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Generalized Poole Frenkel (PF) effect with donors distributed in energy

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Résumé. — Une étape supplémentaire est franchie dans la généralisation de l'effet PF, en considérant l'effet d'une répartition des donneurs, en énergie, dans la bande interdite. Différentes lois de répartition sont étudiées. Les distributions uniformes sont d'abord traitées d'une manière extensive. Les simulations numériques ont révélé des similarités évidentes avec le cas d'un seul niveau donneur. L'ionisation par le champ est ensuite déterminée pour des distributions exponentielles. Au passage, une loi exponentielle, rencontrée quelquefois dans la littérature, est analysée. Les conditions de résolvabilité de l'équation différentielle de base sont indiquées. Le calcul et la simulation sont, en outre, étendus à un système à deux bandes uniformes. Finalement, une méthode de résolution approchée est proposée, lorsque les distributions ont des formes quelconques.

Abstract. — A further step in generalization of PF effect is got over, in considering the effect of a distribution of donors in energy, within the gap. Various laws of repartition are studied. Uniform distributions are first treated extensively. Computer simulations pointed out very conspicuous similarities with the one donor level case. Field-induced ionization is then derived for exponential distributions. An exponential law, given sometimes in literature, is analyzed throughout. Conditions of solvability of the basic differential equation are indicated. Moreover derivation and simulation are extended to a system of two uniform bands. Finally, an approximate method of resolution is proposed, when distributions of any shape are concerned.

1. Introduction. Basic hypotheses.

In theoretical developments dealing with Poole-Frenkel (PF) effect, it is regularly supposed that one donor level alone is present in the gap. Furthermore, as was shown in a preceding paper [1], a PF saturation can be foreseen, when introducing Fermi-Dirac statistics into derivations of field enhanced donor ionization, instead of the usually implemented Boltzmann function.

A step more in generalization can be made, if some kind of distribution of donors in energy is admitted. This is the object of the present paper. We determine here the free electron density when a one-dimensional PF effect is concerned, account being taken of saturation, and for an any shaping of wells, coulombic or not. Thus is obtained a larger based Generalized PF effect.

Two classical types of distributions are considered (Rose [2]) : (i) A uniform distribution ranging from any shallow level, or from the conclusion band edge, down to any deeper arbitrary level. (ii) An exponential distribution starting from any shallow level, singularly from conduction band. In order to achieve the furthermost attainable generalization, two other repartitions are considered : a double-band with uniform donor distribution ; and an arbitrarily shaped distribution.

Fermi-Dirac statistics is used, as required by [1], to describe site population. However, Boltzmann function is retained to write down the density of electrons in conduction band, as no band degeneracy can take place in dielectrics to which PF theories can apply. So that, when simulations are sometimes performed until reaching parameter values that would imply a small degree of degeneracy, these ought to be considered only as describing an asymptotic behaviour. Compensation by acceptors is introduced directly, the case of non-compensated donors being simply a particular case, obtained letting the compensation ratio $q = N_d/N_a$ to tend toward infinity. All acceptors are supposed to lie far below the

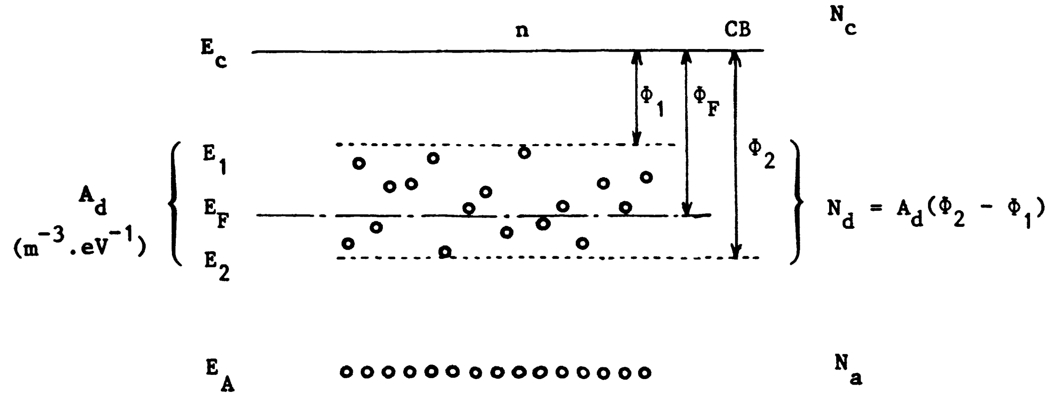

Fig. 1. — Schematic representation of a compensated uniform distribution of donors.

Fermi energy, in such a manner that, as in usual treatments, they can be considered as completely filled, whatever the field F and temperature T. The presence of any other kind of flaws is neglected. Finally it is admitted that the spin degeneracy factor for electrons in donor sites is equal to 1. This is only a matter of convenience, though being not in accordance with the involved monovalent nature of donors. But it can allow numerical fitting of the limiting Boltzmann-type results with those found in literature. Any way, this does not modify significantly the reported behaviours.

2. Uniform distribution.

2.1 MATHEMATICAL FORMULATION. — The model under consideration is represented in figure 1. Sites of constant density A_d per unit volume and unit energy, are distributed between a level E_1 of depth Φ_1 below the conduction band edge, and a level E_2 of depth Φ_2. The total density of donor sites is then given by :

$$N_d = A_d(\Phi_2 - \Phi_1) . \quad (1)$$

Let n_d be the density of electrons coming from the whole of sites, under a given applied field, and n the density of free electrons. Then :

$$n = n_d - N_a . \quad (2)$$

The density dn_d of electrons liberated from an elementary slab $d\Phi$, situated at any depth Φ, can be written

$$dn_d = \frac{A_d \, d\Phi}{1 + \frac{n}{N_c} \exp\left(\frac{\Phi}{kT} - \alpha_p\right)} \quad (3)$$

where $\alpha_p = \Delta\Phi_p/kT$ is the relative field-induced potential lowering for an any kind of well, either coulombic or more steeply shaped. In this equation, n depends upon α_p only. Thus integration can be made readily. Letting $\eta = \Phi/kT$ and $K = A_d kT/N_c$, it becomes :

$$\frac{n_d}{N_c} = K \int_{\eta_1}^{\eta_2} \frac{d\eta}{1 + \frac{n}{N_c} e^{\eta - \alpha_p}} .$$

Taking account of equation (2), yields immediately, in relative quantities :

$$n_r + \frac{s}{q} = \frac{s}{\eta_2 - \eta_1} \ln \frac{e^{-(\eta_1 - \alpha_p)} + n_r}{e^{-(\eta_2 - \alpha_p)} + n_r} , \quad (4)$$

with $n_r = \frac{n}{N_c}$, and $s = \frac{N_d}{N_c}$. This equation reduces readily to equation (4b) of [1], whenever $\eta_1 \to \eta_2$.

2.2 SIMULATED BEHAVIOUR OF THE MODEL. — The behaviour of function (4), studied by computer simulation, allowed to put forward some important peculiarities of the uniform distribution. The leading parameters are $\delta\eta = \eta_2 - \eta_1$ and the maximum relative depth η_2. Their respective influence is studied separately, parameters s and q being chosen so as to facilitate cross-checking with the one-level model results.

2.2.1 *Influence of the maximum donor depth* η_2. — η_2 has a very simple action on the $n_r(\alpha_p)$ behaviour. To put this forward, we drew in figure 2 variations of $\lg n_r$ in terms of α_p, for various η_2 values. We verified by curve superposition that they get rigorously the same form, when the relative band width $\delta\eta$, as well as s and q are left constant. Curves are simply shifted towards right hand side, proportionally to η_2. Saturation occurs as for the one level case, with the same limiting value $s - \frac{s}{q}$. As it could be inferred directly from the model, figure 2 shows that, under a given field, conductivity increases as the impurity band becomes nearer to the conduction band.

