Photoionization cross-section analysis for a deep trap contributing to current collapse in GaN field-effect transistors

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We perform a more incisive numerical analysis of the photon energy dependence of the photoionization cross section of a prominent deep trap (conventionally labeled as Trap 1), which had been found [Klein *et al.*, Appl. Phys. Lett. **75**, 4016 (1999)] to act as a contributor to current collapse phenomena in GaN metal-semiconductor field-effect transistors. The analytical expression for the photoionization cross section of Trap 1 is taken in the form of a convolution of a temperature-*independent* electronic part with a *thermally broadened* Franck–Condon (FC) factor, which also applies to the relevant regime of *large* lattice relaxation. For a direct comparison with earlier results, we specialize the present analysis to an electronic cross-section part represented by the Lucovsky model in combination with the *semiclassical* (Gaussian) approximation for the FC factor. In qualitative accordance with an earlier estimation by Klein *et al.* we obtain a value of $E^O \approx 1.9\,\mathrm{eV}$ for the *classical optical* ionization energy in combination with a full width at half maximum of 0.64 eV. The latter implies, on the assumption for the average phonon energy, to be of order 50 meV, an apparently unusually *large* magnitude, $D \approx 1.1\,\mathrm{eV}$, for the Franck–Condon shift. This parameter constellation is equivalent to a thermal ionization (electron binding) energy, $E^T = E^O - D$, of about $E^T \approx 0.8$ eV. Such a location of Trap 1 near the *middle* of the *upper half* of the fundamental gap of GaN, $E^T \approx E_g/4$, is at clear variance to the earlier suggestion by Klein *et al.* for Trap 1 to be a midgap level. The present estimation offers a chance for detecting the Trap 1 also by deep-level transient spectroscopy measurements. An eventual availability of photoionization cross-section data for *different* temperatures is seen to be the prerequisite for a decisive reduction of residual uncertainties concerning the configuration coordinate diagram. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1753076]

I. INTRODUCTION

Significant progress has been made in recent years in technical developments of GaN-based optoelectronic devices operating in the blue and ultraviolet regions of the spectrum as well as of electronic devices that are also suitable for high frequency, high power, and/or high temperature applications. At the same time, one of the main causes of limitations of their efficiency has been repeatedly found to be due the presence of various *deep* traps, the optical and electrical properties of which are usually not known in due detail. One is presently concerned with such lack of knowledge particularly in cases of traps responsible for current collapse phenomena in GaN metal-semiconductor field-effect transistors.[1–4]

For a theoretical understanding of the electrical properties of such deep traps, particularly for an eventual precalculation of the dependences of their nonradiative multiphonon (NMP) electron capture coefficients (or cross sections) on *lattice* temperature[5,6] and/or *hot* electron energy[7,8] (under high-field conditions), it is necessary to know the magnitudes of certain empirical parameters that use to be represented by a corresponding configuration coordinate diagram. This concerns in particular the *thermal* ionization (=electron binding) energy, E^T, the Franck–Condon (FC) shift, D, the corresponding *classical optical* ionization energy, $E^O = E^T + D$, as well as the effective (average) phonon energy, $\hbar\overline{\omega}$. A basic way for getting corresponding quantitative information consists in numerical analyses of measured photoionization cross-section curves, $\sigma(h\nu, T)$, of the deep trap in question. A variety of successful numerical estimations of basic trap parameters is known from earlier literature, above all, for the frequently encountered regime of *small* ($D < E^T$) lattice relaxation.[9–21]

A brief sketch of foundations of the theory of thermally broadened (multiphonon-assisted) photoionization cross sections of deep traps in semiconductors is given in the appendix. The observable (thermally broadened) photoionization cross-sections, $\sigma(h\nu, T)$, are represented by a sufficiently general version of convolution integrals involving temperature-independent electronic parts with thermally broadened FC factors specialized for the frequently considered regime of *linear* electron-phonon interaction.[13–25] In view of the preliminary nature of the present analysis, we confine ourselves here to the semiclassical (Gaussian) approximation[26–31] for FC factors. This is in analogy to the analyses performed in a variety of earlier articles for cases of *small*[9,10,15] ($D < E^T$) as well as *large*[32–37] ($D > E^T$) lattice relaxation.

For the electronic part of the photoionization cross section we choose in Sec. II (in analogy to Ref. 2) the Lucovsky model.[38] The corresponding special version of the convolu-

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tion integral is used for a least-mean-square fit of the photon energy dependence of the photoionization cross-section data set available for room temperature (293 K) from Ref. 1 for Trap 1. On the basis of the resulting parameter set we are able to construct a physically realistic configuration coordinate diagram for Trap 1, which is qualitatively largely different from those suggested in Refs. 1 or 2. Probable sources of uncertainties of present results, and possible ways for reducing such uncertainties by more comprehensive experimental studies both of the optical and electrical properties of Trap 1, are discussed in Sec. III.

