## Chapter 2

# Physics of Charged Dielectrics: Mobility and Charge Trapping

### 2.1. Introduction

For the lay person, an insulating material is a material which does not conduct electricity. In fact, however, it is necessary to analyse this assertion more closely.

The conductivity of a material is defined by:

$$\sigma = ne\mu \qquad [2.1]$$

where n is the density of the charge carriers and $\mu$ the mobility.

Table 2.1 gives the values, at room temperature, of the conductivity and mobility of the electrons in high purity copper and alumina (aluminum oxide). We note that there are 23 regions between the two conductivities, but the mobility is twice as high in alumina as in copper. These values, which could be surprising, are due to the fact that, from [2.1], alumina contains much less than an electron per $cm^3$ which is used for conduction while copper has about 4.5 x $10^{22}$ electrons per $cm^3$ used for conduction (Table 2.1).

Alumina has, therefore, a very weak conductivity because it has practically no free charges to conduct (and not because it is inept at conducting charges). For a

---

Chapter written by Guy BLAISE and Daniel TREHEUX.

pure material with a large band gap, we have, then, an insulating state, through lack of charge carriers.

For conduction to be observed in an insulator, we need to inject charges into it. Unlike a metal, the bulk of which remains neutral during conduction, an insulating material is thus charged. The injection of charges can be done in many different ways, as will be developed in later chapters of this book. Here, we mention, for example, irradiation (electronic, radiative, etc.), corona discharge, the application of an electrical constraint, and also mechanical or tribological ones.

When we manage to inject charges in a conduction band, the strong mobility of these charges (Table 2.1) is explained by the fact that the electron-electron interactions are reduced to nothing, as a result of the weak density of the free charges. In a perfect insulator, only the electron-phonon interaction remains to limit mobility. But, if the solid contains impurities, they will also reduce the mobility. This explains, as we shall see, the very important role which impurities take in the properties of insulators.

| | **Copper** | **Alumina** |
|---|---|---|
| $\sigma$ ($\Omega^{-1}$cm$^{-1}$) | $5.8.10^{5}$ | $10^{-18}$ |
| $\mu$ (cm$^{2}$.V$^{-1}$.s$^{-1}$) | 80 | 200 |
| n (e$^{-1}$ .cm$^{-3}$) | $4.5.10^{22}$ | $3.1.10^{-2}$ |

**Table 2.1.** *Conductivity $\sigma$ and mobility $\mu$ of pure monocrystalline copper and alumina*

## 2.2. Localization of a charge in an "ideally perfect" and pure polarizable medium

### 2.2.1. *Consideration of the polarization*

Polarization must be taken into account to describe the conduction properties of the dielectrics. The electric field which polarizes the medium is the coulomb field of the charge in motion in the conduction band.

Let us consider an electron introduced into the polarizable medium. It will interact with one of the electrons of the medium situated at a distance r. The potential energy of interaction for two electrons in the permittivity medium $\varepsilon$ is equal to $e^2/4\pi\varepsilon r$. Without polarization of the medium, this same interaction would be that produced in a vacuum, which is $e^2/4\pi\varepsilon_0 r$. The fact of polarizing the medium then lowers the potential energy by a quantity:

$$\Delta W = e^2/4\pi\varepsilon r - e^2/4\pi\varepsilon_0 r \qquad [2.2]$$

We notice that ΔW is negative and that, consequently, the electron is trapped in a potential well. This observation led Landau [LAN 69] to introduce the *polaron concept* in 1933, which will be further analyzed here from an electrostatic as well as a quantum point of view.

Let an electron of kinetic energy $W_e$ interact with an electron connected to the medium whose orbital frequency is $\omega_0 = \hbar/mr_0^2$, where m is the mass of the electron and $r_0$ its orbital extension. The time t taken by the electron to cover the distance r is equal to:

$$r = \sqrt{\frac{2W_e}{m}}\, t \qquad [2.3]$$

For an electron connected to the medium to be able to follow the displacement of the electron over the distance r, it must describe, numerous times, its trajectory during time t, that is to say: $t \geq 2\pi/\omega_0$. So only the electrons situated at a distance greater than $r_e$, defined by the condition $\omega_0 t = 2\pi$, could follow the motion of the electron. Expressing this condition and replacing $\omega_0$ by its value ($\omega_0 = \hbar/mr_0^2$), we get, from equation [2.3]:

$$r_e = 2\pi \frac{r_0^2}{\hbar} \sqrt{2mW_e} \qquad [2.4]$$

Only the electrons situated outside the sphere with radius $r_e$ centered on the moving electron could fit its motion by an electronic polarization.