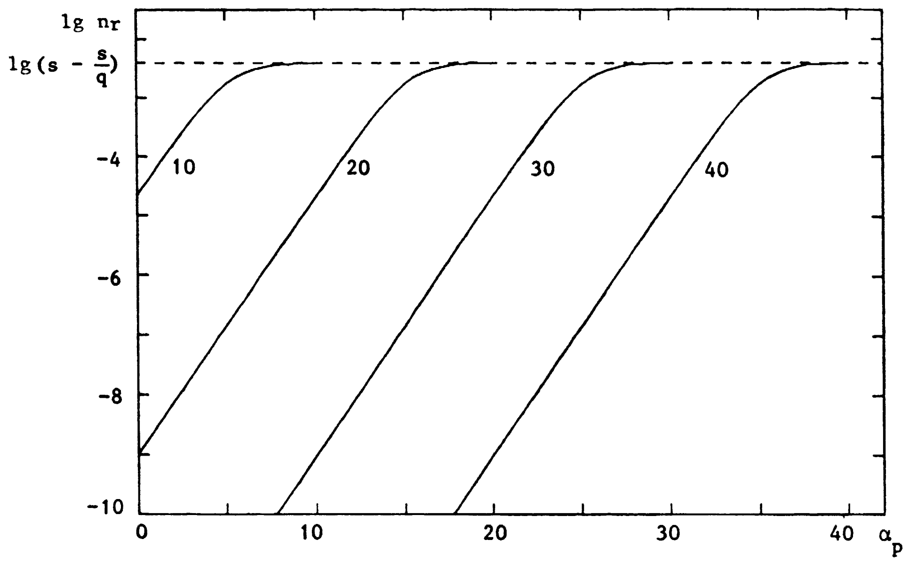

Fig. 2. — Variations of n_r *versus* α_p for bands of equal widths $\delta\eta = 10$, for various depths η_2 (marked on curves). $s = 0.1$; $q = 1.04$ (nearly full compensation).

2.2.2 *Band width influence.* — All curves resulting from the model of uniform distribution are alike the curves given by the one-level model. To show this clearly, we have represented in figure 3a, $\lg n_r = f(\alpha_p)$; with $\delta\eta$ as the leading parameter, η_2 being held constant. Four families of curves are drawn. Families (1) to (3) correspond to $q = 1.04$ (practically full compensation), and distinguish from one each other by $3\,s$ values : 10^{-1}, 10^{-3} and 10^{-6} (decreasing relative density of donors). Family (4) corresponds to a relatively high donor density ($s = 10^{-1}$) and to a very weak compensation ($q = 10^6$). Arrows in the figure indicate increasing band widths. It must be emphasized that the chosen $\delta\eta$ values allow to examplify situations going from a case very close to that of one-donor level ($\delta\eta = 10^{-4}$, or $\delta\Phi = 10^{-4}\,kT$), to the case of a wide band lying in between the conduction band edge and $\Phi_2 (\delta\eta = 40)$.

Moreover, allowing $\delta\eta$ to fall down to values as weak as $\delta\eta = 10^{-7}$, we verified that the lower curve in these families have reached a limiting position, which in addition coincides strictly with the related curve given by the one-level theory of [1]. Hence it is proved that, relative to the one donor level case, a uniform donor distribution exhibits no other effect than curve shifting. This is why, in figure 3b, slopes corresponding to $m = 1$, and to $m = 2$ [1], are obtained as well as transition regions from the former value to the latter. Moreover, when the band of donors approaches its maximum extension ($\delta\eta \lesssim \eta_2$), conditions exist where curves are nearly linear over the overall interval, with a small slope corresponding to slope parameter values $m > 2$. Remembering (see [1]) that stationary values of m greater than 2 cannot be obtained in the frame of the one-level theory, it is interesting to note that such opportunity can arise better with a uniform distribution.

2.2.3 *Variations of the interval of saturation.* — The range of saturation levelling is an increasing function of the relative band width $\delta\eta$, when η_2 is kept constant. This results from two combined effects : (i) curves are shifted upward as $\delta\eta$ is enhanced, because shallower levels are then brought nearer to conduction band edge ; (ii) whereas the maximum value of n_r, amounting to $s - \frac{s}{q}$, does not depend on $\delta\eta$, when in addition, it is implicitly supposed as in figure 3a, that $N_d = A_d\,kT\,\delta\eta$ is kept constant. This figure (families (1) to (3)) shows that, for constant q, the range of levelling off increases as s is decreased. Likewise, for constant s, it increases with q (families (1) and (4)), so that conditions can be met where saturation extends practically over the full range of α_p. Then, and rather paradoxically, a PF regime nearly insensitive to the field can be theoretically imagined.

3. Exponential distribution.

3.1 PRELIMINARY CONSIDERATIONS ABOUT THE MODEL. — The density of sites is supposed to decrease downwards exponentially. The elementary donor density within a slab $d\Phi$, at any depth Φ, is found in literature under two forms.

The first is Rose's [2] expression, which is transcribed here :

$$dN_d = A_d \exp\left(-\frac{\Phi}{kT_0}\right) d\Phi \qquad (5a)$$

A_d being the density of donors per unit energy range, and T_0 a suitable constant having the dimension of a temperature (see also Lampert and Mark [3]).

The second expression is that indicated for example by Pulfrey *et al.* [4]. It can be written :

$$\mathrm{d}N_d = A_d \exp\left(-\frac{\Phi}{bkT}\right) \mathrm{d}\Phi \tag{5b}$$

b being a dimensionless parameter characterizing the distribution sharpness. This form, contrary to that of equation (5a), implies a strong temperature dependence of the distribution steepness.

But actually this formulation should be misleading, as it would lead to an unfaithfull variation of the inter-side distance a, with temperature, at least for the most commonly available dielectrics. This is shown by a simple calculation of the total donor density. This density N_d results readily from any above expression for $\mathrm{d}N_d$. In order to introduce directly the most general case of exponential distribution, we suppose first that sites are distributed