II. ANALYTICAL MODEL AND NUMERICAL RESULTS

For the limiting regime of completely vanishing electron-phonon coupling (i.e., vanishing FC shift, $D \rightarrow 0$), the photoionization spectrum is exclusively due to optical transitions of the *electronic* subsystem. Such a purely electronic absorption regime is typical for shallow (hydrogenic) traps and shows up in experiment, among other things, by an independence of the absorption spectrum, $\sigma_e(h\nu)$, on temperature (apart from a certain shift of the σ_e spectrum as a whole due to a possible temperature-induced shift of the actual trap position[13,14,17–21] with respect to the band edge). In cases where excited (Rydberg-like) states are not involved in the electronic excitation process, the corresponding electronic absorption spectrum, $\sigma_e(h\nu)$, is a continuous function of $h\nu$ whose *edge* (electronic absorption threshold) is coinciding with the *thermal* ionization (=electron binding) energy, E^T. During the past four decades, a variety of more or less plausible analytical models for possible spectral dependences of such purely *electronic* photoionization cross sections, $\sigma_e(h\nu)$, have been developed.[38–49] Not one of these $\sigma_e(h\nu)$ models, however, is capable of providing an acceptable numerical simulation of the $h\nu$ dependence of the photoionization cross-section curve, $\sigma(h\nu,T)$, that has been measured for Trap 1 at room temperature ($T=293$ K). This global statement applies in particular to the familiar Lucovsky model,[38] according to which the dependence of $\sigma_e(h\nu)$ on the photon energy absorbed by the excited electron, $h\nu = E_e$, is given by an expression of the relatively simple form

$$\sigma_e(E_e) = \text{const.}\ \frac{(E_e - E^T)^{3/2}}{E_e^3}. \tag{1}$$

It is seen in particular from Fig. 2 of Ref. 1 that the experimental $\sigma(h\nu,293\,\text{K})$ curve is significantly broader than suggested by a purely electronic excitation model like Eq. (1).

The unusually large extension of the low-energy tail of the $\sigma(h\nu,293\,\text{K})$ curve[1,2] of Trap 1 (see also Fig. 1) is indicative of an obviously rather *strong* electron-lattice coupling. In such cases, the change of the center charge state due to trap-to-band transitions is connected with a pronounced lattice relaxation process (due to shifts of oscillator equilibrium positions) in the vicinity of the trap. Consequently, such transitions are occurring in the form of optical electron excitation processes accompanied by emission or absorption of a variable number of phonons.[16,22–25] The *simultaneous* occurrence of *electron* and *lattice* transitions involves thus a partition of the photon energy absorbed by the total (coupled

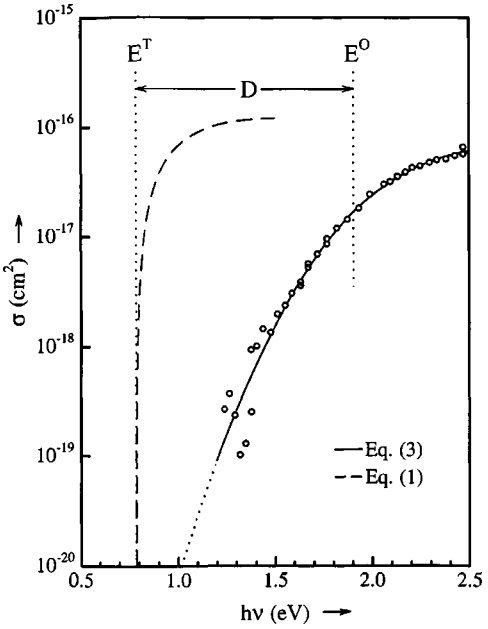

FIG. 1. Fitting of the experimental photoionization cross-section data points, $\sigma(h\nu,293\,\text{K})$ (open circles), that had been presented for Trap 1 by Klein *et al.* (cf. Fig. 2 in Ref. 1 and/or Fig. 3 in Ref. 2). The least-mean-square fit (solid curve) was performed using the specialized (approximate) version (3) of the original convolution integral (2) for thermally activated photoionization cross sections, which followed from the *semiclassical* (Gaussian) approximation (A9) for FC factors in combination with the Lucovsky model, Eq. (1), for the electronic part (dash-dotted curve). The vertical (dotted) lines indicate the estimated positions of the *classical optical* ionization energy, E^O, and of the *thermal* ionization (=electron binding) energy, E^T. The distance between E^T and E^O corresponds to the Franck–Condon shift, D (A7).

electron-phonon) system, $h\nu = E_e + \Delta E_L > 0$, into a certain portion, $E_e > 0$, absorbed by the electronic subsystem, and a complementary portion of heat energy, $\Delta E_L = h\nu - E_e$, that is exchanged with the lattice in form of a multiphonon (MP) emission ($\Delta E_L > 0$) or absorption ($\Delta E_L < 0$) process. We have shown in due detail in the appendix that, under the usual assumption of *linear* coupling[13–25] of the electronic system with *harmonic* lattice oscillators, the observable MP-assisted (thermally broadened) photoionization cross sections, $\sigma(h\nu,T)$, can be represented generally by a convolution integral of the form (A5)

$$\sigma(h\nu,T) = \frac{1}{h\nu}\int dE_e \sigma_e(E_e) E_e R(h\nu - E_e, T), \tag{2}$$

where $R(\Delta E_L, T)$ represents the thermally averaged FC factor (A4). (Note that a somewhat simpler approximate form, $\sigma(h\nu,T) \cong \int dE_e \sigma_e(E_e) R(h\nu - E_e, T)$, for this convolution integral had been used in several preceding papers[18–21] with respect to the familiar regime of *small* lattice relaxation, $D/E^T < 1$. The more general form (2) derived in the appendix for the convolution between the electronic part, $\sigma_e(E_e)$, and the Franck–Condon factor, $R(h\nu - E_e, T)$, applies also to the regime of *large* lattice relaxation,[32–37] $D/E^T > 1$, which is seen from the present analysis to be realized in electron transitions between Trap 1 and conduction band states.)