Numerically, if the energy $W_e$ gets very big, $r_e$ tends to infinity and there is no electronic polarization, and the electron then moves like in vacuum (with permittivity $\varepsilon_0$). Conversely, if the energy of the electron tends to kT, at room temperature, $r_e$ tends to values lower than interatomic distances ($r_e$ less than 0.15 nm for frequencies $\omega_0$ of the order of $10^{15}$ to $10^{16}$ $s^{-1}$ in the UV): the electron then moves in a polarized medium of permittivity $\varepsilon(\omega_0)$.

The ionic polarization around the moving charge can be analyzed in the same way, but as the highest oscillation frequencies of ions ($\omega \cong 10^{12}$ $s^{-1}$) are situated in the IR, the radius associated with this polarization is much greater than $r_e$.

The variation of the polarization with distance is shown in Figure 2.1. Very near the moving charge ($r < r_e$) there is very little polarization and then the permittivity is that of vacuum $\varepsilon_0$. For $r_e < r < r_i$ the electronic polarization is the only one which plays a part. The ionic polarization will come into action for $r > r_i$ and, at lower and lower frequencies, we reach static permittivity $\varepsilon(0)$.

This variation of permittivity leads then, as seen in Chapter 1, to the formation of polarization charges with an opposite sign to the charge in motion. The result is negative interaction energy between the two types of charges, which leads to a confinement of the moving charge.

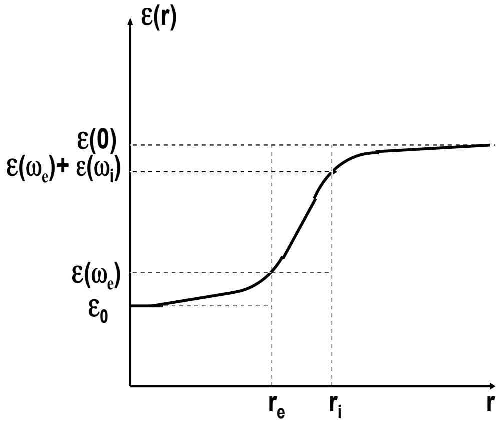


**Figure 2.1.** *Variation of the polarization as a function of the distance r*

### 2.2.2. *Coupling of a charge with a polarizable medium: electrostatic approach*

For simplicity, let us take a fixed charge q, surrounded by a permittivity medium $\varepsilon(r)$ varying radially between $\varepsilon_1 = \varepsilon(\infty)$ for $r < r_1$ and a maximum value $\varepsilon_2$ for $r > r_2$ (see Figure 2.2). Polarization charges appear whose density is given by equation [1.20]:

$$\rho_p(r) = -\mathrm{div}\vec{P}(r) = -\mathrm{div}(\varepsilon_0 \chi \vec{E}_M) = \varepsilon_0\, \varepsilon(r)\vec{E}(r)\ \mathrm{grad}\,[1/\varepsilon(r)] \qquad [2.5]$$

With $\vec{P}(r) = [\varepsilon(r) - \varepsilon_0]\vec{E}(r)$, polarization at distance r and $\vec{E}(r) = \frac{1}{4\pi\varepsilon(r)}\frac{q}{r^2}$, average field in r.

The polarization charges contained between two spheres of radii r and r+dr are:

$dQ_p(r) = 4\pi r^2 \rho_p(r)dr = 4\pi\, \varepsilon_0\varepsilon(r)\, r^2\vec{E}(r)\ d\,[1/\varepsilon(r)]$. It follows after integration:

$$Q_p(r) = \left[\frac{1}{\varepsilon(r)} - \frac{1}{\varepsilon 1}\right] q \qquad [2.6]$$

