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To cite this version:

D. Pons, S. Makram-Ebeid. Phonon assisted tunnel emission of electrons from deep levels in GaAs. Journal de Physique, 1979, 40 (12), pp.1161-1172. 10.1051/jphys:0197900400120116100 . jpa-00209203

HAL Id: jpa-00209203

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Classification
Physics Abstracts
63.20K — 63.20M — 63.70 —
71.50 — 71.55 — 72.20J —
73.40G — 79.70

Phonon assisted tunnel emission of electrons from deep levels in GaAs

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(*Reçu le 8 juin 1979, accepté le 31 août 1979*)

Résumé. — Une théorie a été mise au point pour rendre compte de l'émission d'électrons à partir d'un centre profond dans un champ électrique, en tenant compte de l'effet tunnel ainsi que du couplage électron-phonon. Un modèle numérique utilise cette théorie pour simuler les expériences DLTS capacitives et les variations transitoires de capacité. Les paramètres du modèle pour le piège E3, introduit par irradiation électronique, sont évalués en recherchant les meilleurs ajustements possibles des prévisions théoriques avec les spectres DLTS expérimentaux et avec les variations expérimentales de la capacité. En particulier une estimation est obtenue pour le décalage Franck-Condon. Cette estimation se trouve être consistante avec une autre basée sur l'énergie d'activation mesurée pour la section de capture. Avec les paramètres ainsi obtenus, on montre que le modèle reproduit correctement plusieurs autres résultats expérimentaux pour une grande gamme de températures et d'intensités du champ électrique.

Abstract. — A theory is developed for the electric field emission of electrons from deep levels in GaAs taking into account quantum mechanical tunneling and electron phonon interaction. Using this theory, a numerical model is developed simulating capacitive DLTS and capacitive transient experiments. The parameters of the model for the electron irradiation induced defect E3 are extracted by fitting an experimental DLTS spectrum and an experimental transient capacitance curve. In particular, an estimate is given for the Franck-Condon shift. This estimate is found to be consistent with that obtained by another method based on the measured activation energy of the capture cross-section. With the parameters thus found, the model is shown to reproduce correctly several other experimental results over a wide range of temperatures and electric field intensities.

1. **Introduction.** — Electric field dependent ionization rates of deep levels in semiconductors have been observed by several authors [1-9]. For example, Tash and Sah [1] have experimentally evaluated the field enhancement of the emission rate of a deep acceptor level attributed to gold in silicon. They tentatively explain this enhancement by the Poole-Frenkel effect [10]. Their measurements follow the relationship :

$$e_n = e_{n_0} \exp(\Delta E/kT) \tag{1}$$

between the emission rates e_n in the presence of an electric field and e_{n_0} in the absence of field. In this expression ΔE is the Poole-Frenkel potential barrier lowering, k is the Boltzmann constant and T the absolute temperature. However, they did not succeed in fitting their experimental results with a reasonable value of ΔE.

Lang [4] has also observed a field enhancement of the emission rate of a centre associated with ZnO in GaP. The emission rate was found to depend exponentially on the electric field, but no tentative explanation was given.

Vincent [6] has recently observed field dependent emission rates for a GaAs trap which he ascribed to chromium. To explain the observed emission rates, he develops a theory which bears a close ressemblance to that of the Franz-Keldysh tunneling effect [11, 12].

As it has been shown by Lang [7], field effects can be detected using the DLTS techniques that he had recently introduced [7]. In the depleted region of a reverse biased Schottky barrier or p-n junction, there is a linear distribution of electric field strength. This gives rise to a distribution of field dependent emission rates for a given trapping level. As a consequence,

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Article published online by EDP Sciences and available at http://dx.doi.org/10.1051/jphys:0197900400120116100

one observes in heavily doped samples a deformation in the shape and a shift in the position of DLTS peaks relative to lightly doped samples.

The above observations are common to electron traps in GaAs samples doped above 10^{16} cm^{-3}. For analogous doping levels, field effects seem to be negligible for hole traps [8]. The small effective mass of the electron near the Γ minimum of the conduction band in GaAs may therefore be an important factor and quantum mechanical tunneling may be considered as a likely cause for emission rate enhancement. The aim of this paper is to show that tunneling is effectively the physical mechanism involved and that it can quantitatively explain the observed effects in GaAs.

Recently, Korol' [13] gave an elegant calculation of the probability per unit time for elastic tunneling from a bound state to a free state of the conduction band in the presence of a uniform electric field. The ionization rate $\Gamma(\Delta)$ found by Korol' for an electron trapped in a delta function potential well can be written as

$$\Gamma(\Delta) = \gamma \frac{\Delta}{qK} e^{-K} \tag{2}$$

where Δ is the energy depth of the trap below the conduction band at the trapping site and K is the WKB attenuation of the wave function across the potential barrier separating the trapping site from the free conduction band states. For a uniform field F, the barrier is triangular and K is given by :

$$K = \frac{4}{3} \cdot \frac{(2\, m^*)}{\hbar F} \Delta^{3/2} \tag{3}$$

where q is the electronic charge,
m^* the effective electron mass, and
$\hbar$ Planck's constant divided by $2\,\pi$.

The preexponential factor γ corresponding to Korol's calculations is equal to $q/3\,\hbar$. Calculations similar to those of Landau and Lifshitz [14] for the tunneling ionization rate of the hydrogen atom have been performed by Pons [15] for a delta function potential well. Pons calculations yield an ionization rate in the form of eq. (2) with $\gamma = 8\, q/3\,\hbar$.

Since the coupling with phonons is not accounted for in the above evaluation of the ionization rate $\Gamma(\Delta)$, this quantity is temperature independent. In practice, as we show later, the ionization rates are found to be very sensitive to both temperature and electric field. In part 2 of this paper, we present a theoretical model for the calculation of the emission rate in the presence of an electric field taking into consideration the coupling of the trap with the lattice phonons.

Eq. (2) is used as one of the building blocks for our model. In part 3, we report experimental results obtained for the electron-irradiation induced defect E3 in GaAs [16], and a comparison with theory is made. Lastly, a critical discussion on some salient features of the model is given in part 4.

2. **Theory of phonon assisted tunnel emission.** — Kovarskii and Sinyanskii [17] were the first to formulate a theory for the non radiative capture by multiphonon emission (MPE). Henry and Lang [18] have considerably simplified the theory and put it in a readily usable form. Their work revived the interest in the subject and several authors have discussed different aspects of the MPE theory [19, 21]. The non radiative capture results from lattice vibrations which cause the energy level of the bound state to cross the bottom of the conduction band where free electrons are available. At sufficiently high temperatures, the capture cross section σ can be shown to be thermally activated [15]

$$\sigma = \sigma_\infty \exp(-\, E_\sigma/kT) \tag{4}$$

where
σ_∞ is the value of σ extrapolated to infinite temperature, and
E_σ is an activation energy.

In GaP and GaAs, Henry and Lang [18] have shown that many deep levels give strong evidence for such non radiative transition. We are therefore led to describe the coupling between the centre and the lattice vibrations in terms of MPE theory.

2.1 THE ELECTRON-PHONON INTERACTION. — We now give the assumptions of our model. The deformation of the lattice around the trap is described by a single configuration coordinate Q and coupling is assumed to occur with phonons having a single well defined characteristic angular frequency ω. As shown in (Fig. 1), the electronic energy level E_e of the bound state is assumed to change linearly with Q. When the centre is unoccupied, the value of Q oscillates about an equilibrium position which is taken to be at $Q = 0$. The electronic level E_e of the trap changes with Q according to

$$E_e = E_0 - bQ \tag{5}$$

where E_0 and b are constant.