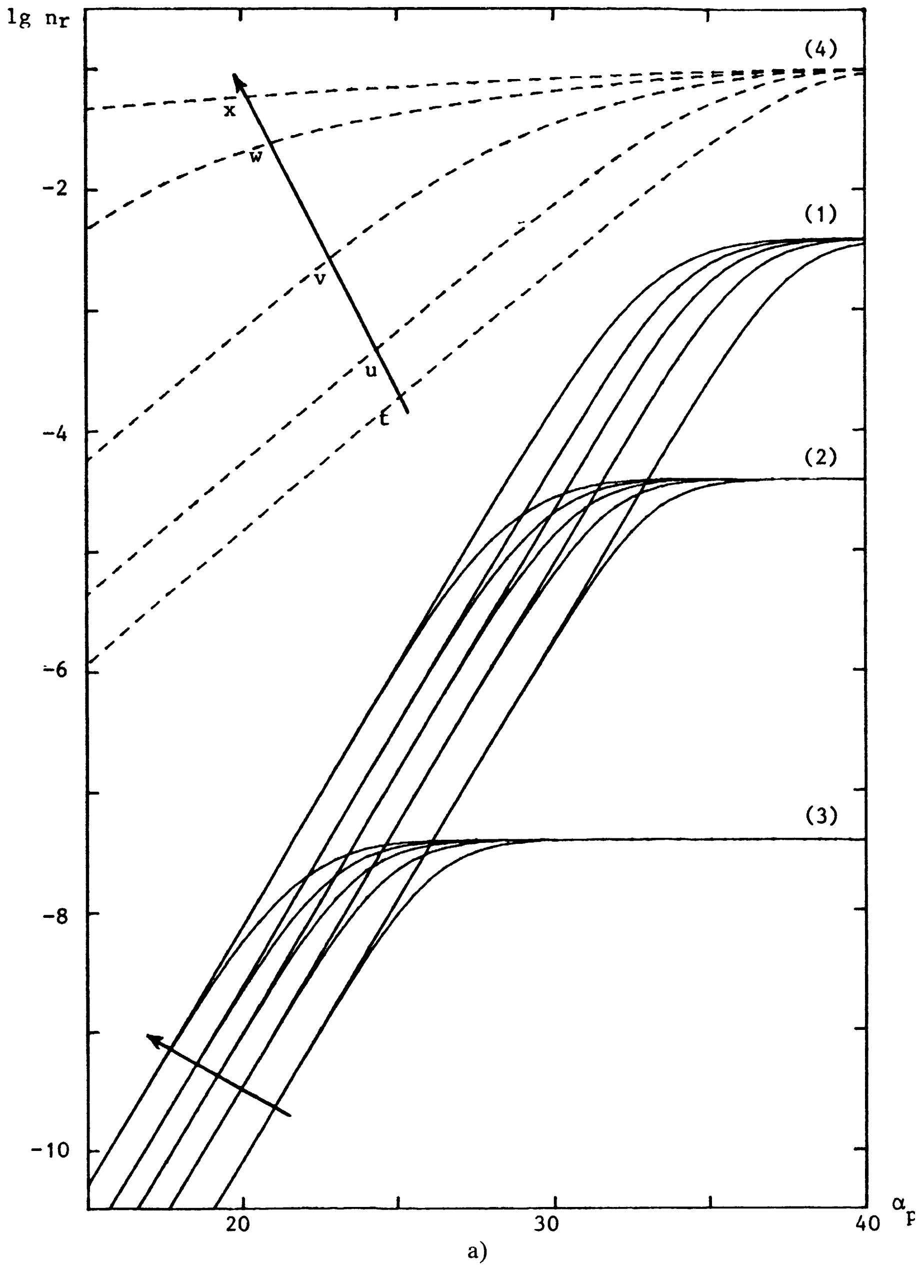

Fig. 3. — lg n_r *versus* α_p for $\eta_2 = 40$ ($\Phi_2 = 1.04$ eV for $T = 300$ K). Arrows indicate increasing $\delta\eta$: (t) 4×10^{-3} ; (u) 4 ; (v) 10 ; (w) 20 ; (x) 40. 3a (———) families (1), (2), (3) : $s = 0.1$; 10^{-3} ; 10^{-6} ; and $q = 1.04$; (----) family (4) : $s = 0.1$; $q = 10^6$ (small compensation). 3b (----) part of family (4) already drawn in figure 3a (———) family (5) : $s = 10^{-6}$; $q = 10^6$. The second ordinate scaling on the left indicates the relative quasi-Fermi level $-\Phi_{F_n}/kT$. Schematic drawing below abscissa visualizes band extensions associated with curves (t) to (x).

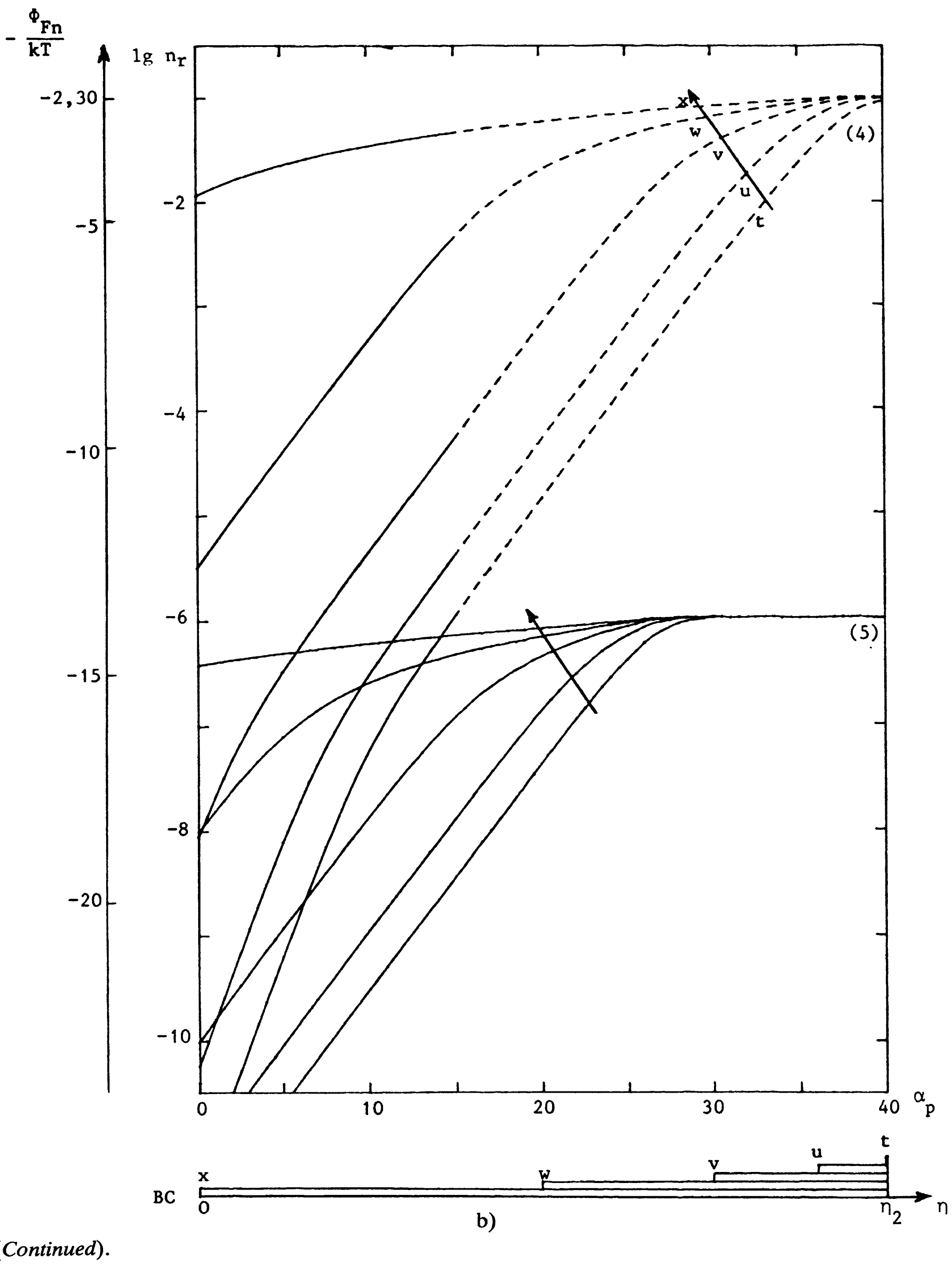

Fig. 3 (*Continued*).

within a band limited by any two potential energies E_1 and E_2, corresponding to depths Φ_1 and Φ_2 ($\Phi_2 > \Phi_1$). Equations (5a) and (5b) give then respectively :

$$N_d = A_d\, kT_0(e^{-\Phi_1/kT_0} - e^{-\Phi_2/kT_0}) \quad (6a)$$

$$N_d = A_d\, bkT(e^{-\eta_1/b} - e^{-\eta_2/b}) \quad (6b)$$

with $\eta_1 = \Phi_1/kT$ and $\eta_2 = \Phi_2/kT$. In the particular, and most commonly admitted situation of a band adjacent to the conduction band $\Phi_1 = 0$ and $\Phi_2 = \infty$.

But as (6) indicates a proportionality to T, apart from the T dependence of A_d, it leads immediately to a variation of the inter-site distance nearly proportional to $T^{-1/3}$. So that a large contraction of the material would result from a growth in temperature. In contrast, expressions (5a) and (6a) of Rose seem more appropriate, as thermal expansion effects are present only through A_d. Such a simple reasoning shows that, even if Pulfrey-type distributions could be advantageous, to describe, in particular, capture cross-sections varying exponentially with T, one should be aware that they lead to an unusual thermal expansion property.