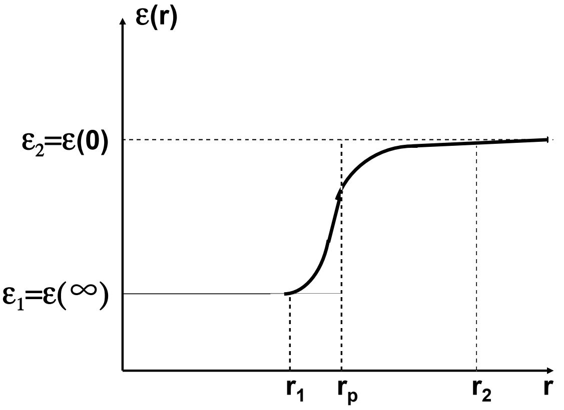


**Figure 2.2.** *Variation of the permittivity of the medium as a function of distance*

The potential energy resulting from the interaction between the charge and the polarization charges is then written as:

$$\mathrm{W}=\frac{q^2}{4\pi\varepsilon_0}\int_{r1}^{r2}\frac{\rho_p(r)}{r}4\pi r^2 dr=\frac{q^2}{4\pi}\int_{r1}^{r2}\frac{d[1/\varepsilon(r)]}{r} \qquad [2.7]$$

Integration by parts leads to:

$$\mathrm{W}=\frac{q^2}{4\pi}\left[\frac{1}{\varepsilon_2 r_2}-\frac{1}{\varepsilon_1 r_1}\right]+\frac{q^2}{4\pi}\int_{r1}^{r2}\frac{1}{\varepsilon(r)r^2}dr \qquad [2.8]$$

If $r_1$ and $r_2$ tend to a common value $r_p$, the second term tends to 0 and consequently:

$$\mathrm{W}=-\frac{q^2}{4\pi r_p}\left[\frac{1}{\varepsilon_1}-\frac{1}{\varepsilon_2}\right] \qquad [2.9]$$

This expression corresponds to the binding energy of the polaron defined by Landau, where $r_p$ is the radius of the polaron. We note that, the smaller $r_p$ is, the more the charge will be localized and the higher the binding energy.

### 2.2.3. *Coupling of a charge with a polarizable medium: quantum approach*

This approach is based on the polaronic concept introduced by Landau in the 1930s [LAN 69], and resumed later by Austin and Mott [AUS 69]. The idea stemmed from a study which expressed the interaction between a given charge q and the longitudinal optical vibrations of a network. In this quantum frame, the localization of an electronic charge (e) in a dielectric medium ensues from its coupling with different polarization fields, which develop:

– a field created by the electronic polarization in the domains of UV frequencies;

– a field stemming from the atomic vibrations (phonons) in the infrared;

– a static field created by the displacement of ions.

#### 2.2.3.1. *Coupling with the electronic polarization field*

Valence electrons are the quickest to react to the action of a field. The time constant, in the order of $10^{-15}$– $10^{-16}$ s, corresponds to the opposite of the orbital frequencies $\omega_{UV}^{-1}$ situated in the ultraviolet range. If the time taken by an electron to traverse the basic cell of the material is greater than $\omega_{UV}^{-1}$, we can consider that all the electrons of the medium can fit the motion of the electron perfectly. It implies that the electron has a kinetic energy less than 10eV. The electron then moves in a medium containing electronic dipoles which produce an electronic polarization field $\vec{P}_e$. Being in motion, the electron can then couple itself with this field, hence the confinement effect according to Landau. It moves at an average speed V, in an electronic permittivity medium $\varepsilon(\omega_e)$ where $\omega_e$ represents the electronic pulsation: it is the electronic polaron which is a very fluid pseudo-particle.

#### 2.2.3.2. *Coupling with the ionic polarization field*

The atomic vibration modes (phonons) of an ionic component are sources of a field. Taking the case of ions vibrating in phase opposition, we see that each couple of ions forms a dipole. When the dipoles are parallel to each other, the field is very intense and the coupling with the charge is very strong. This situation corresponds to the domain of atomic vibrations in IR frequencies $\left(\omega_{IR} \approx 10^{12} - 10^{13}\ s^{-1}\right)$. The result of this coupling is a lattice polaron: it is the usual quantum polaron described by Fröhlich [FRÖ 54], [FRÖ 62] which describes the coupling of a charge with a longitudinal optical phonon.

By definition, the quasi-particle formed by the charge in motion and the polarization charges which surround it in a radius rp form the polaron. The radius rp depends on the force of coupling. We can then understand that the polaron is affected by an effective mass m*, clearly greater than the mass m of the electron, and that its motion is very dependent on its radius rp.