When the trap is occupied by an electron, the electronic level is assumed to be still given by eq. (5) but Q oscillates about a new equilibrium position $\overline{Q}$ and consequently, E_e oscillates about a new equilibrium value E_1. The new equilibrium values $\overline{Q}$ and E_1 can be found by looking for the minimum of the total energy E_{tot} associated with the occupied electron trap. This total energy is the sum of an electronic and an elastic term, hence

$$E_{tot} = E_0 - bQ + \tfrac{1}{2} M\omega^2 Q^2 \tag{6}$$

where the constant M is a reduced mass.

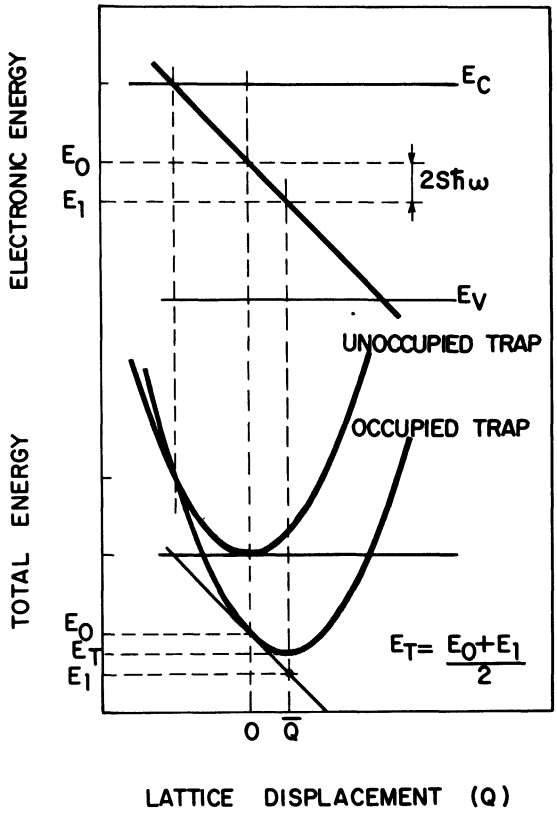

Fig. 1. — Energy diagrams showing the dependence of the electronic and total energy on the configuration coordinate Q. The oscillations of Q occur about the equilibrium values O and $\overline{Q}$ for empty and occupied traps respectively. In each case, the equilibrium value of Q is that corresponding to the minimum of the total energy.

E_{tot} becomes minimum when Q assumes the value

$$\overline{Q} = \frac{b}{M\omega^2} . \tag{7}$$

For a semiclassical model, one may assume that the value of Q oscillates sinusoidally at an angular frequency ω about the equilibrium value. Consequently, for an occupied trap, E_e oscillates about the level E_1 corresponding to $Q = \overline{Q}$ according to

$$E_e = E_1 - bQ_m \cos \omega t , \tag{8}$$

Q_m being the amplitude of oscillation of the coordinate Q. The difference between the levels E_0 and E_1 is easily shown to be equal to twice the Franck-Condon shift $S\hbar\omega$ and can be written as :

$$E_0 - E_1 = M\omega^2 \overline{Q}^2 = 2 S\hbar\omega \tag{9}$$

where S is the Huang-Rhys factor [22]. The amplitude Q_m can be directly related to the total energy in the phonon mode. Assuming that n phonons are involved, we have

$$\tfrac{1}{2} M\omega^2 Q_m^2 = \hbar\omega(n + \tfrac{1}{2}) . \tag{10}$$

Combining eqs. (7), (9) and (10), we obtain

$$bQ_m = 2 \hbar\omega[S(n + \tfrac{1}{2})]^{1/2} \tag{11}$$

for the amplitude of oscillation in the electronic level E_e.

2.2 THE ADIABATIC WAVE-FUNCTION. — In appendix A, we give an adiabatic solution to the electronic time-dependent Schrödinger equation. This solution is shown to be valid in the neighbourhood of the potential well. We now develop this electron wave function in terms of stationary wave functions for the following reasons :

(i) Eq. (2) for the tunnel emission rate applies only to stationary states.

(ii) The emission and capture rates will be related by the principle of detailed balance which only applies to stationary states.

The phase factor $\exp[-i\theta(t)]$ in the electronic wave function in eq. (A.13) of Appendix A can be expanded into a Bessel-Fourier series

$$\Phi(r, t) = \sum_{p=-\infty}^{+\infty} J_p(bQ_m/\hbar\omega) \times \times \exp\left(\frac{i}{\hbar}(E_c - \Delta_p)\, t\right) \cdot \Psi[r, \Delta(t)] \tag{12}$$

where $\Delta_p = E_c - E_1 - p\hbar\omega$, $E_c = E_c(X_t)$ is the bottom level of the conduction band at the trapping site X_t and $E_c - \Delta_p$ is an electronic stationary *quasi-level* as shown in (Fig. 2*a*). It is shown in appendix A that the magnitude $\Psi[r, \Delta(t)]$ of the wave function changes only slightly with Δ in the vicinity of the potential well. Consequently, if the excursion bQ_m of the electronic level is not too large, the modulus $\Psi[r, \Delta(t)]$ of the wave function can be assumed to be time independent. Furthermore, for the values of p yielding non negligible values of the Bessel function $J_p(bQ_m/\hbar\omega)$, we can set

$$\Psi[r, \Delta(t)] \simeq \Psi(r, \Delta_p) . \tag{13}$$

With this approximation, eq. (12) becomes

$$\Phi(r, t) \simeq \sum_{p=-\infty}^{+\infty} J_p(bQ_m/\hbar\omega) \times \times \exp\left(\frac{i}{\hbar}(E_c - \Delta_p)\, t\right) \Psi(r, \Delta_p) \tag{14}$$

showing that, near the potential well, the wave function can be considered as a linear combination of stationary wave functions corresponding to the quasi-levels $E_c - \Delta_p$ ($p = 0, \pm 1, \pm 2, \ldots$).

In order to calculated the probability Π_p of finding the electron at a given quasi-level $E_c - \Delta_p$, we must take into consideration all the allowed values of the

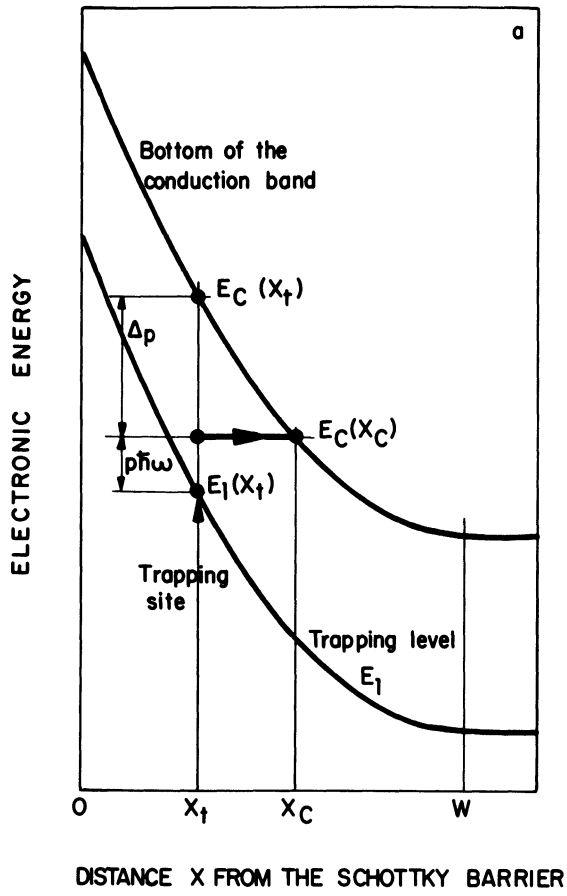

Fig. 2*a*. — Energy diagram showing the profile of the conduction band edge in the depleted region of a $p^+ n$ junction or n-type Schottky barrier diode. This figure shows also the quasi-levels associated with an occupied trapping site.