Nevertheless, it must be noted that variations with T of the shape of the distribution, would not be an anomaly. It is well known that, in many semiconductors, the gap is a function of T which, in the simplest instances, takes the approximate form :

$$E_c - E_v = (E_c - E_v)_0 - \lambda_g T \tag{7}$$

λ_g being a parameter which, as an example amounts to 4×10^{-4} in Ge for $T > 200$ K, following Macfarlane *et al.* [5]. Such variations are commonly attributed to an increase in thermal vibration magnitudes, as well as to an enhancement of inter-atomic distances, resulting from solid expansion (see e.g. Blakemore [6]). But concerning the temperature induced distorsions of distributions of flaws, theoretical as well as experimental foundations seem to be few, though this notion is well stated. Thus for example, Debye and Conwell [7] consider a more general dependance $\Phi(N_d, T)$, for doped semi-conductors like Ge or Si. Moreover, in the domain of amorphous semi-conductors, a form like (7) can be adopted following Mott and Davis [8]. For n-type conduction these authors give an expression which can be transcribed as :

$$\Phi_F(T) = \Phi_F(0) - \lambda T .$$

But now it concerns electrons (holes) excited from localized states into extended states. When applied to the Davis and Mott model [9], where a narrow band of localized states exists in the gap and pins the Fermi energy near the centre of the gap, this relation clearly applies for the depth of any of these states. Thus it appears that in the formulation (5a) of Rose, some dependence $\Phi(T)$ with T can be postulated. With a linear variation, equation (5a) becomes :

$$dN_d = A_d \exp\left(\frac{\lambda}{k}\frac{T}{T_0}\right) \exp\left(-\frac{\Phi}{kT_0}\right) d\Phi .$$

In such a case, and provided that $\lambda T/kT_0 \ll 1$, a linear dilatation of the material is liable to hold.

3.2 CALCULATION OF FREE ELECTRON DENSITIES. — Introducing equations (5a) or (5b) instead of simply A_d into equation (3) yields immediately : either to

$$d\left(\frac{n_d}{N_c}\right) = \frac{A_d}{N_c} \frac{\exp\left(-\dfrac{\Phi}{kT_0}\right) d\Phi}{1 + \dfrac{n}{N_c}\exp\left(\dfrac{\Phi}{kT} - \alpha_p\right)} \tag{8a}$$

or to

$$d\left(\frac{n_d}{N_c}\right) = \frac{A_d}{N_c} \frac{\exp\left(-\dfrac{\Phi}{bkT}\right) d\Phi}{1 + \dfrac{n}{N_c}\exp\left(\dfrac{\Phi}{kT} - \alpha_p\right)} . \tag{8b}$$

Before contriving a fair method of integration, it can be remarked that equation (8a) reduces to equation (8b), if a parameter $b = T_0/T$ is introduced in it. Thus, they differ only through the fact that b is a function of T in the former equation, and a constant in the latter. Their integration can then be treated in the same way, for constant temperature.

Now, in order to integrate, we take as a new variable :

$$v = \left(\frac{N_c}{n}\right)^{1/b} \exp\left(-\frac{\eta - \alpha_p}{b}\right) . \tag{9}$$

Hence, equation (8b) becomes :

$$\frac{n_d}{N_c} = K_b\left(e^{-\frac{\eta_1 - \alpha_p}{b}} - e^{-\frac{\eta_2 - \alpha_p}{b}}\right) + + K_b \left(\frac{n}{N_c}\right)^{1/b} \int_{v_1}^{v_2} \frac{dv}{1 + v^b} \tag{10}$$

with $K_b = A_d\, bkT\, e^{-\alpha_p/b}/N_c$.

3.2.1 *Resolution for some simple Pulfrey-type distributions.* — Equation (10) shows that the remaining quadrature is straightforward for the particular values of b : $b = 1$, $b = 2$ and $b = 3$. Then, the following results obtain.

(a1) For $b = 1$ and with $K_1 = \dfrac{A_d\, kT\, e^{-\alpha_p}}{N_c}$, which parameter reduces to $s\, e^{-\alpha_p}$ for an infinite distribution starting from the conduction band edge, the density of free carriers is given by :

$$n_r + \frac{s}{q} = K_1\left(e^{-(\eta_1 - \alpha_p)} - e^{-(\eta_2 - \alpha_p)} - n_r \ln \frac{e^{-(\eta_1 - \alpha_p)} + n_r}{e^{-(\eta_2 - \alpha_p)} + n_r}\right) . \tag{11a}$$

When $\eta_1 = 0$ and $\eta_2 = +\infty$, this equation becomes :

$$n_r + \frac{s}{q} = s(1 - n_r\, e^{-\alpha_p} \ln(1 + n_r^{-1} e^{\alpha_p})) . \tag{11b}$$

As $n_r^{-1} \gg 1$, and $\alpha_p > \ln n_r$ in order that PF regime exists, it approximates to :

$$n_r + \frac{s}{q} = s(1 - n_r \, e^{-\alpha_p} (\alpha_p - \ln n_r)) . \tag{11c}$$

(a2) For $b = 2$, and with $K_2 = \frac{2 A_d kT}{N_c} e^{-\alpha_p/2}$, the equation for n_r is :

$$n_r + \frac{s}{q} = K_2 \left(e^{-\frac{\eta_1 - \alpha_p}{2}} - e^{-\frac{\eta_2 - \alpha_p}{2}} - n_r^{1/2} \left(\tan^{-1} \left(\frac{e^{-(\eta_1 - \alpha_p)}}{n_r} \right)^{1/2} - \tan^{-1} \left(\frac{e^{-(\eta_2 - \alpha_p)}}{n_r} \right)^{1/2} \right) \right) . \tag{12a}$$

Again, for $\eta_1 = 0$ and $\eta_2 = +\infty$, it becomes :

$$n_r + \frac{s}{q} = s(1 - n_r^{1/2} e^{-\alpha_p/2} \tan^{-1}(n_r^{-1} e^{\alpha_p})^{1/2}) . \tag{12b}$$

As $n_r \ll 1$, this latter equation is resolved readily and gives :

$$n_r = s^2 \frac{\pi^2}{16} e^{-\alpha_p} \left(\sqrt{1 + 16 \frac{q-1}{q} \frac{e^{\alpha_p}}{s \pi^2}} - 1 \right)^2 . \tag{12c}$$

(a3) For $b = 3$, and with $K_3 = \frac{3 A_d kT}{N_c} e^{-\alpha_p/3}$, the related equation is :

$$n_r + \frac{s}{q} = K_3(w_1 - w_2) + \frac{K_3}{3} n_r^{1/3} \ln \left(\frac{w_2 + n_r^{1/3}}{w_1 + n_r^{1/3}} \sqrt{\frac{n_r^{-2/3} w_1^2 - n_r^{-1/3} w_1 + 1}{n_r^{-2/3} w_2^2 - n_r^{-1/3} w_2 + 1}} \right) + $$
$$+ \frac{K_3}{\sqrt{3}} n_r^{1/3} \left(\tan^{-1} \frac{2 n_r^{-1/3} w_2 - 1}{\sqrt{3}} - \tan^{-1} \frac{2 n_r^{-1/3} w_1 - 1}{\sqrt{3}} \right) \tag{13a}$$

with $w_1 = \exp\left(-\frac{\eta_1 - \alpha_p}{3} \right)$ and $w_2 = \exp\left(-\frac{\eta_2 - \alpha_p}{3} \right)$.

This equation simplifies when $\eta_1 = 0$ and $\eta_2 = +\infty$, and gives :

$$n_r + \frac{s}{q} = s \left(1 - \frac{1}{3} n_r^{1/3} e^{-\alpha_p/3} \left(\ln (1 + (n_r^{-1} e^{\alpha_p})^{1/3}) \sqrt{(n_r^{-1} e^{\alpha_p})^{2/3} - (n_r^{-1} e^{\alpha_p})^{1/3} + 1} \right) - \right.$$
$$\left. - \frac{1}{\sqrt{3}} n_r^{1/3} e^{-\alpha_p/3} \left(\frac{\pi}{6} + \tan^{-1} \frac{2(n_r^{-1} e^{\alpha_p})^{1/3} - 1}{\sqrt{3}} \right) \right) . \tag{13b}$$

If the Pulfrey's repartition function should hold, equations (11) to (13) should give the right solutions, but only for very few ranges of the distribution stretching. Now it appears that $b = 1$ is a value which makes the density of sites (5b) to fall off rapidly, i.e. to 10^{-4} of the initial amount within the range $9.2\ kT$. Then it can be appropriate only for very narrow site distributions, typically for restricted band tails in amorphous materials. A value $b = 3$ could be more adequate for some insulating materials, although they would certainly need $b > 3$.

3.2.2 *Research of a general solution in T, for a Rose-type distribution.* — As Rose's law could be preferred to Pulfrey-type law, the above expressions (11) to (13) remain established only for the temperatures $T = T_0$, $T = T_0/2$, and $T = T_0/3$. It can be remarked here that Rose estimated that T_0 should amount to about 10^3 K. Thus, in the present development, this would correspond to $b \cong 3$ at nearly room temperature.