The longitudinal waves respond at best to the solicitations of the field and consequently maintain a better coupling. Fröhlich uses the approximation of a coupling with only one optical mode of vibration, the dispersion being neglected. The expression for the infrared polarization is written:

$$\vec{P}_{IR} = \varepsilon_0 \left[ \frac{1}{\varepsilon(\infty)} - \frac{1}{\varepsilon(0)} \right] \vec{D} \qquad [2.10]$$

where $\vec{D}$ is the electric induction, $\varepsilon(\infty)$ the optical (electronic) permittivity and $\varepsilon(0)$ the static permittivity.

The total potential energy (potential energy of the charge carrier q surrounded by the polarization charge whilst taking into account the polarization energy of the surrounding medium) which ensues is, then:

$$W_p = - \frac{1}{8\pi} \left[ \frac{1}{\varepsilon(\infty)} - \frac{1}{\varepsilon(0)} \right] \frac{q^2}{r_p} \qquad [2.11]$$

We note that equation [2.11] has the same form as equation [2.9] deduced from the electrostatic approach.

The result is that, since $\varepsilon(\infty) << \varepsilon(0)$, the bonding effect is controlled by electronic permittivity, i.e. the permittivity of the medium very near the charge. Besides, the potential deduced from [2.11] does not preexist on all the sites likely to receive a polaron. It is only present at the site where the polaron is, and, in this way, we say that the charge “digs its own potential well”.

We distinguish, in fact, two types of situations:

– *a large polaron*: if the perturbation region around an electron is of an order of size greater than the lattice parameter, we talk about a large polaron. In this case, the electron-phonon interaction and the effective mass are both weak. The polaron conserves, in its potential well, a notable kinetic energy $W_c$ which must be added to the potential energy $W_p$: $W_t = W_c + W_p$. The radius of the large polaron is:

$$r_p = 2\pi^2 \frac{\varepsilon_p m}{\varepsilon_0 m^*} r_B \qquad [2.12]$$

with: $\frac{1}{\varepsilon_p} = \frac{1}{\varepsilon(\infty)} - \frac{1}{\varepsilon(0)}$ and $r_B$, Bohr radius.

For reasonable values, we find $r_P$ of the order of $20\, r_B$, and thus clearly greater than the interatomic distances. The large polaron especially affects the semiconductors.

– *a small polaron*: this is the case where the electron-phonon interaction is strong. The effective mass of the polaron is then very big. The kinetic energy of the electron localized in its potential well is weak and negligible to a first approximation ($W_t \approx W_p$), so $r_P$ becomes smaller than the interatomic distance. Its radius is estimated from a simple approximation of the optical phonon spectrum:

$$r_p \cong \frac{1}{2}\left(\frac{\pi}{6N}\right)^{1/3} \qquad [2.13]$$

where N is the number of centers per unit volume on which the polaron can form.

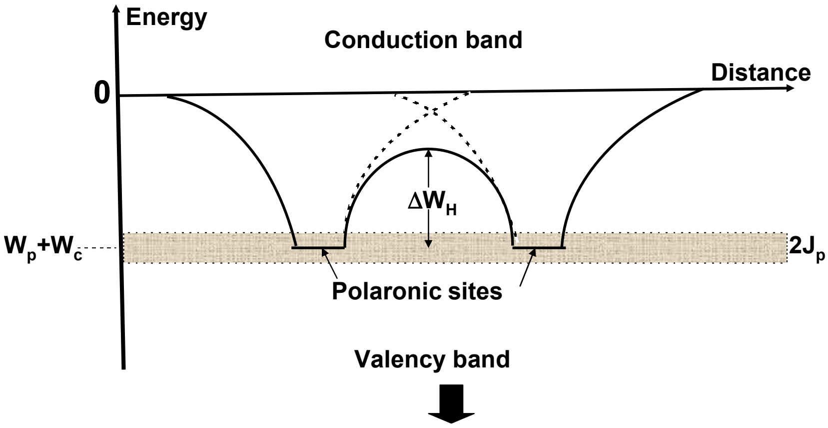


**Figure 2.3.** *Potential wells associated with the polaronic sites in a medium with uniform polarisability forming a polaronic band, shaded, of width* $2\, J_P$

In the case of simple orderly insulators (MgO, $Al_2O_3$), we are dealing with small polarons. The density of polaronic sites is equal to the density of cationic sites, which is approximately half of the atomic density. This strong density leads to a certain recovery between two adjacent sites (see Figure 2.3): this recovery leads to the formation of a polaronic band, situated at $W_t = W_c + W_p$ below the conduction band and due to a recovery of the orbital wave functions of the different adjacent polaronic sites. The polaronic sites possess the periodicity of the cristalline structure, and the recovery of the wave functions form a narrow band of width $2\,J_P$ such that $\frac{m^*}{m} \propto \frac{1}{2} J_P$, which results in values of the order of $10^{-3}$ eV for $J_P$.