amplitude bQ_m given in eq. (11), the probability of finding an integer number of phonons n following the canonical distribution. Straightforward calculations yield

$$\Pi_p = (1 - e^{-\hbar\omega/kT}) \sum_{n=0}^{+\infty} e^{-n\hbar\omega/kT} J_p^2(2\sqrt{S(n+\tfrac{1}{2})}) . \tag{15}$$

Π_p is, roughly speaking, a bell-shaped function of p as shown in the sketch of (Fig. 2*b*). The above calculations were performed for an occupied trap. The calculations for an empty trap are identical except that the corresponding quasi-levels are located at $E_c - \Delta'_p$ ($p = 0, \pm 1, \pm 2, \ldots$) and :

$$\Delta'_p = E_c - E_0 - p\hbar\omega . \tag{16}$$

2.3 Calculation of emission and capture rates. — When the trap is occupied, the electron can be field emitted from any of the quasi-levels $E_c - \Delta_p$. This is an elastic tunneling transition from a localized quasi-stationary state to a free conduction band state. The probability for this process is the product of three factors. The first factor is the probability Π_p of finding the trapped electron at the quasi-level $E_c - \Delta_p$. The second factor is the tunneling emission probability $\Gamma(\Delta_p)$ for an electron at this quasi-level. The third factor is the Fermi-Dirac probability $(1 - f_{1,p})$ of finding an empty conduction band state of energy $E_c(X_c) = E_c(X_t) - \Delta_p$ (see Fig. 2*a*). The net field ionization probability e_F is considered as the sum of the ionization probabilities for all the different quasi-levels and can be written as

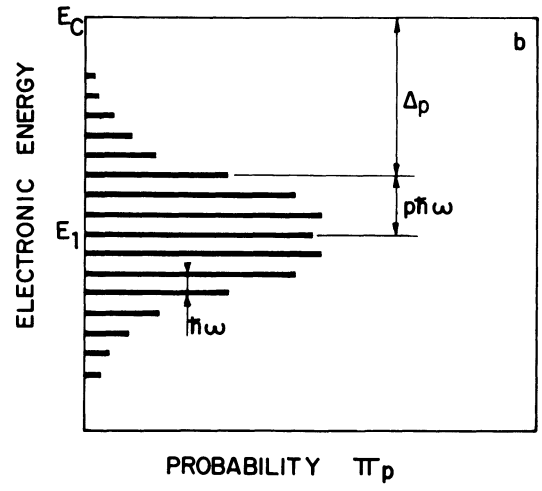

Fig. 2*b*. — Probability of occupation Π_p of each quasi-level of energy $E_c - \Delta_p$.

$$e_F = \sum_p \Pi_p . \Gamma(\Delta_p) . (1 - f_{1,p}) . \tag{17}$$

The above sum is restricted to quasi-levels having an energy $E_c - \Delta_p$ in the forbidden band at the trapping site. Therefore, expression (17) for e_F is restricted to electronic levels for which an elastic transition to the conduction band can occur only through tunneling. To obtain the total emission rate e_n, we must add to e_F the thermal emission rate e_{n_0} which is present even at zero electric field, thus

$$e_n = e_{n_0} + e_F . \tag{18}$$

Similar calculations can be performed for tunnel assisted capture rate c_F, we only have to replace the level E_1 by E_0 and the probability $(1 - f_{1,p})$ appearing in eq. (17) by the Fermi-Dirac probability $f_{0,p}$ of finding the electronic conduction band level

$$(E_c(X_c) = E_c(X_t) - \Delta'_p)$$

occupied, Δ'_p being defined by eq. (16). The counterpart of eq. (17) for c_F is thus

$$c_F = \sum_p \Pi_p . \Gamma(\Delta'_p) . f_{o,p} . \tag{19}$$

As for eq. (17), the summation of eq. (19) is restricted to terms for which the energy $E_c - \Delta'_p$ is located in the forbidden band at the trapping site. The total capture rate c_n can be written as

$$c_n = c_{n_0} + c_F \tag{20}$$

where c_{n0} is the thermal capture rate which is prevalent at low fields.

The thermal emission and capture rates e_{n0} and c_{n0} can be related by the detailed balance equation :

$$e_{n0} = c_{n0} . \exp\left(\frac{E_T - E_F}{kT}\right) \tag{21}$$

where E_F is the Fermi level and E_T is the Gibbs energy of the *level* and is given by [23]

$$E_T = \tfrac{1}{2}(E_1 + E_0) = E_1 + S\hbar\omega . \tag{22}$$

2.4 FIELD AND TEMPERATURE DEPENDENCE OF THE EMISSION RATE. — An approximate analytical expression for the field emission rate e_F can be obtained by approximating the sums in eqs. (15) and (17) by integrals. The details are given in Appendix B. For temperatures higher than $\hbar\omega/k$, e_F approximates to :

$$e_F \simeq (2\pi/A_\nu)^{1/2} \exp(-2\,SkT/\hbar\omega) \times \times \Gamma(\Delta_\nu) . I_\nu(2\,SkT/\hbar\omega) \tag{23}$$

where $I_\nu(x)$ is the modified Bessel function of order ν. The values of ν and of A_ν are given in Appendix B. With the above approximations, we note that the emission rate e_F depends on the Huang-Rhys factor S and on temperature T only through the product ST. In (Fig. 3) we have plotted the emission rate e_F *versus* the electric field using the full expressions (15) and (17) and the approximate expression (23). In both cases, the preexponential factor γ appearing in expression (2) for $\Gamma(\Delta)$ was taken as $q/3\,\hbar$, corresponding to Korol's calculations. In the example of (Fig. 3), we deal with traps having an electronic level 0.35 eV below the conduction band. The phonon energy $\hbar\omega$ is taken to be 10 meV. The choice of this value corresponds to the Transverse Acoustic phonon mode in GaAs and will be justified later.

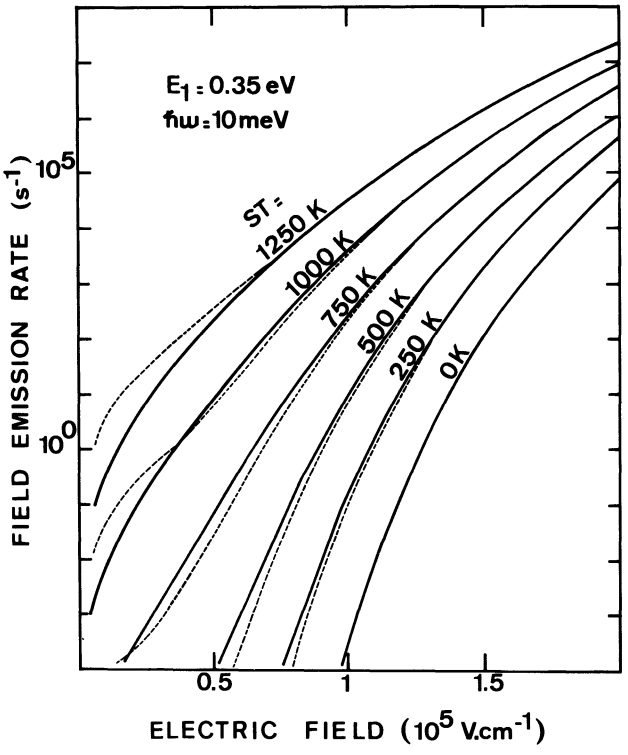

Fig. 3. — Electric field dependence of the field emission rate e_F, as a function of the product ST. Full and dotted lines correspond respectively to the « exact » and *approximate* expression for e_F. The case labelled $ST = 0$ is evaluated after Korol's expression.