Concerning the choice between qualitatively different analytical approximations for the FC factor [cf. Eqs. (A9),

(A13), and (A14)], we limit ourselves in the present study to the familiar *semiclassical* approximation.[26–31] This means a representation of $R(\Delta E_L, T)$ by a Gaussian (A9), whose first moment (center of gravity), $D \equiv \langle \Delta E_L \rangle$ (A7), corresponds to the well known FC shift (which has been denoted alternatively in various earlier papers by Δ,[10] Δ_{FC},[13] d_{FC},[15,34,49,50,51] A,[5–7,16–21] or S[24,31]). The associated second moment, $M^{(2)}(T) \equiv \langle (\Delta E_L - D)^2 \rangle$ (A8), reduces in effective-phonon energy approximation[7,31] to an expression of the form (A11). (Note that even for a deep trap in hexagonal GaN, where the transition-specific degree of phonon dispersion may be large when significant electron-phonon coupling contributions are made both by the *low*- and *high*-energy sections[52] of the total phonon energy spectrum, the effective phonon energy approximation (A12) for the second moment (A11) can be expected to work reasonably above liquid nitrogen temperature.)

Adopting, henceforth, the semiclassical approximation (A9) for the FC factor in combination with the effective phonon energy approximation (A11) for the second moment, and the Lucovsky formula (1) for the electronic part, we reduce the general convolution integral (2) to the special (approximate) form

$$\sigma(h\nu, T) \cong \frac{\text{const.}}{h\nu\sqrt{2\pi D\varepsilon \coth(\varepsilon/2k_BT)}} \times \int_0^{(+\infty)} dE_k \frac{E_k^{3/2}}{(E_k + E^O - D)^2} \times \exp\left[-\frac{(h\nu - E^O - E_k)^2}{2D\varepsilon \coth(\varepsilon/2k_BT)} \right]. \quad (3)$$

Here we have denoted by $E_k \equiv E_e - E^T \geqslant 0$ the kinetic energy of the excited electron and by

$$E^O \equiv E^T + D \quad (4)$$

the associated *classical optical* ionization energy.[5,26,29,42,46,49,53] The latter is seen to be shifted from the associated *thermal* ionization energy, E^T [=electronic absorption edge; cf. Eq. (1)], towards higher photon energies by the FC shift, D (A7). From Eq. (3) we see that the resulting $h\nu$ and T dependences of the thermally broadened photoionization cross sections, $\sigma(h\nu, T)$, are given in terms of *three* trap-specific parameters, namely: the classical optical ionization energy, E^O (4), the FC shift, D (A7), and the effective phonon energy, $\varepsilon \equiv \hbar\overline{\omega}$ (A12). However, it is a matter of principle that the magnitude of the latter can be determined only when $\sigma(h\nu, T)$ data are available for at least *two* different temperatures (e.g., for room and liquid nitrogen temperature). This is, unfortunately, not the case for Trap 1 in question.[1–3] Nevertheless, for the sake of an (at least) order-of-magnitude estimation of the FC-shift, D, in combination with the classical optical ionization energy, E^O, via a numerical fit of the available $\sigma(h\nu, 293\,\text{K})$ data set[1] using Eq. (3), we choose here for the effective phonon energy an apparently reasonable magnitude of $\varepsilon \rightarrow 50$ meV. (Note that the phonon energy spectrum of hexagonal GaN is known[52] to consist of a low- and a high-energy section extending from 0 to about 45 meV and from 65 to about 90 meV, respectively. Assuming that *both* sections are making significant contributions to the first and second moments, (A7) and (A8), of the FC factor curve, one can expect the effective phonon energy to be located near the middle of the total phonon energy spectrum. Accidentally, a magnitude of about 50 meV had been estimated to be characteristic also for the temperature-induced shrinkage[54] of the fundamental band gap in h-GaN). Owing to this fixation of the effective phonon energy, $\varepsilon = 50$ meV, we obtain from our least-mean square fit of the $\sigma(h\nu, 293\,\text{K})$ data set[1] (see Fig. 1) for the two remaining parameters occurring in Eq. (3) the values $E^O = 1.91$ eV and $D = 1.12$ eV. Consequently, in accordance with Eq. (4), we obtain for the *thermal* ionization (=electron binding) energy, $E^T = E^O - D$, of Trap 1 a magnitude of $E^T = 0.79$ eV. The latter is thus found to be by a factor of order 1/4 *smaller* than the fundamental band gap of h-GaN at room temperature, $E_g \approx 3.4$ eV. The corresponding configuration coordinate diagram of Trap 1 is shown in Fig. 2.