Now, their would be needed for a general solution, valuable whatever T. Such a solution does not seem to exist, at least when Fermi-Dirac function is used. Instead, a lot of solutions can theoretically be found, each for a suitably defined relative temperature $b^{-1} = T/T_0$. Because the remaining integral in (10) can receive analytical solutions for any rational value of b :

$$b = \frac{c}{d}$$

c and d being integers. Letting $v^b = -t^c$, transforms (10) into the integrable form :

$$\int \frac{dv}{1+v^b} = -c \int \frac{(-t)^{d-1}\,dt}{1-t^c} . \tag{14}$$

However, solutions become somewhat untractable for large c and d values. Nevertheless it stands that, theoretically speaking, determination of $n_r(T)$ is achievable for a large set of T (and T_0). But a discrete variation with T, determined through as many equations as many b values involved, is substituted for the usual continuous variation.

Thus, expressed in terms of b, our model would lead to a general law $n_r(b, s, q, F)$, known through a set of numerical values. Moreover T_0 being a constant characteristic of the investigated material, or at least of the trap « freezing in » temperature, it must be known for any actual application.

The above development reveals so awkward to handle that it can be asked whether a direct computation of equation (10) should not be more advantagious, after an appropriate choice of T_0. Yet it constitutes a throughrough analysis of what is possible to do with an exponential distribution, when the use of Fermi-Dirac statistics is not ruled out by « at hand » hypotheses, as did Rose and many other later authors.

3.3 SIMULATED BEHAVIOUR. — Simulation was performed in terms of the applied field only. Two cases of donor distributions are treated. The case investigated mostly is that where $\eta_1 = 0$ and $\eta_2 = +\infty$, b being chosen equal to 1, 2 and 3. The other case corresponds to $\eta_1 = 8$ and $\eta_2 = +\infty$, b being taken equal to 3. These are represented in figure 4 which, as seen above, is interpretable differently following the chosen formulation of the exponential distribution. In the approach of Pulfrey *et al.*, the three given values of b allows to concretize the influence upon $n_r(\alpha_p)$ of the distribution stretching. In that of Rose, these same values of b, and hence the same curves, examplify only the behaviour resulting from a given exponential distribution at the three relative temperatures $b^{-1} = 1$, 1/2 and 1/3.

Figure 4 involves mainly three types of curves. The first represents (curves (1), (2) and (3)) an example of the effect of a variation of b, for $s = 10^{-1}$ and $q = 1.04$ (nearly full compensation). The second type is a family for which $b = 3$ (curves (3) to (3d)) and $q = 1.04$, generated by a choice of 5 values of s, respectively 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4} and 10^{-6}. These curves show that the overall variation of $n_r(\alpha_p)$, which is the greater the higher the compensation, decreases with s. The height of the plateau of saturation reduces accordingly, as it amounts to $s - \frac{s}{q}$. The third type of curves is examplified by curve (3e) which shows that, even when s is high, the overall variation of n_r is greatly reduced when compensation decreases ($q = 10.4$).

The general tendency of curve evolution, when s and q are modified, is as follows. At constant q, a decrease in s results simply in an oblique sliding down of curves, parallel to their linear initial parts. This fact could already to observed with curves of figure 3a, when a band with a uniform distribution was concerned. In order to bring out further the degree of similarity in behaviour between exponential and uniform distributions, two more kinds of curves were drawn. First we built a curve (dashes) generated by a uniform band of depth 14 kT (with $s = 0.1$ and $q = 1.04$), adjacent to conduction band. This curve remains very close to curve (3) until the onset of saturation. Secondly, we drew a family (dotted curves) deduced directly from the family of curves (3), by taking simply $\eta_1 = 8$ instead of $\eta_1 = 0$. This results only in a curve shifting along the α_p axis, as in figure 2. At constant s, any enhancement of q is equivalent to a stretching of the α_p scaling in the left direction. The observed reduction of the overall variation of n_r is contributed for these kinds of displacements, originating in s or q modifications.

The physical explanation of these facts is involved but, fundamentally, a high compensation « consumes » almost all the electrons thermally excited out from the shallower donors, which are also the most numerous. A detailed interpretation of behaviour observed in figure 4 would need, every time, a knowledge of the pseudo-Fermi level position. Now, this figure displays also, on a second ordinate scaling, the relative variations Φ_{F_n}/kT of this level. To take one example only, let us remark that, as far as a band contiguous to conduction band is dealt with, the position of Φ_{F_n} with no field applied remains practically unchanged, when s is decreased from 10^{-1} to 10^{-4} ($q = 1.04$). So, the density $n_r(0)$ of free electrons, originating from thermal excitation only, is practically constant. Consequently, every N_d lowering entails a reduction in the density of sites that remain filled. Their subsequent emptying by the field brings then, in proportion, less further free electrons and the difference between $n_r(\infty)$ and $n_r(0)$ is reduced.

The above results allow to conclude that, when distributions starting from the conduction band edge are concerned, only those with slow enough decrement ($b \geqslant 3$) are liable to bring about a well characterized PF regime. In addition, two more conditions are prescribed, except eventually for very large b : a high compensation must be achieved, together with a high total donor density (family of curves (3)). Hence, it looks very improbable for such donor distributions, to be effectively invoked when a PF regime is stated as a possible interpretation of permanent currents. Conditions to obtain a well-