As with the approximate expression (23), the exact calculation of eq. (17) for e_F depends on S and T through the product ST provided $T > 50$ K. We see that the agreement between exact and approximate expression for e_F is good for the different values of the product ST except at small field strengths. The case $ST = 0$ reduces simply to Korol's ionization rate $\Gamma(E_c - E_1)$. We note that coupling with the lattice increases the field emission rate e_F to a great extend especially at low fields. For $ST = 500$ K, and at a field of 10^5 V.cm^{-1}, the field emission rate is five orders of magnitude larger than for $ST = 0$.

2.5 CALCULATION OF CAPACITIVE TRANSIENTS. — In a $p^+ n$ junction or Schottky barrier, the electric field F varies linearly across the depleted junction width W according to a law of the form

$$F = \frac{q}{\varepsilon_0\,\varepsilon_r} N_D(W - X) \tag{24}$$

where $\varepsilon_0\,\varepsilon_r$ is the dielectric constant, qN_D the net charge density of shallow ionized donors assumed to be uniform in the depleted region, X is the distance from the junction or the Schottky barrier. The variable field strength in the depleted region will give rise to a distribution of emission rates. In the following, we outline the calculations for the transients following the application of a rectangular refilling pulse in the diode bias. This pulse serves the purpose of filling a fraction of the traps in the depleted region. The transients are subsequently studied under the conditions of a constant bias voltage. The occupation of an electron trap at any position X can be deduced from the differential equation

$$\frac{\partial f(t)}{\partial t} = c_n[1 - f(t)] - e_n\, f(t) \tag{25}$$

where $f(t)$ is the occupation ratio of the traps at the position X and at any time t. The rates c_n and e_n are the capture and emission rates for the trap at the position X including field effects. The solution of eq. (25) can be written in the form

$$f(t) = f_\infty + [f(t_0) - f_\infty] \times \times \exp[-(e_n + c_n)(t - t_0)] \tag{26}$$

where t_0 is an arbitrary reference time and f_∞ is the limiting value of $f(t)$ at steady state given by

$$f = \frac{c_n}{c_n + e_n} . \tag{27}$$

The capacitance transients that we simulate are obtained just after the application of a rectangular refilling pulse which reduces the value of the reverse bias and reduces consequently the depletion layer width. The transients occurring during and after the refilling pulse are both governed by eqs. (24) to (27) except that the depletion layer width is changed when the pulse is removed and consequently c_n and e_n assume different values.

In a DLTS experiment, the refilling pulses of duration t_p are applied periodically with period t_r. Assuming that e'_n and c'_n are the emission and capture rates for a trap during the refilling pulse and that e_n and c_n are these values after the removal of the pulse, and taking for the time origin the instant of application of the refilling pulse, eq. (26) yields

$$f(t_p) = f'_\infty + [f(0) - f'_\infty] \exp[-(e'_n + c'_n)\, t_p] \tag{28a}$$

and

$$f(t_r) = f_\infty + [f(t_p) - f_\infty] \times \times \exp[-(e_n + c_n)(t_r - t_p)] \tag{28b}$$

where f_∞ is given by eq. (27), whereas

$$f'_\infty = \frac{c'_n}{c'_n + e'_n}. \tag{29}$$

If the heating rate during the DLTS experiment is sufficiently low, one can assume that

$$f(t_r) = f(o). \tag{30}$$

This condition together with eqs. (28*a*) and (28*b*) easily yield the value of $f(t_p)$. The case of a one shot refilling pulse can be treated as a limiting case for which the repetition period t_r is made to go to infinity.

The transient behaviour of $f(t)$ is given by eq. (26) with t_p replacing t_0. The corresponding capacitive transients are obtained by using Poisson's equation, the solution of which has the form

$$V = \frac{q(N_D - N_T)}{2\,\varepsilon_0\,\varepsilon_r} W^2 + \frac{qN_T}{\varepsilon_0\,\varepsilon_r} \int_0^W [f(t_p) - f_\infty] \times \times \exp[-(e_n + c_n)(t - t_p)]\, X dX \tag{31}$$

where N_T is the concentration of traps per unit volume assumed to be uniform. These traps are assumed to be neutral when unoccupied. V is the electrostatic potential across the depletion region and includes the diffusion potential. The depth of the depletion layer W can now be calculated at any instant t and the capacitance C is deduced from the formula

$$C = \frac{\varepsilon_0\,\varepsilon_r . A}{W} \tag{32}$$

where A is the diode area.

We have developed a computer model calculating the emission and capture rates under different temperature and electric field conditions after the full formulae given by eqs. (17) to (20). The computer model then predicts the capacitive transients according to the method outlined above.

3. **Comparison between theoretical and experimental results.** — 3.1 TECHNIQUES. — We have studied field effects on the irradiation induced defect E3 [16]. For this study, irradiations with 1 MeV electrons have been performed on three different vapour phase epitaxy layers of GaAs (dopant concentrations of the starting materials : 1.5×10^{15}, 1.8×10^{16}, 5×10^{16} cm^{-3}) and on one layer of bulk Czochralski material (dopant concentration of the starting material : 1×10^{17} cm^{-3}). Irradiation doses range from 2×10^{14} cm^{-2} for the material with the lowest dopant concentration to 2×10^{16} cm^{-2} for the material with the highest dopant concentration. After irradiation, the layers are lightly etched (1 μm) and a 1 000 Å thick layer of gold is evaporated onto their surface. (Area of the Schottky diodes : 5.8×10^{-3} cm^2.)

Capacitance transients have been recorded at fixed temperatures using a Boonton model 72 B capacitance bridge monitored by a computer [24]. « Deep Level Transient Spectroscopy » (DLTS) [7] experiments have also been performed with both capacitance and current transients. The transient signals are analysed with a two phase lock-in amplifier [25, 26] ; the difference between the in-phase component and the quadrature component of the transient is recorded as the DLTS signal [27].

3.2 EXPERIMENTAL RESULTS. — Capacitance transients have been recorded at five temperatures ranging from 108 K to 163 K for a sample with a free electron concentration equal to $N_D = 4.7 \times 10^{16}$ cm^{-3} after electron irradiation, with a fixed reverse bias equal to 3.5 V and after a refilling pulse of 100 μs duration. The results are given in (Figs. 4*a* and 4*b*). A somewhat unusual linear scale for capacitance and a logarithmic scale for time have been used. For the lowest temperature a linear dependence of the capacitance on the logarithm of the time is observed over more than five orders of magnitude of time, giving clear evidence of a large distribution of time constants in the depleted region of the Schottky diode. Let us note the increasing slopes of the curves with increasing temperatures, which obviously shows that the effect is temperature dependent.