### 2.2.4. *Conduction mechanisms*

In the process of conduction described by Austin and Mott, the moving charge "carries away" with it the polarization cloud as though it were a heavy particle of given effective mass. Generally, we distinguish two conduction mechanisms: band conduction and hop conduction. The transition between these two mechanisms occurs at a temperature $\left(T_t = {}^{T_D}\!/\!_2\right)$; ($T_D$ represents the Debye temperature).

#### 2.2.4.1. *Low-temperature conduction* $\left(T \prec {}^{T_D}\!/\!_2\right)$

At low temperature, the charge moves by band conduction mechanism, which does not bring into play the activation energy, analogous to the motion in a conduction band with a mobility $\mu = e\tau/m^*$, where $\tau$ is the average time between two collisions. All states of the polaronic band are equally populated, the band being narrow and less than kT. Consequently the mobility takes the form:

$$\mu \cong \frac{e\,a^2}{\hbar^2}\tau\frac{J_P}{k_B T} \qquad [2.14]$$

where $a$ represents the lattice parameter, and $\tau$ represents average time between two collisions (diffusion by the phonons).

Consequently, at very low temperature, the mobility is inversely proportional to the absolute temperature.

#### 2.2.4.2. *Conduction at high temperature* $\left(T \succ {}^{T_D}\!/\!_2\right)$

At higher temperature, we observe a conduction mechanism by hops (*hopping*) from one polaronic site to the other. This second process requires the overstepping of a barrier of energy $W_H$ (see Figure 2.3) which can be supplied by the phonons (thermal activation).

The mobility is expressed by:

$$\mu = \mu_0 \exp\left(-\frac{W_H}{k_B T}\right) \qquad [2.15]$$

where $W_H$ is the *hopping* energy between the different adjacent polaronic sites.

The detailed analysis of the mobility given by [2.15] is complicated because we must distinguish the adiabatic displacement process, by quantum tunnelling, from the non-adiabatic process:

– if the process is adiabatic by the tunnel effect, we have: $\mu_0 = \dfrac{ea^2\omega_0}{kT}$,

– if the process is non-adiabatic, the electron is directly excited by a phonon, and we then have: $\mu_0 = \dfrac{\sqrt{\pi}}{2}.\dfrac{e\,a^2}{\hbar}.\dfrac{{J_p}^2}{\sqrt{W_H}}.\dfrac{1}{(k\,T)^{3/2}}$.

Whatever the process brought into play, there is always a possibility of displacement for the polaron: a polaron (free or free polaron) is thus a moving charge, contrary to the bonded polaron, described later, trapped on an impurity.

2.2.4.3. *Comments*

In a polarizable medium, the total energy of the carrier is lowered by Wp. The binding energy of a polaron being negative, the polaronic band is situated in the forbidden band. This energy is quite weak and of the order of 0.1eV for oxides.

## 2.3. Localization and trapping of carriers in a real material

### 2.3.1. *Localization and trapping of the small polaron*

For a small polaron, let us remember that the kinetic energy is negligible, and only the potential energy $W_p$ remains, to a first approximation. In expression [2.11], which gives the potential energy, $\varepsilon(\infty)$ is systematically at least 2 to 4 times smaller than $\varepsilon(0)$; consequently the bonding effect is controlled by the electronic permittivity, i.e. by the polarisability of the atoms of the cell occupied by the polaron. We can understand, then, how a polaron can get trapped. Indeed, let us consider the electronic polarisability $\alpha_{\text{elec}}(\vec{r},\infty)$ (Chapter 1) at the point $(\vec{r})$ and the corresponding permittivity $\varepsilon(\vec{r},\infty)$: if the electronic polarisability on a given site $(\vec{r}_i)$ (impurity, for example) is $\alpha_{\text{elec}}(\vec{r}_i,\infty) < \alpha_{\text{elec}}(\vec{r},\infty)$, with $(\vec{r}_i) \neq (\vec{r})$, that is to say if $\varepsilon(\vec{r}_i,\infty) < \varepsilon(\vec{r},\infty)$, we see from [2.11] that the binding energy on the site $(\vec{r}_i)$ is reinforced (see Figure 2.4), so: $|W_P(\vec{r_i})| > |W_P(\vec{r},\infty)|$, and Wp is then lowered by ΔWp.