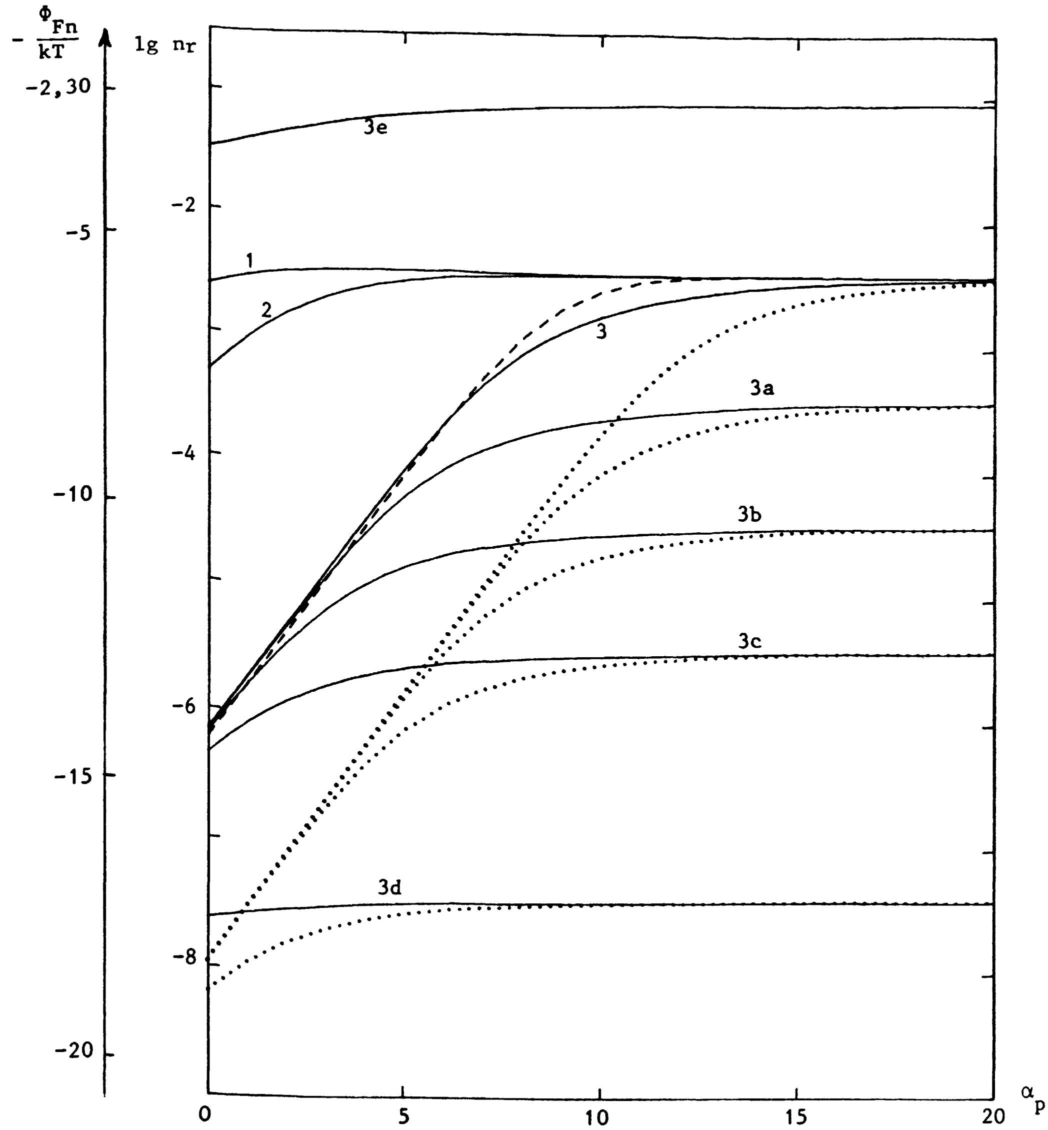

Fig. 4. — Variations of n_r *versus* α_p for exponential distributions of donors. $\eta_2 = \infty$. (———) $\eta_1 = 0$ band adjacent to conduction band.

s	0.1			10^{-2}	10^{-3}	10^{-4}	10^{-6}	0.1
q	1.04							10.4
b	1	2	3					
curve labelling	(1)	(2)	(3)	(3a)	(3b)	(3c)	(3d)	(3e)

(....) band with $\eta_1 = 8$ and same parameters as curves (3a)-(3d) ; (----) uniform distribution from 0 to 14 kT: $s = 0.1$; $q = 1.04$.

shaped PF regime with an exponential distribution are less severe when the band begins at a depth $\eta_1 \neq 0$. But such a case is hardly considered in literature for, when a band is disconnected from conduction band, it is most often regarded as a uniform band.

4. Generalization for any kind of distribution.

Calculations performed in the preceding subsections can be generalized, either exactly or approximately, whatever the shape of the distribution. As a matter of interest, the simple case of two separated bands of

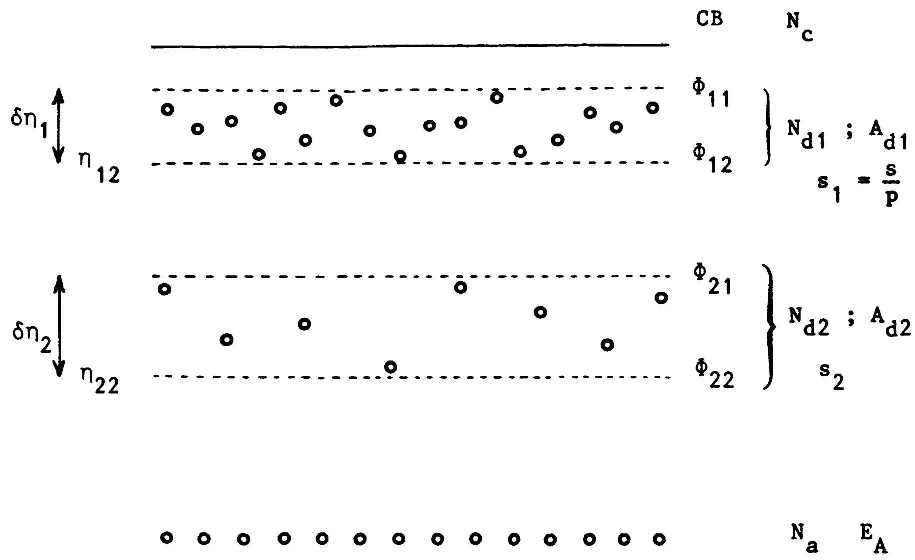

Fig. 5. — Schematic representation of a uniform compensated donor distribution splitted in two bands.

donors is first treated exactly. Next, the case of a continuous arbitrarily shaped distribution is developed, with the help of a suitable approximation.

4.1 DONORS UNIFORMLY DISTRIBUTED WITHIN TWO BANDS. — Donors are supposed to be shared within two arbitrary disconnected bands, in which a uniform distribution prevails (Fig. 5). In the shallower band, lying in between Φ_{11} and Φ_{12} ($\Phi_{11} < \Phi_{12}$), the constant donor density per unit energy is A_{d1}. It amounts to A_{d2} in the deeper band limited by Φ_{21} and Φ_{22} ($\Phi_{21} < \Phi_{22}$). Calculations of paragraph 2 above apply then readily for the two bands, and one obtains immediately :

$$n_r + \frac{s}{q} = \ln \left(\left(\frac{e^{-(\eta_{11} - \alpha_p)} + n_r}{e^{-(\eta_{12} - \alpha_p)} + n_r} \right)^{\frac{s_1}{\eta_{12} - \eta_{11}}} \times \right. \left. \times \left(\frac{e^{-(\eta_{21} - \alpha_p)} + n_r}{e^{-(\eta_{22} - \alpha_p)} + n_r} \right)^{\frac{s_2}{\eta_{22} - \eta_{21}}} \right) . \quad (15a)$$

In this equation :

$$s_1 = \frac{N_{d1}}{N_c} = \frac{A_{d1}}{N_c} (\Phi_{12} - \Phi_{11}) ;$$

$$s_2 = \frac{N_{d2}}{N_c} = \frac{A_{d2}}{N_c} (\Phi_{22} - \Phi_{21}) ;$$

$$s = s_1 + s_2 = \frac{N_d}{N_c} ; \text{ and } N_d = N_{d1} + N_{d2} .$$

To make easier the analysis of behaviours resulting from this equation we transform it into :

$$n_r + \frac{s}{q} = \frac{s}{p} \ln \left(\left(\frac{e^{-(\eta_{11} - \alpha_p)} + n_r}{e^{-(\eta_{12} - \alpha_p)} + n_r} \right)^{\frac{1}{\delta\eta_1}} \times \right. \left. \times \left(\frac{e^{-(\eta_{21} - \alpha_p)} + n_r}{e^{-(\eta_{22} - \alpha_p)} + n_r} \right)^{\frac{p-1}{\delta\eta_2}} \right) \quad (15b)$$

where $\delta\eta_1 = \eta_{12} - \eta_{11}$; $\delta\eta_2 = \eta_{22} - \eta_{21}$; and $p = s/s_1$ a dimensionless parameter characterizing the fraction of total donor density present in the first band ($p > 1$).

Figure 6 gives some examples of curves obtainable with the above model, in a (lg n_r, α_p) plot, when the first band is contiguous to conduction band. Here, the principal aim is mainly to try to take out the most characteristic features of this system. The overall donor density is supposed relatively high ($s = 10^{-1}$). The relative proportions of the densities in the two bands $N_{d2}/N_{d1} = s_2/s_1 = p - 1$, are modified through p, at constant s. The (second) deeper band keeps a constant width $\delta\eta_2 = 2$. Its maximum depth is fixed to $\eta_{22} = 40$, except for curves (b) for which $\eta_{22} = 30$. The width of the (first) shallower band is more often taken as $\eta_{12} = 3$. Yet, larger values are used whenever the effect of band widening is studied.

It is to be noticed that the final levelling, at large α_p, is the now well-known saturation levelling of the deeper band. Let us recall that its magnitude is equal to $s - s/q$, so that it moves downward and widens as s decreases (see [1], Fig. 3).