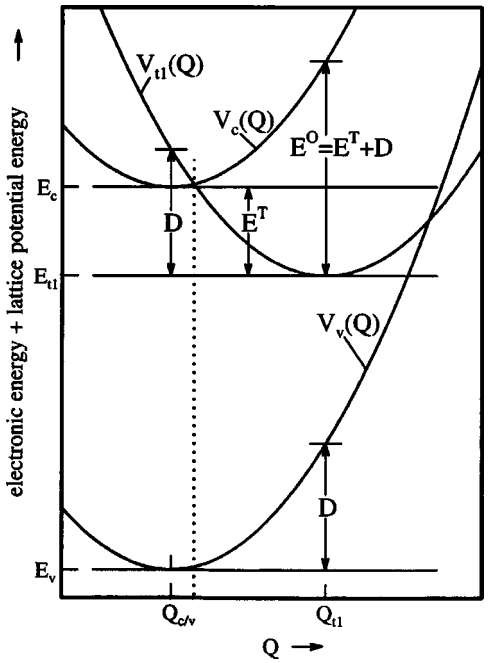

FIG. 2. Configuration coordinate diagram of Trap 1 in GaN. The thermal ionization (electron binding) energy, E^T, followed from the present analysis to be of order $E^T \approx E_g/4$, which is in clear contrast to the original picture of a midgap trap (cf. Fig. 3 in Ref. 1). The classical vibrational barrier energy (see Refs. 5–8, 12) for NMP *capture* of electrons from the vicinity of the conduction band edge into Trap 1 is seen to be very low, $(E^T - D)^2/4D = 0.024$ eV. This involves a high efficiency of Trap 1 in NMP electron capture processes.

III. DISCUSSION

The results of the present analysis of the $\sigma(h\nu, 293\,\text{K})$ data set[1] show, above all, that the Trap 1 is located near the *middle* of the *upper* half of the band gap (cf. Fig. 2). This means in particular that, at variance to earlier suggestions,[1,3] the Trap 1 can by no means be looked upon as a midgap level. Moreover, the associated FC shift versus thermal ionization energy ratio is larger than unity, $D/E^T \approx 1.4$. This confirms the above suggestion for electron transitions (i.e.,

excitation as well as capture processes[5–8]) from/into Trap 1 to pertain to the regime of *large* lattice relaxation.[7,8] This feature is reflected in Fig. 2, among other things, by the peculiarity that the point of crossing between the potential parabolas for the electron in Trap 1, $V_{t1}(Q)$, and the conduction band edge, $V_c(Q)$, is located *between* the vertex positions, Q_{t1} and Q_c, of both parabolas (as indicated by the dotted line in Fig. 2). At variance to this, the points of crossing between the corresponding potential curves in Fig. 3 of Ref. 1 or Fig. 4 of Ref. 2 are located *outside* the interval limited by the vertex positions Q_{t1} and Q_c.

In order to clearly identify the origin of the pronounced qualitative difference between the present version (Fig. 2) of the configuration coordinate diagram and earlier versions, it is instructive to compare directly the parameter values quoted in Refs. 1 and 2 with their counterparts obtained in the present study. First of all we observe that there is only a relatively small difference (of about 6%) between the present estimation of $E^O \cong 1.9\,\mathrm{eV}$ and the earlier estimation[1,2] of $E^O \cong 1.8\,\mathrm{eV}$ for the *classical optical* ionization energy. Curiously, a similar observation can be made also with respect to the associated full width at half maximum (FWHM) values, $W(T)$ (A10). Actually, inserting $D = 1.12\,\mathrm{eV}$ in combination with $\varepsilon = 50$ meV into Eq. (A11), we obtain for the second moment at room temperature a value of $M^{(2)}(293\,\mathrm{K}) = 0.074\,(\mathrm{eV})^2$. The latter corresponds to a FWHM value (A10) of $W(293\,\mathrm{K}) \cong 0.64\,\mathrm{eV}$, which differs from the earlier estimation[2] of $W \cong 0.6\,\mathrm{eV}$ by only about 7%. Thus it is not surprising that the fitted $\sigma(h\nu, 293\,\mathrm{K})$ curve (solid curve in Fig. 1) is almost indistinguishable from its predecessor (shown in Fig. 2 of Ref. 1 and Fig. 3 of Ref. 2).

The origin of the qualitative difference between the present configuration coordinate diagram (Fig. 2) and its predecessors (in Refs. 1 and 2) can thus readily be identified as a result of a further step of our numerical analysis, an analogy of which was completely absent in Refs. 1 and 2. Actually, on the background of the present analytical framework (displayed in the appendix), the basic qualitative difference between the present analysis procedure and the preceding one[2] can readily be seen to be due to

(i) the general (unambiguous) connection (A10) between the FWHM value of $W(293\,\mathrm{K}) = 0.64\,\mathrm{eV}$ and the corresponding second moment of $M^{(2)}(293\,\mathrm{K}) = 0.074\,(\mathrm{eV})^2$, in combination with

(ii) the approximate representation (A11) of $M^{(2)}(T)$ in terms of *two* basic trap parameters, namely: the FC shift, D (A7), and the effective phonon energy, ε (A12).