Differentiating equation [2.11], and neglecting $1/\varepsilon(0)$ in front of $1/\varepsilon(\infty)$ gives:

$$\Delta \mathrm{Wp} = \frac{q^2}{8\pi r_p}\left[\frac{\Delta\varepsilon(\infty)}{\varepsilon^2(\infty)}\right] \qquad [2.16]$$

where, for an electron of charge e:

$$\Delta \mathrm{Wp} = E_R\left[\frac{\Delta\varepsilon(\infty)}{\varepsilon^2(\infty)}\right]\frac{r_B}{r_p} \qquad [2.17]$$

$r_B$ : *Bohr radius* of the order of 0.05 nm

$E_R$ : *Rydberg Energy*: $E_R = e^2/8\pi\varepsilon_0 r_B = 13.6$ eV

In other words, if $\Delta\varepsilon(\infty) = \varepsilon(\vec{r}_i,\infty) - \varepsilon(\vec{r},\infty) < 0$, a polaron will stabilize on the site $(\vec{r}_i)$ because the charge is more bonded, so its hopping frequency is reduced and its maintenance time on this site is longer. We can then speak of carrier localization, associated with a reduction of its mobility. But, if the carrier is thus localized during a sufficient time so the ions can move, the ionic polarization is to be added to the electronic polarization and consequently the energy of the carrier is reduced again by $\Delta W_m$ (see Figure 2.4). The electron-lattice binding energy therefore becomes more and more negative, which reinforces the bonding between the electron and the polarization charges thus contributing to the stable trapping of the carrier.

### 2.3.2. *Localization and intrinsic trapping of the carriers*

In an ideal structure where all sites are equivalent, there is no possible carrier localization: this is the case with pure monocrystalline annealed MgO [VAL 99]. In pure corindon (monocrystalline $Al_2O_3$) we observe a strong localization of low-temperature charges (<-20°C) which can be likened to trapping on unoccupied octaedric sites of the hexagonal structure of aluminum. This has been confirmed by a molecular dynamic calculation [RAM 97]. Thus, Figure 2.5 shows that at 200K an electron is *confined* on a site of the hexagonal structure. On the other hand, at 300K the electron can migrate from one site to another. Thus even in a very pure and orderly material, there can be trapping, but with an energy variation of the polaron of less than 1eV, which allows easy thermal detrapping.

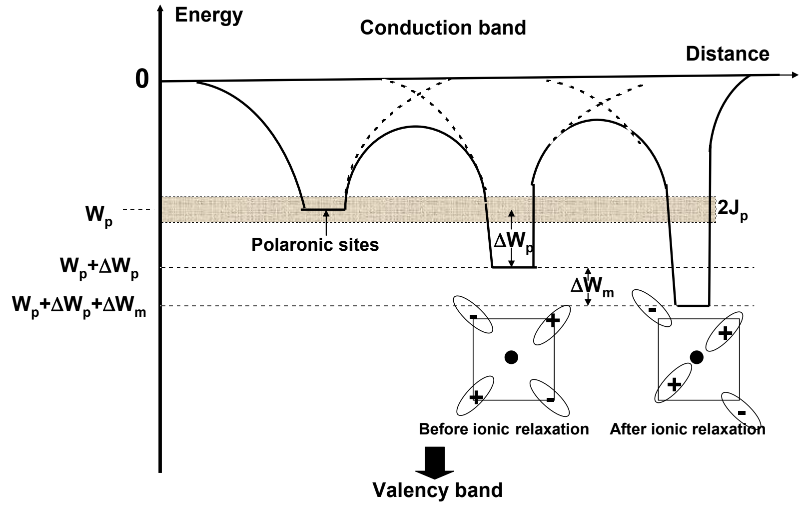


**Figure 2.4.** *Illustration of the localization and trapping of a carrier before and after relaxation of the ions around the charge*

### 2.3.3. *Trapping on structure defects and impurities*

The intrinsic point defects (vacancies, interstitials, etc.) or extrinsic (impurities) will then also be potential trapping sites. In oxides (MgO, $Al_2O_3$, $ZrO_2$, etc.), studies show that vacancies are particularly important to consider and in particular the oxygen vacancies whose formation energy is weaker than that of cationic vacancies (25 eV for oxygen vacancies against 55 eV for aluminum vacancies in alumina). An oxygen vacancy in alumina is doubly charged, by the absence of an $O^{2-}$ ion. This center, known as $F^{2+}$, is then likely to trap 1 (center $F^+$) or 2 electrons (center F). The trap is very stable, with a binding energy of 3.8 eV in the first case, and 3eV in the second.