DLTS curves have also been recorded from the same sample, with a fixed reverse external bias equal to 4.0 V, with refilling pulses of variable amplitude ΔV, and with two different emission rate-windows [7] (Fig. 5). With increasing amplitude of the pulses, the additional filled traps are submitted to increasing electric fields. As a consequence, shifts in the position and deformations in the shape of the DLTS peaks

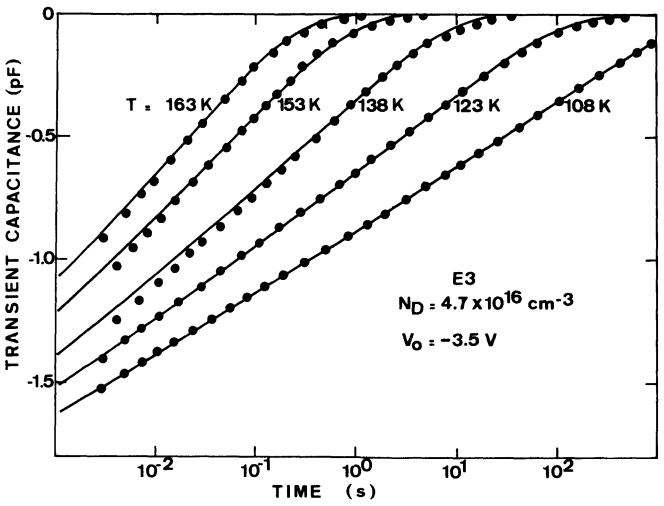

Fig. 4*a*. — Transient capacitance changes at different temperatures for a Schottky barrier diode made on n-type GaAs with a dopant concentration of 4.7×10^{16} cm^{-3}. The transients correspond to a reverse bias of 3.5 V, the refilling pulse has a height $\Delta V = 4$ V and a duration of 100 µs. The reference capacitance level has been taken to be equal to the steady state value. The points correspond to measurements and the full lines to the simulated transients.

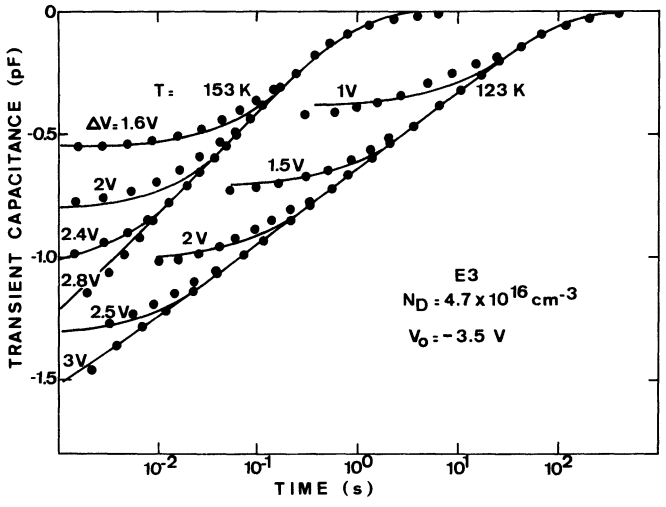

Fig. 4*b*. — Transients recorded in the same conditions as for (Fig. 4*a*), but with different values of the refilling pulse height ΔV.

towards low temperatures are observed. A saturation of the peaks is reached for amplitudes of the refilling pulses larger than 2.0 V. The *signatures* [28] of E3 in four different samples with dopant concentrations ranging from 1.5×10^{15} to 9×10^{16} cm^{-3} have been recorded using both capacitance and current transients (Fig. 6). For the samples with the larger dopant concentrations, we note strong deviations of the signatures from that recorded from the sample with the lowest dopant concentration. It can be noticed that this effect is less pronounced for large emission rates or for high temperatures.

3.3. Evaluation of the physical parameters by curve-fitting method. — The different physical parameters entering the model are : the Gibbs energy

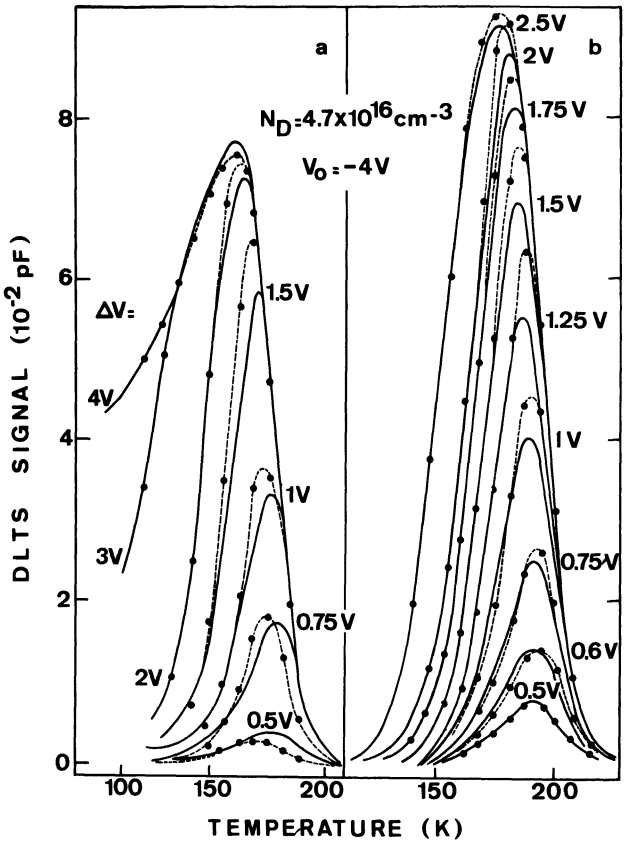

Fig. 5. — DLTS curves for the same sample as in (Fig. 4), with a 4 V reverse bias and different values of the refilling pulse height ΔV. The emission rate windows and pulse durations are respectively : (*a*) 17 s^{-1} and 100 µs, (*b*) 140 s^{-1} and 50 µs. Dotted curves correspond to the model simulations.

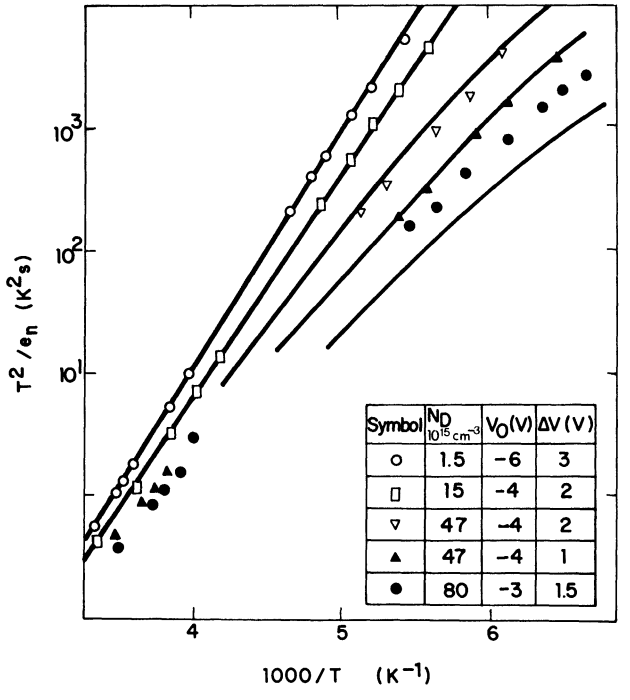

Fig. 6. — *Signatures* of E3 for four samples with different dopant concentrations N_D, reverse bias V_b and refilling pulse heights ΔV; e_n is the experimental emission rate window, yielding a DLTS peak with a maximum at the temperature T. Curves correspond to model simulations and points to experimental determinations. (Points with $1\,000/T < 4.5$ are determined from current transients.)

E_T of the trap, its concentration N_T, the phonon energy $\hbar\omega$, the Huang-Rhys factor S, the effective mass m^* for the trapped electron, the preexponential factor γ and the dopant concentration N_D.

We have assumed that m^* is identical to the effective mass for the density of state of the Γ minimum of the conduction band ($m^* = 0.068\ m_0$) and that the energy of the phonons corresponds to the peak of density of state for the T.A. mode ($\hbar\omega = 10$ meV). These choices will be discussed later.