A simultaneous determination both of D and ε from Eq. (A11) would be possible, of course, only when the second moment $M^{(2)}(T)$ is known for (at least) *two* different temperatures ($T_1 \neq T_2$). This would require corresponding photoionization cross sections, $\sigma(h\nu, T)$, to be measured at different temperatures. In the present case, however, $M^{(2)}(T)$ is known only for room temperature,[1–3] so that there remains naturally an appreciable uncertainty for both parameters. Fortunately, due to the obviously *monotonic* (inverse) relation (A11) between D and ε, at fixed $M^{(2)}(T)$, one can determine in an unambiguous way at least a *lower* as well as an *upper* bound for the magnitude of FC shift, D. This is useful for general qualitative conclusions.

(A) The cutoff energy, $\varepsilon_{\max.}$, of the phonon energy spectrum of h-GaN is known[52] to be about $\varepsilon_{\max.} \cong 90\,\mathrm{meV}$. Inserting the latter value into Eq. (A11) we obtain, at fixed $M^{(2)} = 0.074\,(\mathrm{eV})^2$ and $T = 293\,\mathrm{K}$, a *lower* bound of $D_{\min.} \cong 0.78\,\mathrm{eV}$.

(B) In the $\varepsilon \to 0$ limit, Eq. (A11) takes the limiting form $M^{(2)}(T) \to 2Dk_BT$ (in accordance with the high-temperature limiting transition leading to the *classical* expression (A13) for the FC factor). Thus we obtain, at fixed $M^{(2)} = 0.074\,(\mathrm{eV})^2$ and $T = 293\,\mathrm{K}$, an *upper* bound of $D_{\max.} \cong 1.46\,\mathrm{eV}$.

From these two estimations it follows that, for any magnitude of the effective phonon energy (ranging somewhere within the total phonon energy interval of $0 < \varepsilon < 90$ meV), the FC shift is strictly limited to an interval of

$$0.78\ \mathrm{eV} < D < 1.46\ \mathrm{eV}. \tag{5}$$

This implies, at fixed magnitude of the *classical optical* ionization energy, $E^O = 1.91\,\mathrm{eV}$ (cf. above), that the *thermal* ionization (=electron binding) energy, $E^T = E^O - D$, is strictly limited to an interval of

$$1.13\ \mathrm{eV} > E^T > 0.45\ \mathrm{eV}. \tag{6}$$

This rigorous limitation of E^T can be looked upon as a definitive proof that the Trap 1, instead of being a midgap level,[1,2] is located fairly *within* the *upper third* of the fundamental band gap of h-GaN. At the same time we can state that, accidentally, the particular value of $E^T = 0.79\,\mathrm{eV}$, which we have obtained above due to the particular choice of $\varepsilon = 50$ meV for the effective phonon energy, happens to be coincident with the *middle* of the interval (6). This coincidence can be considered as a further hint that our preliminary choice for the hitherto unknown effective phonon energy was not unreasonable.

In view of the relatively small differences (<7%) between the E^O and $W(293\,\mathrm{K})$ values quoted in Ref. 2 in comparison with their counterparts obtained in the present study one can assess that, by starting alternatively from the former ones,[2] one would come to rather similar constellations of D and E^T values, provided one uses essentially the same relationships [i.e., equations of type (4), (A10), and (A11)] for connecting the relevant parameters. One can state in particular that an account of the inherent *correlation* (A11) between the magnitudes of the *first* and *second* moments of the FC curve is *absolutely indispensable* for a reasonable estimation of the FC shift, including a physically realistic construction of a configuration coordinate diagram. It was this correlation, by a relationship of type (A11), which had *not* been taken into consideration in Refs. 1 and 2. The resulting lack of numerical information, especially on the unusually large magnitude of the FC shift for Trap 1, was the main reason for obvious misconstructions of configuration coordinate diagrams for Trap 1 in Refs. 1 and 2.

On the other hand, we must be also conscious of the fact that even the present version (Fig. 2) of this configuration

coordinate diagram cannot yet be considered as a definitive one. There remain various numerical uncertainties due to the following reasons.

(1) The present choice of $\varepsilon=50$ meV for the effective phonon energy [in Eqs. (3) and (A11)] is only a preliminary one. A certain modification of this value can be envisaged in conjunction with forthcoming analyses of more comprehensive experimental data sets [provided that $\sigma(h\nu,T)$ data will be available in future for at least two different temperatures]. Any change of ε would automatically also induce correlated changes of other parameters, especially of the FC shift, D, [cf. Eq. (5)] and, consequently, of the thermal ionization energy, $E^T=E^O-D$ [cf. Eq. (6)].