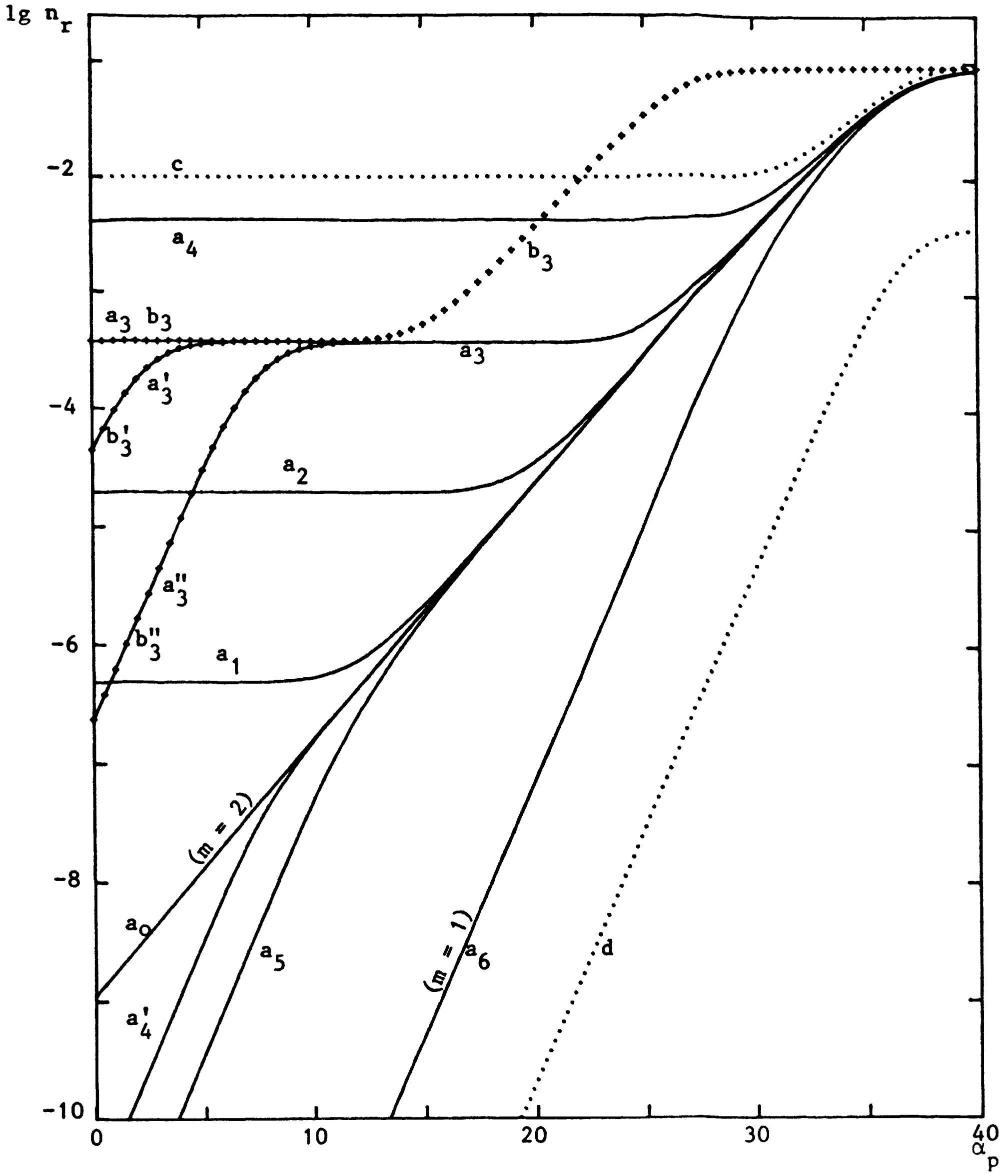

Fig. 6. — Variations of n_r *versus* α_p for a double uniform distribution $s = 0.1$; $\eta_{12} = \delta\eta_1$; $\delta\eta_2 = 2$. Family a : $\eta_{22} = 40$. Family b : $\eta_{22} = 30$. For curves (c) and (d) : $\eta_{22} = 40$.

$\delta\eta_1$	3							9	15		3	
p	10	9.9995	9.98	9.63	7	10.0005	40	9.63		10		
q	10										10^5	1.04
curve labelling	(a_0)	(a_1)	(a_2)	(a_3), (b_3)	(a_4)	(a_5)	(a_6)	(a'_3), (b'_3)	(a''_3), (b''_3)	(a'_4)	(c)	(d)

4.1.1 *Influence of a variation of the relative densities* $\frac{s_2}{s_1}$. — Curves drawn in full line in the figure result from p variations, the other parameters being held constant. They show that an initial levelling can occur or not following the chosen value of the ratio p/q. An extended simulation put forward that a threshold value $p/q = 1$ separates curves displaying an initial plateau from that which have none. Curve (a_0) is then obtained which slope corresponds to $m = 2$. When $p/q < 1$, this plateau occurs, and its height is a decreasing function of p/q, very sensitive to the ratio variations in the vicinity of 1. Conversely, when $p/q > 1$ the related curves display two linear parts, the initial straight line getting a slope parameter $m = 1$. Any ratio enhencement results in a right hand side shift of this initial line (curves (a_4'), (a_5) and (a_6)). Curve (a_6), on which the straight line with $m = 1$ remains alone, has practically overtaken a limiting position, actually reached when $p/q \gtrsim 40$.

In order to precise further conditions for the abrupt changing, occurring at the threshold, approximations that can be made on equation (15b) were investigated. Suppose that a rough estimation of n_r on any initial plateau is made for, say $\alpha_p = 10$. Equation (15b) writes then :

$$n_r + \frac{s}{q} = \frac{s}{p} \ln \left(\left(\frac{e^{10} + n_r}{e^7 + n_r} \right)^{1/3} \left(\frac{e^{-28} + n_r}{e^{-30} + n_r} \right)^{\frac{p-1}{2}} \right)$$

$$= \frac{s}{p} \ln (I_1 I_2) \qquad (16)$$

As $10^{-1} > n_r > 10^{-8}$, I_2 is very close to 1, while I_1 approaches e. It results that :

$$n_r \cong \frac{s}{p} \left(1 - \frac{p}{q} \right) = s_1 \left(1 - \frac{p}{q} \right) . \qquad (17)$$

To take an example, the initial value of n_r in the particular case of curve (a_2) is given by :

$$n_r = 0{,}1 \left(\frac{1}{9.98} - \frac{1}{10} \right) = 2 \times 10^{-5} .$$

It appears then that an initial levelling can exist under the condition $s_1 > \frac{s}{q}$. This means physically that $N_{d1} > N_a$. Given the respective band positions, the first band alone supplies practically all the electrons that filled the acceptors. Condition $N_{d1} > N_a$ is then simply that which ensures that free electrons, coming from the first band, can exist in conduction band. As the former is a very narrow band, the enclosed donor sites are almost entirely empty. Thus a low field applied is nearly unefficient. When it becomes large enough some deep donors begin to tempty, and the increasing part of curves sets in.

When $p/q > 1$, shallow donors are not sufficiently numerous to fill completely the acceptor sites. Fermi level deepens, and a weak electron density only is present in conduction band. This is why the related curves are very close to curves given by a deep band alone.

The distance apart the initial and the final plateaus is independent of s, for :

$$\Delta(\lg n_r) = \lg \frac{1 - \frac{1}{q}}{\frac{1}{p} - \frac{1}{q}} = \lg \left(1 + \frac{N_{d2}}{N_{d1} - N_a} \right) .$$

It depends only on p and q, that is finally on the ratio of the deep donor density to the density of shallow donors in excess on acceptor density.

We built, in addition, curve (b_3) corresponding to $\eta_{22} = 30$. The final saturation is shifted accordingly, while the initial levelling remains unchanged, as it depends only on shallow donors.

Moreover we drew, as a simple illustration, the effect of a variation of q. Insofar as typification of curves, with or without an initial plateau, is only dependent on p/q, p was given the value $p = 10$. So, curves (c) and (d) are obtained for $q = 10^5$ and $q = 1.04$ respectively. They must be brought together with curve (a_0) for which $q = 10$.

4.1.2 *Influence of the shallower band width.* — To get a somewhat deeper insight into the subject, we examined the effect of a variation of width $\delta\eta_1$ of the shallower band, the relative densities $s_2/s_1 = p - 1$ being held constant as well as s ($s = 0.1$).

It is then observed that enlarging the band makes an initial ascending line to appear, which slope corresponds to $m = 1$. This straight line shifts toward right hand side as $\delta\eta_1$ increases (curves : (a_3') for $\delta\eta_1 = 9$; (a_3'') for $\delta\eta_1 = 15$). The initial levelling is reduced accordingly.

