IOP PUBLISHING SEMICONDUCTOR SCIENCE AND TECHNOLOGY

Semicond. Sci. Technol. **23** (2008) 125031 (4pp) doi:10.1088/0268-1242/23/12/125031

Centers with low correlation energy in deep-level transient spectroscopy studies

Nikolai Yarykin

Institute of Microelectronics Technology, RAS, Chernogolovka 142432, Russia

E-mail: nay@iptm.ru

Received 25 August 2008, in final form 2 October 2008
Published 7 November 2008
Online at stacks.iop.org/SST/23/125031

Abstract

The application of deep-level transient spectroscopy (DLTS) for the investigation of multi-level defects is considered in detail. In the case of a low absolute value of the effective correlation energy U, the amplitude of a DLTS signal is predicted to be a complex function of U, which can result in erroneous determination of the defect concentration. The magnitude of the effect is shown to be mainly controlled by the shape of a weighting function used to produce the DLTS peak. The DLTS technique is applied for the study of the zero-U center in electron-irradiated silicon. In agreement with the theoretical consideration, the amplitude of the DLTS peak determined by the concurrent emission of two charge carries is observed to be *more* than two times higher as compared to a single-level defect of the same concentration.

1. Introduction

Deep-level transient spectroscopy [1] (DLTS) is nowadays a common technique for quantitative characterization and identification of electrically active defects in semiconductors. In all its modifications, the technique detects the rate and intensity of thermal emission of non-equilibrium charge carriers from deep levels. In general, each deep level produces a DLTS peak whose amplitude is proportional to the defect concentration. This also holds true for centers which introduce two levels in the gap, if the effective correlation energy U of the centers is well positive (more than several kT for relevant temperatures). By definition, $U = E_2 - E_1$, where E_1 and E_2 are the energies required for the first and second ionizations of the center, respectively. Anderson assumed [2] that U can be negative in solids, if the energy gain due to a large lattice relaxation around a charged center exceeds the loss due to the Coulomb repulsion of two charge carries. The order of levels in the gap is inverted in the case of negative U, and the thermal emission of one charge carrier is followed by fast emission of a second carrier, resulting only in one DLTS peak of double amplitude [3, 4].

In agreement with the above reasonings, experiments show that two clearly resolved DLTS peaks of equal amplitude originate due to electron emissions from the first and second acceptor levels of the divacancy in silicon (an example of a positive-U center) [5, 6], while only one DLTS peak of double amplitude appears owing to simultaneous emissions of two charge carriers from the isolated vacancy or the interstitial boron atom in silicon (the known negative-U systems) [3]. Such an ideal behavior is obviously determined by the fact that absolute values of the effective correlation energy $|U|$ are high enough in all these examples, or in other words, the emission rates for two charge carriers differ strongly. However, competing energies of the Coulomb repulsion and the lattice relaxation are, generally speaking, not related to each other. Therefore, centers with low $|U|$ are also possible to exist.

Indeed, the defect with two coincident deep levels has been recently reported in electron-irradiated oxygen-rich silicon [7]. The new experimental data presented below show that amplitude of the DLTS-peak determined by emission of two charge carriers from this defect is unexpectedly high. The experimental results are explained using a simple theoretical consideration of the behavior of the centers with a low absolute value of correlation energy under DLTS studies.

2. Theoretical consideration

Consider a double donor in p-type silicon, both levels being located in the lower half of the gap. The equilibrium charge state of such a defect is neutral inside the space charge region (SCR) formed, for example, by a reverse-biased Schottky diode. Due to a long enough DLTS filling pulse which removes the SCR, the center traps two holes and becomes double positive. Emission of the holes after termination of

the filling pulse at $t = 0$ is described by the system of rate equations:

$$\frac{\mathrm{d}f_2}{\mathrm{d}t} = -r_1 f_2, \tag{1}$$

$$\frac{\mathrm{d}f_1}{\mathrm{d}t} = r_1 f_2 - r_2 f_1, \tag{2}$$

$$f_2(t=0) = 1, \qquad f_1(t=0) = 0, \tag{3}$$

where f_1, f_2 are the fractions of defects in the single and double positive charge states, respectively. The hole emission rates $r_i = \gamma_i T^2 \exp(-E_i/kT)$ $(i = 1, 2)$, where energies E_1 and E_2 correspond to the (++/+) and (+/0) transitions, respectively. (The more elaborate system of equations, which describes the carrier exchange for a double-level center including the capture processes, has been solved in [8].)

DLTS analyzes the diode capacitance variations ΔC resulting from the emission of charge carriers from deep levels. For double donors, $\Delta C \propto 2f_2 + f_1$, assuming the defect concentration is low as compared to the doping level. Solving system (1)–(3), we obtain an expression for the capacitance transient:

$$\Delta C \propto (1 + K)\exp(-r_1 t) + (1 - K)\exp(-r_2 t), \tag{4}$$

where $K = r_2/(r_2 - r_1)$. (The case of $r_1 = r_2$ does not introduce any new physics.) The limits of $r_2 \ll r_1$ $(K \approx 0)$ and $r_2 \gg r_1$ $(K \approx 1)$ for well-positive and well-negative U, respectively, have been considered earlier [3, 4]. Below we focus on the centers with $r_1 \simeq r_2$.

As seen from (4), ΔC could be deconvoluted into two exponential transients at any temperature and, generally speaking, all parameters of the defect could be obtained in that way. However, the methods based on direct deconvolution, such as the Laplace DLTS [9], require a very low noise-to-signal ratio to produce reliable results. Therefore, conventional DLTS is used in most studies.

The signal of conventional DLTS, S, is formed by the convolution of a capacitance transient $\Delta C(t)$ with a weighting function F:

$$S = \frac{1}{P}\int_0^P \Delta C(t) F(t)\,\mathrm{d}t, \tag{5}$$

where P is the time interval after termination of the filling pulse when the transient is recorded. Due to the linearity of (5) with respect to ΔC, the DLTS spectrum of a double-level defect could be represented as a combination of two peaks determined by two single-level centers with activation energies E_1 and E_2. However, the amplitudes, shapes and even sign of these peaks are strongly modified by the temperature-dependent pre-exponential factors in (4). Since the shape and temperature position of a DLTS peak are determined (in addition to the level parameters) also by the weighting function, the manifestation of the double-level nature of a defect in DLTS studies has to be investigated separately for different weighting functions. We concentrate below on two widely used weighting functions which are shown in figure 1 and represent filters of the first and second order, respectively [10].

The DLTS curves calculated for several double-donor centers are shown in figure 2. To compose the figure, E_2 was

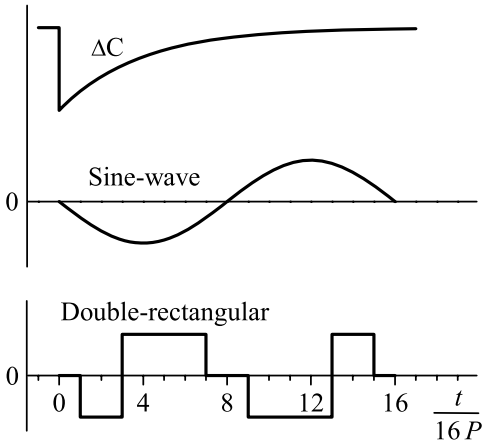

Figure 1. The sine-wave and double-rectangular weighting functions. The capacitance transient is also schematically shown.