(2) The present choice of the Lucovsky model[38] for the electronic part of the photoionization cross section can neither be considered as the uniquely admissible one nor as the most reasonable one (among a variety of possible competitors[39–49]) for a deep trap. This model[38,47] is known to correspond to optical excitation that are *forbidden* (in dipole approximation). However, the wave function of a *deep* trap is generally expected to be represented by a superposition of wave function components from *several* bands, which involves the presence of some *allowed* component in optical trap-to-band transitions (cf. various alternative models suggested in Refs. 41–49). Moreover, when a center in consideration is *attractive* or *repulsive*, with respect to the excited electron, the incorporation of a corresponding Sommerfeld (or Coulomb) factor[18–21,44–46] into the electronic part, $\sigma_e(E_e)$, is necessary. Any modification of $\sigma_e(E_e)$, however, is generally accompanied by a more or less pronounced shift of the parameter set determining the configuration coordinate diagram.

(3) Finally one must bear in mind that the original (nonapproximate) FC factor curves (A4) show throughout a pronounced *asymmetry* between their low- and high-energy wings, which is not accounted for by the completely symmetric, semiclassical (Gaussian) approximation (A9). This deficiency of (A9) can cause falsifications of basic parameters, particularly for cases[16–21] of *small* lattice relaxation [when $\sigma(h\nu,T)$ data from the vicinity of the electronic absorption edge, $h\nu\approx E^T$, are taken into consideration]. A physically adequate alternative to the semiclassical formula (A9) is known to be given by the duly elaborate FC factor formula[18–21] (A14) [including (A15) and (A16)], which resulted from the effective phonon approximation developed in Ref. 31. One cannot exclude that an eventual substitution of the Gaussian (A9) by the theoretically consistent (asymmetric) FC factor (A14) in Eq. (2) causes more or less pronounced parameter shifts also in cases of large lattice relaxation.

Nevertheless, even in view of the incompleteness of the experimental material[1–3] available hitherto, and of the obviously preliminary character of the present numerical analysis, we can assess that residual numerical uncertainties of the thermal ionization energy are likely limited to an order of ± 0.2 eV. Thus we can assess definitively that the Trap 1 must be located somewhere in an interval between about 0.6 and 1.0 eV below the conduction band edge. With respect to forthcoming experimental studies, this seems to be a favorable energy region, since it is known to be possible to detect deep traps with activation energies up to about 1 eV by the familiar deep-level transient spectroscopy (DLTS) technique (provided that the range of measurements is extended up to temperatures of order 500 K.) Accidentally, a series of deep *electron* traps, with activation energies ranging between 0.6 and 1.1 eV, have been detected by various DLTS studies[55–69] in GaN-based systems. It cannot be excluded that, accidentally, one of the numerous deep traps quoted in Refs. 55–69 might be found by forthcoming studies to be identical with Trap 1.

In any case, a much better insight into both the electrical and optical properties of Trap 1 could be achieved by an eventual combination of DLTS studies with additional measurements of photoionization cross sections, for *different* temperatures.

APPENDIX: CONVOLUTION OF ELECTRONIC PARTS WITH F-C FACTORS

For nonvanishing electron-phonon coupling, transitions from an initial electronic (deep trap) state, $|\varphi_i\rangle$, into a set of final (excited trap and/or band) states, $|\varphi_f\rangle$, are generally accompanied by transition between associated initial and final vibrational states of lattice oscillators, $|\chi_{n,i}\rangle$ and $|\chi_{n',f}\rangle$, that are adjusted to the respective average electron-phonon interaction potentials.[24] The corresponding photoionization cross sections are known to be given, in standard dipole (long-wavelength) approximation[39,44] for the electronic transition matrix element, by an expression of the type[34]

$$\sigma(h\nu,T)=\frac{C}{h\nu}\sum_f\sum_{n'}\sum_n P_{n,i}(T)\left|\langle\chi_{n',f}|\langle\varphi_f|\hat{\mathbf{p}}|\varphi_i\rangle|\chi_{n,i}\rangle\right|^2 \times\delta(E_f+E_{n',f}-E_i-E_{n,i}-h\nu) \tag{A1}$$

involving a summation over the excited (final) states f of the electronic subsystem as well as an average and a summation over the initial and final states n and n', respectively, of the vibrational system.[16,24] Here we have denoted by E_i and E_f the effective energy levels of the electronic system (represented by the vertices of the configuration-coordinate curves associated with the initial and final electronic states, $E_i<E_f$), and

$$E_{n,i}=\sum_\mu \hbar\omega_{\mu,i}\left(n_\mu+\frac{1}{2}\right)$$

and

$$E_{n',f}=\sum_\mu \hbar\omega_{\mu,f}\left(n'_\mu+\frac{1}{2}\right) \tag{A2}$$

are the corresponding vibrational energy levels[70] of the adjusted lattice subsystem (ensemble of individual harmonic oscillators labeled by μ, with circular frequencies $\omega_{\mu,i}$ or $\omega_{\mu,f}$ adopted prior and after the transitions, respectively). Further we have denoted by[16,24]

$$P_{n,i}(T)=\exp\left(-\frac{E_{n,i}}{k_BT}\right)\Big/\sum_{n'}\exp\left(-\frac{E_{n',i}}{k_BT}\right) \tag{A3}$$

the occupation probabilities of the initial vibrational energy levels, $E_{n,i}$.