Impurities are equally responsible for the apparition of deep trap levels for the charges. They can be of a positively charged empty donor character or an empty neutral acceptor character. It appears, here again, that the traps are very deep and the detrapping possibility by thermal activation is weak.

When the defects density is fairly high, an impurity band can appear localized in the forbidden band. We can then envisage conduction in this impurity band.

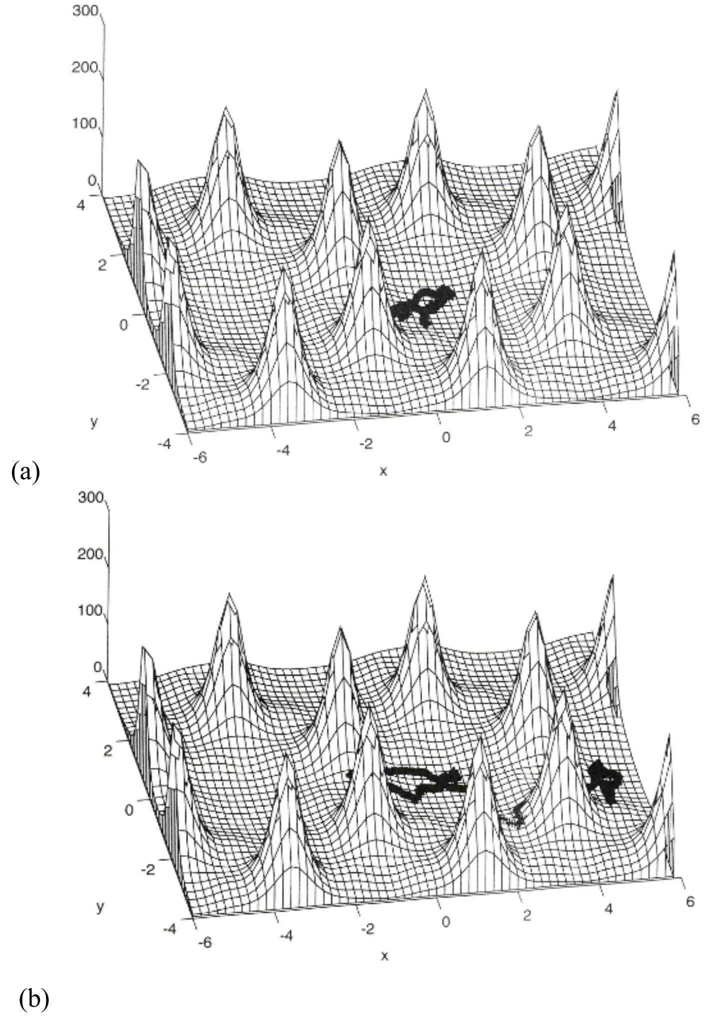


**Figure 2.5.** *Modeling by molecular dynamics of the motion of an electron in ideally pure alumina $\alpha$, (a) at 200K, and (b) at 300K (from [RAM 97])*

Extended defects, such as the interfaces between phases, are places where there is a variation of dielectric susceptibility and so trapping possibility, but the deepness of this type of trap remains weak (<0.1 eV), so the detrapping is at first sight easy.

We note, however, that these extended defects can themselves be the segregation place of impurities or intrinsic defects, which can lead to a large range of trap deepness.

### 2.3.4. *Localization related to disorder*

Electron theory in the lattice has been established for a crystalline material. However, in non-crystalline materials we find conducting materials and insulating materials. We must conclude that the existence of bands and forbidden energy gaps is not something specific to crystals. Anderson [AND 58] has modeled disorderly matter by processing the problem of an electron located in a "random potential" (see Figure 2.6).