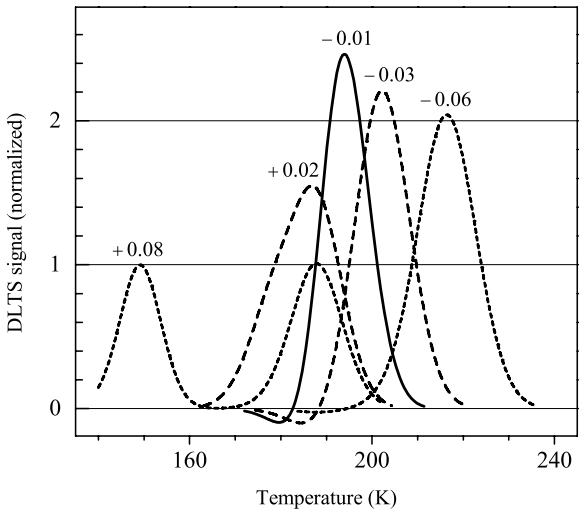

Figure 2. The DLTS signatures simulated for double-donor centers using the double-rectangular weighting function. The unit amplitude corresponds to the maximum signal for a single-level center. E_2 is fixed at 0.36 eV, while U serves as a parameter and is shown in figure in the electronvolt units. $\gamma = 2 \times 10^6$ s^{-1} K^{-2} for both levels.

fixed at 0.36 eV, while the E_1 value varied as a parameter from 0.28 to 0.42 eV. In accordance with the previous consideration, the DLTS spectrum consists of two well-resolved peaks of unit amplitude when U is well-positive (the curve labeled +0.08). In the case of a well-negative U, a single peak of the double amplitude appears in the spectrum (the curve labeled −0.06).

The most exciting feature in figure 2 is the amplitude of a DLTS peak at $U \approx 0$. The maximum signal is about 2.47 when the double-rectangular weighting function is used. Even presuming the negative-U nature of a defect, the defect concentration can be overestimated by more than 20% if the effect is not taken into account.

The amplitude of a capacitance transient never exceeds 2 as seen from (4). Therefore, it is clear that the higher DLTS signal is a result of using the normalization factor which was calculated for the given weighting function assuming a pure exponential transient. Indeed, similar calculations for the sine-wave weighting function show that the maximum

DLTS signal is only about 2.27 in this case. The maximum DLTS signals arise when $r_2/r_1 = 1.57$ ($r_2/e_p = 1.94$) and $r_2/r_1 = 1.88$ ($r_2/e_p = 2.43$) for the double-rectangular and sine-wave weighting functions, respectively, where e_p is the 'rate window' [1] of the corresponding weighting function. The discrepancy in the sets of r_1 and r_2 values, which provide the maximum signals for different weighting functions, shows again that the unexpectedly high DLTS signal for low-$|U|$ defects is totally determined by an interplay between a given weighting function and capacitance transients consisting of two exponents of close rates.

The non-exponential transients inherent to the low-$|U|$ centers open up the possibility of detecting the low-$|U|$ nature of a given and *a priori* unknown defect by means of careful analysis of the shape of the corresponding DLTS peak. Simulations show that the peak shape for the low-$|U|$ center differs from that for two single-level defects with close activation energies. In general, variations in the peak shape are rather small and very accurate measurements are required to make a distinction. In some cases, however, qualitative variations can be found. In particular, a small negative peak preceding the positive one can be noted in figure 2. This feature, which occurs due to the negative second term in (4) at $K > 1$, can be observed only for weighting functions providing a higher resolution.

3. Experimental verification

To experimentally verify the above predicted properties of DLTS signatures, we need a low-$|U|$ center for which such parameters as concentration and emission rates were independently determined. A good candidate is the recently discovered radiation defect in oxygen-rich silicon (M-center) [7, 11, 12], which reveals the charge-driven bistability. In one of its configurations, M_A, the M-center acts as a zero-U double donor. It was found using DLTS filling pulses of different duration that both levels are located at $E_v + 0.36$ eV [7] (where E_v is the top of the valence band). Since r_2 is about 12 times higher than r_1 because of the difference in pre-exponential factors [7], this system is referred to as negative-U-like. In another configuration, M_B, the M-center behaves as a single donor with the level at $E_v + 0.12$ eV. Total switching between the two configurations is easily performed by cooling the studied diode from room temperature down to the measurement temperature either with or without the reverse bias applied. The bistable nature of the M-center allows one to measure the true defect concentration using the single-donor configuration, and to compare it with the amplitude of the DLTS peak determined by the emission of two holes in the zero-U configuration.