Some of the other parameters can be deduced from experimental results : the dopant concentration is obtained from careful $C(V)$ profiling. Measurements at the same temperature of the emission and capture rates with negligible electric field effects provide the Gibbs energy E_T of the trap, from eq. (21). Direct measurements of the capture cross section of E3 have been published by Henry and Lang [18] who interpreted the results in terms of their MPE theory. The temperature dependence of σ follows eq. (4) with parameters

$$\sigma_\infty = 1 \times 10^{-14}\,\mathrm{cm}^2 \quad \text{and} \quad E_\sigma = 0.10\,\mathrm{eV}\,.$$

DLTS experiments have been performed on a sample with the low dopant concentration

$$N_D = 1.5 \times 10^{15}\,\mathrm{cm}^{-3}\,,$$

with several emission rate windows [7] ranging from $6.9\ \mathrm{s}^{-1}$ to $1.7 \times 10^5\ \mathrm{s}^{-1}$ using both capacitance and current transients (Fig. 6). The emission rates have been checked to be uniform in the depleted region and insensitive to the external bias. Numerical simulations of these experiments have been performed, and assuming that the Gibbs energy E_T varies with temperature according to a law similar to that of the gap [29], we set

$$(E_C - E_T) = (E_C - E_{T_0}) - \frac{\alpha T^2}{T + 204} \qquad (33)$$

where the parameters determined for best fits are given by :

$$E_C - E_{T_0} = 0.305\,\mathrm{eV}$$
$$\alpha = 3.3 \times 10^{-4}\,\mathrm{eV.K}^{-1}\,.$$

In order to determine the remaining unknown parameters of the models, we have fitted, with the computer model described in section (2.4), the experimental results described above for a sample having a uniform dopant concentration measured to be

$$N_D = 4.7 \times 10^{16}\,\mathrm{cm}^{-3}$$

by careful C-V profiling.

For such a dopant concentration, because of field effects, only a rough estimation of the concentration of the trap can be deduced from the amplitude of the DLTS peaks. Hence, the concentration of the trap N_T is an unknown parameter, together with S and γ. For a fixed value of N_T, we can determine the values of S and γ required to yield a least square fit for the capacitance transient at 123 K of (Fig. 4*a*). In fact, this curve is very close to a straight line over four orders of magnitude of time, and in our numerical model, the slope of the linear part of the plot depends only on S, and increases when S is made to increase. Changing γ results in a mere translation of the computed transients along the logarithmic time scale. Everything else being fixed, the parameters S and γ can be considered as single valued functions of N_T.

For a range of values of N_T from 1.5×10^{15} to $2.1 \times 10^{15}\ \mathrm{cm}^{-3}$, we find that the parameters required to fit the transient at 123 K of (Fig. 4*a*) will also reasonably fit the transients recorded at other temperatures, and the corresponding values of S range from 4 to 10.

In order to reduce the uncertainty in S and to check the validity of our model over wider temperature and electric field ranges, we have developed a computer program to perform DLTS simulations. These simulations allow us to determine the trap concentration N_T which remains undetermined after the curve-fitting procedure described above. This is achieved by seeking the model parameters which simultaneously yield a best fit for the 123 K capacitive transient of (Fig. 4*a*) and of the DLTS curve of (Fig. 5*a*) which corresponds to the pulse height $\Delta V = 2.5$ V. The consistent set of parameters is thus found to be

$$N_T = 1.7 \times 10^{15}\,\mathrm{cm}^{-3}$$
$$S = 7.5$$
$$\gamma = 9 \times 10^{12}\,\mathrm{s}^{-1}\,\mathrm{eV}^{-1}\,.$$

With the above parameters, all the capacitive transients of (Fig. 4*a* and 4*b*) as well as all the DLTS curves of (Fig. 5*a* and 5*b*) have been simulated. One notices the good agreement between calculations and measurements even for the cases which have not been initially selected for curve-fitting purposes.

We have applied our model to simulate DLTS experiments in other samples with different dopant concentrations. The computed signatures, deduced from the position of the maximum of the simulated peak for a given emission rate window are compared to the experimental signatures in (Fig. 6).

4. **Discussion.** — 4.1 SENSITIVITY ANALYSIS OF THE MODEL. — Uncertainties in some parameters entering the model cause errors in the parameters S, γ and N_T that we have deduced by our curve fitting method. Convincing values of the uncertainties in m^*, E_{T_0}, α and N_D have been assumed to investigate the sensitivity of our model. We have determined the parameters S, γ and N_T using extreme values of m^*, E_{T_0}, and N_D. The results are given in table I. It is clear from the above table that the parameters S and N_T can be obtained within an uncertainty of about $\pm$ 25 %, whereas γ can only be located within a four orders of magnitude range. We note that this range

Table I. — *Values of the model parameters S, γ and N_T, deduced by curve-fitting for extreme and average values of the parameters m^*, E_{T_0}, α and N_D assumed in the model.*

m^*/m_0	0.066	0.068	0.070
$E_c - E_{T_0}$ eV	0.290	0.305	0.320
α 10^{-4} eV.K^{-1}	3.8	3.3	2.8
N_D 10^{16} cm^{-3}	4.9	4.7	4.5
S	10.2	7.5	5.4
γ 10^{14} s^{-1} eV^{-1}	1.2×10^{-3}	9×10^{-2}	42
N_T 10^{15} cm^{-3}	1.45	1.7	2.2

includes the theoretical value $q/3\hbar$ corresponding to Korol's calculations for a delta function potential well.

4.2 Comparison with other results. — From our evaluation of the different parameters, we can obtain a rough estimate of the Franck-Condon shift

$$S\hbar\omega = 75 \pm 22 \text{ meV}.$$

It is interesting to compare this estimation with the value deduced from the activation energy of the capture cross-section after the MPE theory. As mentionned earlier, measurements by Henry and Lang [18] yield an activation energy of 0.10 eV for the capture cross-section of trap E3. Using the theoretical formula of these authors for σ, one obtains the measured capture cross-section activation energy for

$$S\hbar\omega = 90 \text{ meV}.$$

This estimate is seen to be consistent with ours.

4.3. Choice of phonon energy. — The procedure outlined in section 3.3 has been repeated for different values of $\hbar\omega$. For values of $\hbar\omega$ between 9 and 12 meV, reasonably good agreement between theory and experiment is obtained. For other values of $\hbar\omega$, we find that agreement is only possible in a narrow temperature range. Although the phonon mode could be a local one, the range of acceptable values of $\hbar\omega$ seems to be consistent with the transversal-acoustic mode having a sharp peak of density of state at 9.8 meV [30].

4.4. Effective mass. — In our treatment of electron tunneling, we have assumed the effective mass of the trapped electron to be constant and identical to the effective mass for the density of state of the Γ minimum of the conduction band. Two types of objections can be made about this assumption :

(i) As noted by Kohn [31], the electron effective mass cannot be used to describe the electron wave function in the immediate vicinity of the potential well of a deep trap. It can only be used to describe the asymptotic behaviour of the wave function away from the potential well. This may explain the discrepancy between the value of the preexponential factor γ given by Korol's theory :

$$\gamma = q/3\hbar = 5.06 \times 10^{14} \text{ eV}^{-1} \text{ s}^{-1}$$

and the average value that we have determined. From table I, it can be seen that the determined values of γ are between 8 times too large and 4 000 times too small.

(ii) In the forbidden band, the dispersion law $E(\mathbf{k})$ is not parabolic, which invalidates the use of a constant effective mass in the gap. However, according to the theoretical calculations of Kane [32] and Chaves *et al.* [33], experimentally confirmed by Padovani and Stratton [34] and by Conley and Mahan [35], deviation from the parabolic dispersion law occurs only for energies deeper than 0.4 eV below the conduction band. Consequently, our theory should be applied with caution to trapping levels deeper than that of E3.