As a final remark, let us indicate that curve (a_0), obtained with $\delta\eta_1 = 3$ and $p/q = 1$ is not of a special kind which would display one straight line only, with slope parameter $m = 2$. Because as a matter of fact, curve (a_4') results when $\delta\eta_1 = 15$, this curve being akin to curves (a_1) to (a_6).

4.1.3 *Conclusive comments on the model.* — The account above allowed to put forward some important features deriving from the double-band model, with one band adhering to conduction band. In particular, this model brought a new way of interpretation of curves displaying an initial levelling (ohmic regime) followed by an « original » PF regime ($m = 2$). Now, it is well known that many authors tried to find theoretical formulations of such a kind of behaviour, in terms of PF effect. Some introduced for that corrections of the basic formulation through a three dimensional PF effect (Hartke, [10] ; Hill, [11] ; Ieda *et al.*, [12] ; Connell *et al.*, [13]). While others brought along additional hypotheses ; for example the existence of free carriers excited from two flaw species : coulombic sites on the one hand, and any kind of traps undistortable by the field on the other hand. Then, under the condition that with no field applied, the latter provides a larger amount of conduction electrons than the former, an initial ohmic conductivity prevails (Hirai and Nakada, [14]).

In our model where donors and acceptors are exclusively introduced, only the « original » PF regime can be associated with this initial regime. However, it is certainly possible to find conditions where such an association can hold with any other kind of PF regime ($1 \leq m \leq 2$). For it is believed that it would suffice to add to coulombic sites some kind of traps insensitive to the field, in order to shift the Fermi level to a suitable position. This is the point of view of Mark and Hartman [15] that we admit provisionally as we did not yet perform calculations corresponding to the related model.

4.2 LEVEL DISTRIBUTION ACCORDING TO AN ARBITRARY FUNCTION. — It is possible to determine in a convenient approximate manner, and with the help of computer calculation, theoretical $n_r(\alpha_p)$ variations corresponding to any kind of donor distribution. The related function giving the density of sites per unit energy can be written as :

$$A_d\, f(\Phi) \qquad (18)$$

where f is a well-behaved function, which remains bounded over any suitable interval in Φ.

Now, the exact solution $n_r(\alpha_p)$ can be derived readily from calculations of the preceding subsection. It is sufficient for that to use the geometrical definition of integrals, that is to replace integration associated with $f(\Phi)$ by a discrete summation over an infinitely great number of adjacent rectangular areas, dΦ wide. Calculation reduces then to a direct generalization of equation (15). But the infinite series so obtained is quite untractable. Fortunately this can be reduced to few terms only, without entailing large deviations, owing to the relative insensitivity of $n_r(\alpha_p)$ towards the effective shape of the distribution. For, it was shown in figure 4 that an exponential distribution could be roughly approximated with only one uniform band (curves 3, 4), except in the saturation region. Some testing simulations allowed us to verify that a set of two or three bands is sufficient to ensure a convenient fitting in this region (maximum local departure < 20 %).

Consider then figure 7 in which the area under an arbitrarily shaped $f(\Phi)$ function was approximated by a few joined rectangular slabs, of equal thickness

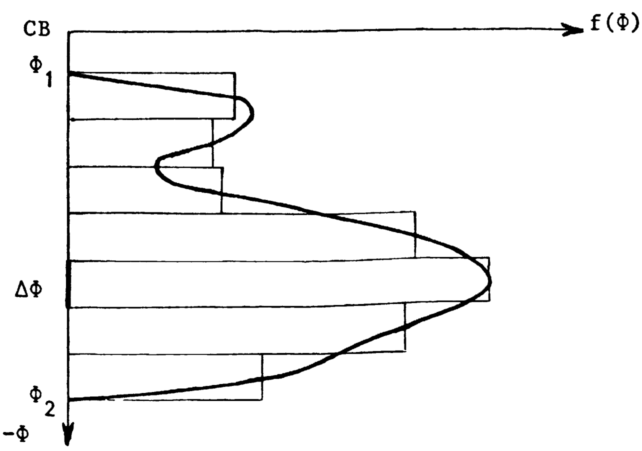

Fig. 7. — Any shaped donor distribution.

$\Delta\Phi$. Each area represents a density of sites, which can be written for the ν-th rectangle :

$$N_{d\nu} = A_d\, f\left(\Phi_1 + \left(\nu - \frac{1}{2}\right)\Delta\Phi\right)\Delta\Phi .$$

Hence, the total density of sites is given by :

$$N_d = A_d(\Phi_2 - \Phi_1)\sum_{\nu=1}^{N} f\left(\Phi_1 + \left(\nu - \frac{1}{2}\right)\Delta\Phi\right) \qquad (19)$$

where : Φ_1 and Φ_2 are the limiting depths of the distribution. They are generally zeros of $f(\Phi)$. A straightforward generalization of (15) leads to :

$$n_r + \frac{s}{q} = \ln\left(\prod_{\nu=1}^{N}\left(\frac{e^{\alpha_p - (\nu-1)\Delta\eta} + n_r}{e^{\alpha_p - \nu\Delta\eta} + n_r}\right)^{\frac{s_\nu}{\delta\eta}}\right) \qquad (20)$$

with $s_\nu = \dfrac{N_{d\nu}}{N_c}$; $s = \dfrac{N_d}{N_c}$ and $\Delta\eta = \dfrac{\Delta\Phi}{kT}$.

As N can be limited to a few units, equation (20) becomes practically as easily tractable as (15).

So as to emphasize how much this approximated method of resolution can be relevant let us recall that, when $f(\Phi)$ is a power function, with either an integer or a fractional exponent, the integrals of differential equations derived accordingly from (3) are Dirac functions, taken over a finite interval. Some of them are tabulated. Moreover, series expansions have been proposed for example by Sommerfeld [16], and then by Rhodes [17] or Dingle [18]. But these processes of calculation do not seem to bring, as easily as does equation (20), a solution of equations of type (3).

We did not attempt in the present work any simulation of the approximated method of resolution of (3). Namely, we did not try to precise further the numerical divergence with regard to the exact result, issuing from the choice of a more or less reduced number of slabs.

5. Conclusion.

The above developments showed that it was possible to obtain some mathematical expressions, rather easily tractable on a numerical view-point, when Fermi-Dirac statistics is used. For the most conventional repartitions, either uniform or exponential, exact solutions could be found. It was also shown throughout, that some expression of exponential distribution, found in literature, is hardly admissible. It was established moreover that calculation remains tractable for any kind of distribution if an approximate formulation is used. Moreover, we put forward an alternative interpretation of currents, often found experimentally, which admit an initial ohmic regime followed by a PF regime.

It must be emphasized that, as far as we know it, very few attemps have been made before to give such a general treatment of site distributions. The work of Pulfrey *et al.* for example, or that of Viger *et al.* [19] based uppon a Rose-type distribution, can be cited among the exceptions. The scarcity of such treatments in literature seems attributable to two main reasons. First, the general tendency, quite natural before the advent of computational facilities, was to reduce at a maximum the calculation complexity, by a fair choice of suitable simplifying assumptions. This is typically the case for Boltzmann function which, introduced early on, leads always to very simple equations admitting graphical straightforward representations. The second reason is that the greatest wealth of information, contained into Fermi-Dirac statistics, seems to have remained largely under-estimated, perhaps sometimes unsuspected, as it was shown about saturation [1], though authors like Blakemore [6] put it forward throughout.

At the outlet, the thourough investigation presented above leads to ask the following important question. Is an experimentalist provided with an available means, getting him a reasonable ability to aknowledge some distribution of sites in the gap. Our response is twice. Firstly, as we saw that different shapes of distribution can get very close forms for $n_r(\alpha_p)$, a major difficulty would arise in distinguishing them. Especially, because the range of larger divergence is in the vicinity of saturation. Now, this saturation does not seem, as yet, to have been found experimentally. So that attempts of fitting data, with an apparently convenient model, should not be considered more than plausible ways of interpretation. Secondly, as we shall see in a following paper, the same difficulty arises from Arrhenius diagrams. It will be shown there that such plots does not bring undoubtless proofs of effectiveness of any energetic site distributions in the gap. This will probably be the most prominant consequence of our calculations, and of the assigned simulations, developed along the present article.

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