The DLTS measurements have been performed on p-type electron-irradiated oxygen-rich silicon samples using the sine-wave weighting function. The experimental details and general appearance of the DLTS spectra were given in [12] and [11], respectively. The apparent depth profiles of the M_A and M_B centers have been calculated from the dependencies of the DLTS peak amplitudes on the filling pulse voltage (figure 3). Before these measurements the defects were

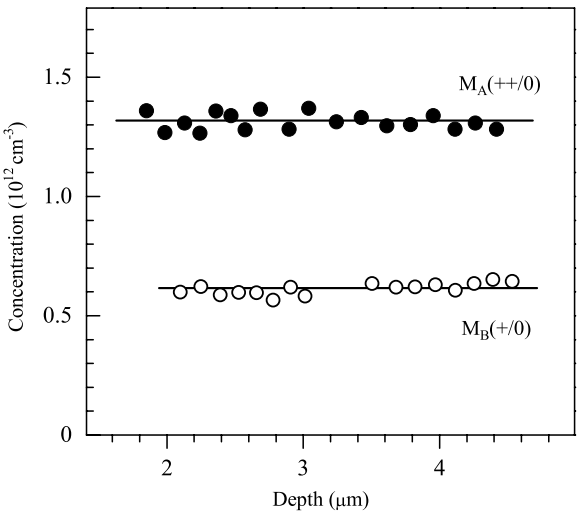

Figure 3. The apparent depth profiles of the M-center in different configurations. The concentrations were calculated using the amplitudes of the DLTS peaks produced by the sine-wave weighting function. Horizontal lines are the best fits to the data.

totally converted into the M_A or M_B configuration using proper cooling conditions [11]. The essentially flat profiles, as it was actually expected for the highly uniform damage produced by fast electrons, demonstrate that the most important factors, such as the existence of static and dynamic λ-layers [13], have properly been taken into account during the calculations.

The true M-center concentration is about 6×10^{11} cm^{-3} as found from the peak amplitude in the M_B (single donor) configuration. This fairly low value (as compared to the doping level of about 10^{15} cm^{-3}) justifies the quantitative analysis of the DLTS data. In the M_A configuration the DLTS peak is determined by emission of two holes, but the apparent concentration is found to be 2.14 times higher. The relative uncertainty of the latter value is estimated to be less than 3%. This rather low error bar is determined (i) by the bistable nature of the M-center, which excludes any possible contributions from other (stable) defects to the DLTS peak amplitudes, and (ii) by the use of the same diode, which strongly reduces uncertainties due to the unknown diode parameters. The normalized apparent concentration of the M_A-centers and the error bar are shown in figure 4 with a horizontal line and a hatched region, respectively.

For a given weighting function the DLTS peak amplitude of zero-U centers depends only on the γ_2/γ_1 ratio. Such dependence is shown by the thick curve in figure 4 for the sine-wave weighting function. It is seen that for the centers with $\gamma_1 \gg \gamma_2$ (positive-U-like centers) the amplitude of the peak is close to unity. (In fact, in this case, the DLTS spectrum consists of two peaks similar to those shown in figure 2 by the curve labeled +0.08. However, we are interested in the amplitude of the high-temperature peak only.) In the opposite case of $\gamma_1 \ll \gamma_2$ (negative-U-like centers) the peak amplitude equals 2. In the range where γ_1 and γ_2 are comparable, the peak amplitude exhibits a maximum.