The temperature dependence of thermally broadened photoionization cross sections (A1) is well known to be controlled by the thermal averages of the absolute squares of overlap factors[16,23–25,70]

$$R(\Delta E_L,T)=\sum_{n'}\sum_{n} P_{n,i}(T)|\langle\chi_{n',f}|\chi_{n,i}\rangle|^2 \times\delta(E_{n',f}-E_{n,i}-\Delta E_L), \tag{A4}$$

where ΔE_L represents the difference between final versus initial heat energy that is due to a multiphonon (MP) emission ($\Delta E_L>0$) or absorption ($\Delta E_L<0$) process. [Note that these MP spectral functions (A4), which are frequently referred to as Franck–Condon factors, are normalized exactly to unity,[24] $\int d(\Delta E_L)R(\Delta E_L,T)=1$, for any T.] Assuming, henceforth, that the absolute squares of the individual overlap factors, $|\langle\chi_{n',f}|\chi_{n,i}\rangle|^2$, in (A4) are the same for all final states, $|\varphi_f\rangle$, of the electronic system (which is the case when both the individual equilibrium positions, $Q_{\mu,f}$, and circular frequencies, $\omega_{\mu,f}$, are the same for all *f*), we can rewrite the thermally broadened photoionization cross sections (A1) in the form of a convolution integral of the form

$$\sigma(h\nu,T)=\frac{1}{h\nu}\int dE_e\sigma_e(E_e)E_eR(h\nu-E_e,T). \tag{A5}$$

The latter involves the FC factor (A4), with heat energy argument $\Delta E_L=h\nu-E_e$, and an electronic cross-section part that is given, consequently, by an expression of the standard form[34,40–43,47–49]

$$\sigma_e(E_e)=\frac{C}{E_e}\sum_f |\langle\varphi_f|\hat{\mathbf{p}}|\varphi_i\rangle|^2\delta(E_f-E_i-E_e). \tag{A6}$$

In Eqs. (A5) and (A6) we have denoted by $E_e\equiv h\nu_e>0$ the energy portion that is absorbed by the *electronic* subsystem. The difference $h\nu-E_e=\Delta E_L$ between $E_e>0$ and the energy $h\nu>0$ of the photon absorbed by the total (electron-phonon) system is canceled out by the *phonon* subsystem. In the limiting case of vanishing electron lattice coupling, the FC factor (A4) reduces to a δ function, $R(\Delta E_L,T)\to\delta(\Delta E_L)$. Consequently, as expected, the observable photoionization cross section (A1) reduces in this limit automatically to the electronic part (A6), $\sigma(h\nu,T)\to\sigma_e(h\nu)$.

Consider now the regime of *linear* interaction[13–25,44] of the electronic subsystem with *harmonic* modes, within the frame of which the circular frequencies remain unchanged during an electronic transition, $\omega_{\mu,f}=\omega_{\mu,i}=\omega_\mu$. In such cases, the first order moment (center of gravity) of the FC factor curve (A4) is independent[31,71] of T

$$\int d(\Delta E_L)\Delta E_L R(\Delta E_L,T)=\sum_\mu S_\mu\hbar\omega_\mu\equiv D. \tag{A7}$$

This quantity D (A7) corresponds to the familiar FC-shift (which had been denoted in various earlier articles alternatively by Δ,[10] Δ_{FC},[13] d_{FC},[15,34,49,50,51] A,[5–7,16–21] or S[24,31]). Here we have denoted in (A7) by S_μ the mode-specific Huang Rhys factors (dimensionless quantities characterizing the strengths of electron-phonon coupling of the individual oscillators, with phonon energies $\hbar\omega_\mu$), and $D_\mu\equiv S_\mu\hbar\omega_\mu$ are the mode-specific contributions to the resulting (total) FC shift D (A7). The associated second moment, with respect to D (A7), is given accordingly by[31]

$$M^{(2)}(T)\equiv\int d(\Delta E_L)(\Delta E_L-D)^2R(\Delta E_L,T) =\sum_\mu S_\mu(\hbar\omega_\mu)^2\coth(\hbar\omega_\mu/2k_BT). \tag{A8}$$

In terms of these two lowest-order moments D (A7) and $m^{(2)}(T)$ (A8), we can represent the ΔE_L dependence of the FC factor curve (A4) in the vicinity of the center of gravity, $\Delta E_L\approx D$, by the familiar semiclassical (Gaussian) form,[15,27–31,72]

$$R(\Delta E_L,T)\cong\frac{1}{\sqrt{2\pi M^{(2)}(T)}}\exp\left(-\frac{(\Delta E_L-D)^2}{2M^{(2)}(T)}\right). \tag{A9}$$

The full width at half maximum of this Gaussian (A9) is given in terms of the second moment (A8) by[15,29]

$$W(T)=2\sqrt{2M^{(2)}(T)\ln 2}. \tag{A10}$$

It is necessary to bear in mind, however, that the Gaussian approximation (A9) for the FC factor ceases to be adequate at distances $|\Delta E_L-D|$ significantly larger than $2\sqrt{M^{(2)}(T)}$ [$\approx W(T)$; cf. (A10)] from the center of gravity. The original FC factor curve (A4) is known to show at larger distances a pronounced *asymmetry* between the corresponding low-and high-energy wings [cf. Fig. 1 in Ref. 31 and see below Eqs. (A14)–(A16)].