4.5 Poole-Frenkel effect. — Assuming that the E3 centre is neutral when unoccupied (acceptor type), we have neglected in our calculation the Poole-Frenkel effect [10]. To evaluate the error caused by this neglect we may calculate the increase in the emission rate due to this effect, with the formula of Hartke [36]. For a spherical potential well having a radius $a = 5$ Å (of the order of the interatomic spacing), we see that the thermal emission rate at 123 K is increased for an electric field of 10^5 V.cm^{-1} by only 30 %. This is a very small correction when compared with the observed increase in emission rate for this temperature and electric field range which is more than five orders of magnitudes.

5. **Summary and conclusions.** — We have developed a theory of electric field ionization by means of quantum mechanical tunneling for deep traps in semiconductors. The theory takes into account interaction with phonons. Our field emission model is particularly simple because of the use of the adiabatic approximation for the wave function of the trapped electron. This approximation is justified on the ground that the crossing between the bound and free energy levels is not involved in the transition.

We have applied our theory to the trap E3 which is introduced by electron irradiation into GaAs. Capacitance transients and DLTS curves have been obtained for several samples with different dopant concentrations. Our experimental results give clear evidence of electric field dependent emission rates for this trap. A complete computer calculation has been elaborated to simulated the above mentioned experiments, which are accurately reproduced in a large range of temperature and electric fields. In particular, the Huang-Rhys factor and the energy of

the phonon mode coupled to the trap are evaluated by careful curve fitting. The value of the Franck-Condon shift which can be deduced is consistent with the one obtained from the activation energy of the capture cross-section after the work of Henry and Lang.

Acknowledgments. — The authors wish to express their gratitude to A. Mircea for his encouragements and relevant remarks and to D. Bois and G. Vincent for exchanging information with the authors. They thank J. Bok for stimulating discussions and J. Bourgoin who supervised sample irradiation. Thanks are also due to R. Duchesne for skilful technical assistance. The authors acknowledge partial financial support from the Délégation Générale à la Recherche Scientifique et Technique (contract n° 77 40028-440 f).

APPENDIX A

The adiabatic approximation for the electron wavefunction. — We wish to evaluate, in this Appendix, the error involved in using the adiabatic solution of the Schrödinger wave equation for the electron.

The time dependent Schrödinger equation for the trapped electron is

$$\frac{i\hbar}{\Phi}\frac{\partial\Phi}{\partial t} + \frac{1}{\Phi}\frac{\hbar^2}{2\,m^*}\nabla^2\Phi - V = 0 \qquad (A.1)$$

where V represents the potential energy of the trap which is time-dependent due to interaction with lattice phonons. In the immediate vicinity of the trap, the changes in potential energy due to the electric field are negligible compared to the trap potential. The trap potential V is assumed to be a function of time t and of the distance r from the centroid of the trap.

If the time derivative appearing in eq. (A.1) is neglected, a possible solution of this equation would be an energy eigenfunction for the fundamental electronic eigen energy E_e. For an occupied trap, E_e is assumed to change sinusoidally with time according to eq. (8) of the text. At any instant t, the instantaneous energy level E_e lies at an energy depth $\Delta(t)$ below the conduction band E_e at the trapping site, that is

$$\Delta(t) = E_c - E_1 + bQ_m \cos t\,. \qquad (A.2)$$

Assuming the instantaneous potential well V yields an eigen energy level $E_c - \Delta$, let $\Psi(r, \Delta)$ represent the corresponding real normalized solution of the stationary Schrödinger equation. We now attempt to find the solution of the full Schrödinger eq. (A.1) in the form

$$\Phi(r, t) = \Psi[r, \Delta(t)]\exp[-\,i\theta(t)] \qquad (A.3)$$

where $\theta(t)$ is a phase angle to be found. Substituting this tentative solution into the left hand side of eq. (A.1), we obtain, instead of zero, an error ΔE having the units of energy in the form

$$\Delta E = \frac{i\hbar}{\Psi}\frac{\partial\Psi}{\partial\Delta}\cdot\frac{\partial\Delta}{\partial t} + \hbar\frac{\partial\theta}{\partial t} - E_c + \Delta(t)\,. \qquad (A.4)$$

The real part of the above error ΔE can be made to vanish by choosing for $\theta(t)$ the value

$$\theta(t) = \int^t \frac{E_c - \Delta(t)}{\hbar}\,dt \qquad (A.5)$$

Eqs. (A.3) and (A.5) completely define the adiabatic solution $\Phi(r, t)$. We readily see that $\Phi(r, t)$ satisfies the normalization condition if $\Psi(r, \Delta)$ satisfies this condition for all values of Δ. However, the above solution $\Phi(r, t)$ still leaves us with an error which is the imaginary part of ΔE in eq. (A.4).

We assume for simplicity that the potential well of the trap has a constant depth V_0 inside a sphere of radius a centered at the trap centroid, the potential being zero outside this sphere. We adopt the simple phonon-electron interaction picture of Henry and Lang [15] by assuming that V_0 is time-dependent whereas the radius is time-independent. With the above assumption, we get for the ground state with zero angular momenta

$$\begin{aligned} \Psi(r, \Delta) &= \frac{A}{r}\cdot\sin(kr) && \text{for} \quad r < a \\ \Psi(r, \Delta) &= \frac{A'}{r}\exp[-\,\chi(r - a)] && \text{for} \quad r \geqslant a \end{aligned} \qquad (A.6)$$

where

$$k^2 = \frac{2\,m^*(V_0 - \Delta)}{\hbar^2} \quad \text{and} \quad \chi^2 = \frac{2\,m^*}{\hbar^2}\Delta$$

and A and A' are constant related by the condition of continuity of $\Psi(r, \Delta)$ at $r = a$, which yields

$$A' = A\sin(ka)\,. \qquad (A.7)$$

The values of A and A' are determined by the normalization condition for $\Psi(r, \Delta)$. In order to satisfy the condition of continuity of the gradient of $\Psi(r, \Delta)$ at $r = a$, the potential well depth V_0 and the energy depth Δ must be related by the implicit relation

$$\tan(ka)/(ka) = -\,1/\chi a\,. \qquad (A.8)$$

For a potential well with a small radius and large depth, the value of ka which satisfies eq. (A.8) is very nearly equal to $\pi/2$. Furthermore, one easily gets

$$A' \simeq A \simeq (\chi/2)^{1/2}\,. \qquad (A.9)$$

From eqs. (A.2), (A.5), (A.8) and (A.9), we can calculate the time derivative of the wave function

$\Psi[r, \Delta(t)]$. Straight-forward algebra yields

$$\frac{1}{\Psi}\frac{\partial\Psi}{\partial\Delta}\frac{\partial\Delta}{\partial t} = -\frac{b\omega Q_m}{2\,\Delta(t)}\sin(\omega t) \times \left[\frac{1}{2} + \frac{kr}{\tan(kr)}\frac{\chi}{\chi + a(\chi^2 + k^2)}\right] \quad \text{for} \quad r < a$$

$$= -\frac{b\omega Q_m}{2\,\Delta(t)}\sin(\omega t)\left[\frac{1}{2} - \chi(r - a)\right] \quad \text{for} \quad r \geqslant a\,. \qquad (A.10)$$

We note in particular that the time derivative is very small outside the potential well and near the spherical shell defined by

$$r = a + 1/2\,\chi\,. \qquad (A.11)$$

We can now evaluate the residual imaginary part of the error ΔE given in eq. (A.4). One can easily obtain an upper bound for the logarithmic derivative of $\Psi(r, \Delta)$ given in eq. (A.3) and we deduce

$$|\,\Delta E\,| = |\,\mathrm{Im}\,(\Delta E)\,| < \frac{\hbar\omega}{2}\cdot\frac{bQ_m}{E_e - E_1 - bQ_m} \times \left[\chi(r + a) + \frac{1}{2}\right] \qquad (A.12)$$

which shows that when the amplitude of the energy level oscillation is not too large, the error is a fraction of the phonon energy multiplied by a factor of the order of (χr). For trap E3 and for temperatures under 200 K, the average value for the amplitude excursion bQ_m is smaller than 65 meV. This can be obtained from an evaluation of the parameter S and $\hbar\omega$ as is explained in the text.