As seen in figure 4, the experimentally observed peak amplitude can be implemented when the γ_2/γ_1 ratio is about either 0.8 or 7.2. The latter value is rather close to the ratio

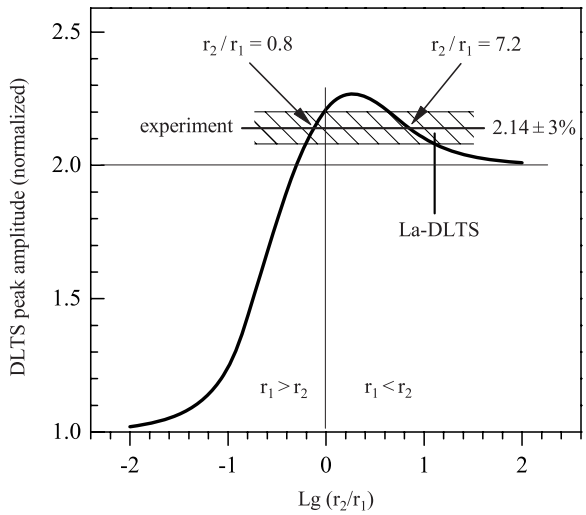

Figure 4. Dependence of the DLTS peak amplitude for the sine-wave weighting function on the r_2/r_1 ratio for zero-U centers (curve). The horizontal line and hatched region around it show the experimentally observed apparent concentration of the M-centers in the zero-U configuration and the estimated uncertainty of this value, respectively. The vertical line marks the r_2/r_1 ratio from the Laplace-DLTS measurements [7].

based on direct measurements of the emission rates reported in [7] (shown in figure 4 with a vertical line).

4. Conclusion

We have analyzed how the kinetics of charge carrier emission from two-level centers affects the DLTS analysis. The total charge captured by such centers is found to reveal a strongly non-exponential transient in the case of close emission rates from the two levels. The convolution of the corresponding capacitance transient with a weighting function in DLTS studies results in a complex relationship between the DLTS peak amplitude and the concentration of traps. In particular, the concentration of low-$|U|$ centers could be overestimated by more than 20% for certain weighting functions if the effect is not properly taken into account.

The apparent concentrations of the zero-U M-center in different metastable configurations have been measured in electron-irradiated silicon samples. The experimentally observed ratio of the apparent concentrations is found to be in good agreement with the theoretically predicted value.

Acknowledgments

The author is grateful to Professor E B Yakimov for valuable discussions.

References

[1] Lang D V 1974 *J. Appl. Phys.* **45** 3023
[2] Anderson P W 1975 *Phys. Rev. Lett.* **34** 953
[3] Watkins G D and Troxell J R 1980 *Phys. Rev. Lett.* **44** 593
[4] Bourgoin J C and Lannoo M 1983 *Point Defects in Semiconductors II: Experimental Aspects (Springer Series in Solid State Science* vol 35*)* (Berlin: Springer)
[5] Evwaraye A O and Sun E 1976 *J. Appl. Phys.* **47** 3776
[6] Svensson B G and Willander M 1987 *J. Appl. Phys.* **62** 2758
[7] Markevich V P *et al* 2005 *Solid State Phenom.* **108-109** 273
[8] Dobaczewski L and Kaczor P 1991 *Semicond. Sci. Technol.* **6** B51
[9] Dobaczewski L, Kaczor P, Hawkins I D and Peaker A R 1994 *J. Appl. Phys.* **76** 194
[10] Istratov A A, Vyvenko O F, Hieslmair H and Weber E R 1998 *Meas. Sci. Technol.* **9** 477
[11] Markevich V P, Murin L I, Lastovskii S B, Medvedeva I F, Komarov B A, Lindström J L and Peaker A R 2005 *J. Phys.: Condens. Matter* **17** S2331
[12] Yarykin N and Weber J 2007 *Physica* B **401–402** 483
[13] Stievenard D and Vuillaume D 1986 *J. Appl. Phys.* **60** 973