Comparing Eq. (A8) with Eq. (A7) one finds that these two relevant lowest order moments can be connected by an approximate relation of type[15,29]

$$M^{(2)}(T)\cong D\varepsilon\coth\frac{\varepsilon}{2k_BT}, \tag{A11}$$

where we have denoted by ε an effective phonon energy defined by[7,24]

$$\varepsilon\equiv\hbar\bar{\omega}\equiv\sqrt{\sum_\mu S_\mu(\hbar\omega_\mu)^3\Big/\sum_\mu S_\mu\hbar\omega_\mu}. \tag{A12}$$

An approximation of type (A11) uses to be adequate when it is used in a region of elevated (intermediate to high) temperatures, $k_BT>\varepsilon/3$. Moreover, one can readily see that in the *high* temperature limit, $k_BT\gg\varepsilon$, the second moment $M^{(2)}(T)$ tends to a linear function of temperature, $M^{(2)}(T)\to 2Dk_BT$. This corresponds to the familiar classical limit[12,31,42,50,51,72,73] for FC factors

$$R(\Delta E_L,T)\to\frac{1}{\sqrt{4\pi Dk_BT}}\exp\left(-\frac{(\Delta E_L-D)^2}{4Dk_BT}\right). \tag{A13}$$

However, properly speaking, this limiting expression (A13) would have a chance to be applicable only to temperatures of order 10^3 K. Thus it is as a rule irrelevant for practical applications. This statement applies in particular to wide band

gap materials like GaN, AlN, diamond, SiC, and ZnO, where the phonon energies for the upper optical bands are rather high, $\hbar\omega_{\mathrm{TO/LO}}>70\,\mathrm{meV}$.

In general, the use of the classical approximation (A13) involves a significant *overestimation* of D. As we have seen, e.g., in Sec. III [under point (B)], the classical limit $M^{(2)}(T)\rightarrow 2Dk_BT$ would give for the FC shift a magnitude of $D_{\mathrm{max.}}\cong 1.46\,\mathrm{eV}$, which is obviously much too high. In analogy to this one can obtain, e.g., from analyses of the $\sigma(h\nu,90\,\mathrm{K})$ data set given in Ref. 73 for the E2 level in GaN via the *semi*classical approximation (A9) [in combination with alternative models[44–47] for the electronic part, $\sigma_e(E_e)$, in Eq. (A5)] magnitudes for D in the range of 0.1 to 0.2 eV, whereas the fit according to the classical approximation (A13) of this data set in Ref. 74 gave a magnitude of $D_{\mathrm{max.}}\cong 0.3\,\mathrm{eV}$. In view of such a significant over estimation, $D\rightarrow D_{\mathrm{max.}}$, in practically all cases of physical interest (for $T<500\,\mathrm{K}$), it would be best to avoid *a priori* any application of the classical approximation (A13) to numerical analyses.

Particularly for the regime of small lattice relaxation,[19–21] $D/E^T<1$, even the semiclassical approximation (A9) does often not give satisfactory results owing to the fact that it does *not* account for the inherent *asymmetry*[31] of the *low*-energy wing, $\Delta E_L<D-2\sqrt{M^{(2)}(T)}$, versus the *high*-energy wing, $\Delta E_L>D+2\sqrt{M^{(2)}(T)}$, of the original FC factor curve (A4). Adequate $R(\Delta E_L,T)$ values for these wing regions can be obtained via a FC-factor expression of the sufficiently elaborate form

$$R(\Delta E_L,T)\cong \frac{1}{\sqrt{2\pi\varepsilon F(\Delta E_L,T)}} \times\exp\left[\frac{F(\Delta E_L,T)-F(T)}{\varepsilon} -\frac{\Delta E}{\varepsilon}\ln\frac{\Delta E_L+F(\Delta E_L,T)}{D+F(T)}\right], \tag{A14}$$

where the functions $F(\Delta E,T)$ and $F(T)$ have been defined as

$$F(\Delta E_L,T)\equiv\sqrt{\left(\frac{D}{\sinh(\varepsilon/2k_BT)}\right)^2+(\Delta E_L)^2} \tag{A15}$$

and

$$F(T)\equiv F(\Delta E_L\rightarrow D,T)=D\coth(\varepsilon/2k_BT). \tag{A16}$$

The latter representation resulted from the effective phonon energy approximation developed in Refs. 24 and 31, and has successfully been used for detailed analytical and numerical descriptions both of nonradiative multiphonon (NMP) carrier capture processes[5–8] as well as thermally broadened (MP-assisted) photoionization processes[16–21] occurring at deep traps in various group-IV and III–V materials. This elaborate $R(\Delta E_L,T)$ representation might also be of considerable use for future theoretical descriptions of analogous processes associated with deep traps in GaN (and other wide band gap materials), especially when more comprehensive experimental information on their optical and electrical properties will be available.

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