The error ΔE in this case is of the order of 1 meV times (χr). Since, furthermore, ΔE is in phase quadrature with the other energy terms of eq. (A.4), we conclude that the adiabatic approximation yields the correct wave function near the potential well and the errors become important only in regions where the wave function is very small.

We may write this adiabatic wave function in the form

$$\Phi(r, t) = \Psi[r, \Delta(t)] \times \exp\left[-\frac{i}{\hbar}(E_c - E_1)\,t + \frac{ibQ_m}{\hbar\omega}\sin\omega t\right]. \qquad (A.13)$$

APPENDIX B

Analytical approximation for the field emission rate. — It is possible to get an analytical closed form expression for the field emission rate, avoiding the double summation in eq. (17) of the text.

We assume that the density of free carriers in the conduction band is low enough so that the Fermi-Dirac probability of finding an empty conduction band state having an energy $E_c - \Delta_p$ is equal to unity for any value of p subject to the condition

$$\Delta_p > 0\,. \qquad (B.1)$$

The field emission rate can be written as :

$$e_F = [1 - \exp(-\hbar\omega/kT)]\sum_{n=0}^{+\infty}\sum_p \exp(-n\hbar\omega/kT) \times \Gamma(\Delta_p)\,J_p^2\left\{2\left[S\left(n + \frac{1}{2}\right)\right]^{1/2}\right\}. \qquad (B.2)$$

The summation over n can be replaced by an integral, which is justified for high temperatures ($kT \gtrsim \hbar\omega$)

$$W_p \equiv \sum_{n=0}^{+\infty}\exp(-n\hbar\omega/kT)\,J_p^2\left\{2\left[S\left(n + \frac{1}{2}\right)\right]^{1/2}\right\} \simeq \int_0^{+\infty} J_p^2\left\{2\left[S\left(n + \frac{1}{2}\right)\right]^{1/2}\right\}.\exp(-n\hbar\omega/kT)\,dn \qquad (B.3)$$

with the transformation

$$2\left[S\left(n + \frac{1}{2}\right)\right]^{1/2} = x^{1/2}\,p\,, \qquad (B.4)$$

we get

$$W_p \simeq \frac{p^2}{4\,S}\exp(\hbar\omega/2\,kT)\int_{2S/p^2}^{+\infty} J_p^2(x^{1/2}\,p) \times \exp(-xp^2\,\hbar\omega/4\,SkT)\,dx\,. \qquad (B.5)$$

For large enough values of p, the lower limit of the integral can be replaced by zero, thus

$$W_p \simeq \frac{p^2}{4\,S}\exp(\hbar\omega/2\,kT)\int_0^{+\infty} J_p^2(x^{1/2}\,p) \times \exp(-xp^2\,\hbar\omega/4\,SkT)\,dx$$
$$\simeq (kT/\hbar\omega)\exp(\hbar\omega/2\,kT)\exp(-2\,SkT/\hbar\omega) \times I_p(2\,SkT/\hbar\omega) \qquad (B.6)$$

where I_p is the modified Bessel function of integer order p [34]. We deduce

$$e_F \simeq (2\,kT/\hbar\omega)\,\sinh(\hbar\omega/2\,kT) \times \exp(-2\,SkT/\hbar\omega)\sum_p \Gamma(\Delta_p)\,I_p(2\,SkT/\hbar\omega)\,. \qquad (B.7)$$

The term under the summation sign in the above equation will be shown to have a maximum for a value of $p = \nu$. In fact, we can approximate this term by expanding its logarithm by means of a Taylor

series, yielding a Gaussian expression of the form

$$\Phi(p) \equiv \Gamma(\Delta_p)\, I_p(2\, SkT/\hbar\omega)$$
$$\simeq \Phi(\nu) \exp[-\, A_\nu (p - \nu)^2/2]\,. \qquad (B.8)$$

The value of ν is found by looking for the solution $p = \nu$ of the transcendental equation

$$\left[\frac{\partial}{\partial p} \ln \Phi(p)\right]_{p=\nu} = \left[\frac{\partial}{\partial p} \ln \Gamma(\Delta_p) + \frac{1}{I_p}\frac{\partial I_p}{\partial p}\right]_{p=\nu} = 0 \qquad (B.9)$$

and A_ν is defined as

$$A_\nu = -\left[\frac{\partial^2 \ln \Phi(p)}{\partial p^2}\right]_{p=\nu}. \qquad (B.10)$$

The summation in eq. (B.7) can now be evaluated by approximating is to an integral yielding

$$e_F \simeq (2\,\pi/A_\nu)^{1/2}\,(2\,kT/\hbar\omega)\sinh(\hbar\omega/2\,kT)\,\times$$
$$\times \exp(-\,2\,SkT/\hbar\omega)\,\Gamma(\Delta_\nu).I_\nu(2\,SkT/\hbar\omega)\,. \qquad (B.11)$$

The above evaluation of e_F therefore requires the calculation of ν and A_ν.

We first evaluate ν by solving eq. (B.9). Neglecting the dependence on Δ_p of the preexponential factor of $\Gamma(\Delta_p)$, we get

$$\frac{\partial \ln \Gamma(\Delta_p)}{\partial p} \simeq 3\,K\hbar\omega/2\,\Delta_p \qquad (B.12)$$

where K is given by eq. (3) in the text.

A good approximation for $\partial I_p/\partial p$ can be obtained from the recurrence relation

$$I_{p-1}(x) - I_{p+1}(x) = 2\,pI_p(x)/x\,. \qquad (B.13)$$

From

$$\partial I_p/\partial p \simeq (I_{p+1} - I_{p-1})/2 \qquad (B.14)$$

we get

$$\frac{\partial \ln \Phi(p)}{\partial p} \simeq \frac{3\,K\hbar\omega}{2\,\Delta_p} - \frac{p\hbar\omega}{2\,SkT}\,. \qquad (B.15)$$

An elementary calculation yields, from eq. (B.9)

$$\nu\hbar\omega = 2(E_c - E_1)\,\{\,1 + [1 + (F/F_c)^2]^{1/2}\,\}^{-1} \qquad (B.16)$$

where the *critical* electric field F_c is given by

$$F_c = \frac{2\,SkT\hbar\omega}{\hbar q}\left(\frac{2\,m^*}{E_c - E_1}\right)^{1/2}. \qquad (B.17)$$

The parameter A_ν is deduced from eqs. (B.10) and (B.15)

$$A_\nu \simeq \frac{3}{4}K\left(\frac{\hbar\omega}{\Delta_\nu}\right)^2 + \frac{\hbar\omega}{2\,SkT}\,. \qquad (B.18)$$

For high temperatures ($kT \gtrsim \hbar\omega$), a further simplification can be made

$$(2\,kT/\hbar\omega)\sinh(\hbar\omega/2\,kT) \simeq 1 \qquad (B.19)$$

and the field emission rate is written as

$$e_F = (2\,\pi/A_\nu)^{1/2}\exp(-\,2\,SkT/\hbar\omega)\,\Gamma(\Delta_\nu)\,\times$$
$$\times\, I_\nu(2\,SkT/\hbar\omega)\,. \qquad (B.20)$$

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