excess time-domain capacitance at the short times of observation has been documented for the anomalous kinetics. An experimental verification of the prediction raises the problem of distinguishing between the two *constant* contributions to the overall capacitance. The first contribution is due to the constant (independent of t_2) term in equation (6) as a result of correlating the anomalous transient charge, competing with charging the instantaneous (geometrical) capacitance $C(0)$ of

the junction by the pulse ΔU. In other words, it is impossible to reconstruct the two quantities involved while only their difference is available.

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Queries

(1) Author: Please verify equation (1).
(2) Author: Please verify equation (5).