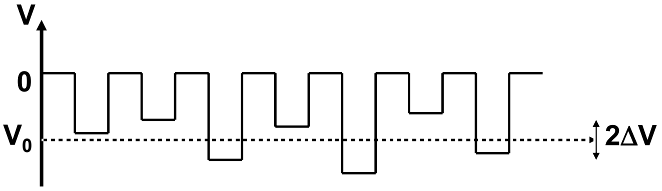


**Figure 2.6.** *Anderson's random potential*

Figure 2.6 is made up of a collection of square wells, centered at the geometric points of the crystal but non-identical: their deepness V varies randomly around an average value $V_0$, with a distribution width ΔV. The disorder is characterized by the parameter ΔV. Once ΔV is not null, *localized states* appear at the bottom of the bands (valence and conduction bands). These are "Anderson states" which exist from the apparition of a disorder, whether the material is crystalline, or amorphous.

In these conditions, the true electronic configuration of a real material will be characterized (see Figure 2.7):

– by delocalized or extended states (valence and conduction bands);

– by Anderson's localized states at the bottom of the bands, whose expanse depends on the disorder;

– by states known as impurity states (from impurities but also structure defects in general) for electrons or holes, localized in the forbidden band.

We then see that the classic description of *conduction band–band gap–valence band* is very simplistic and the reality is more complex. In these conditions, it is the boundaries between the forbidden band and the Anderson state bands which become badly defined. Mott has introduced critical energies $E_C$ and $E_{C'}$ [MOT 74] which delimit the extensive states from the states localized at the bottom of the bands (see Figure 2.7).

Blaise studied the mobility in disorderly materials by using Mott's work. Figure 2.8 summarizes this work and shows the evolution of the effective mobility $\mu^* = \mu^*_{ext} + \mu^*_{hop}$ where $\mu^*_{ext}$ and $\mu^*_{hop}$ are respectively the mobilities in extended and in localized states. The disorder is expressed with respect to $N_C/N$ where $N_C$ is the density of the localized states at the bottom of the conduction band and N the atomic density of the material. We can conclude that the mobility in extended states decreases with disorder, whereas the mobility in localized states increases with disorder.

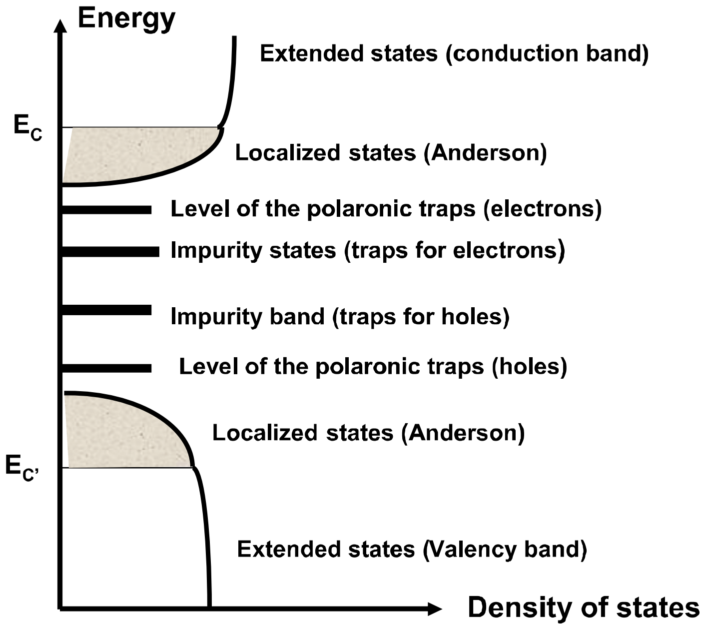


**Figure 2.7.** *Sketch of the energy bands in an insulating material. The position and the amplitude relative to the levels are given for information only*

Thus for a pure material without disorder, such as pure monocrystalline alumina, the insulator can assimilate and evacuate charges towards the mass at room temperature. It is clear that it would be useless to carry out metallization to observe the material using a Scanning Electron Microscope; on the other hand, if we lower the temperature, trapping of intrinsic sites of the material could be seen.

Conversely, for a high disorder ($N_C/N > 5.10^{-2}$), the mobility which prevails is that of Anderson's localized states. It can lead to a current within the sample and an expansion and diffusion of the injected charges.

For intermediate disorders ($10^{-2} < N_C/N < 5.10^{-2}$), the effective mobility passes through a minimum, and we see a strong accumulation of charges. The relaxation of these charges will be extremely slow; the secondary electronic emission could be a way of regulating this charge excess.

The same reasoning can be applied to the holes, but as they are much less movable than electrons, the accumulated positive charges will release more slowly.

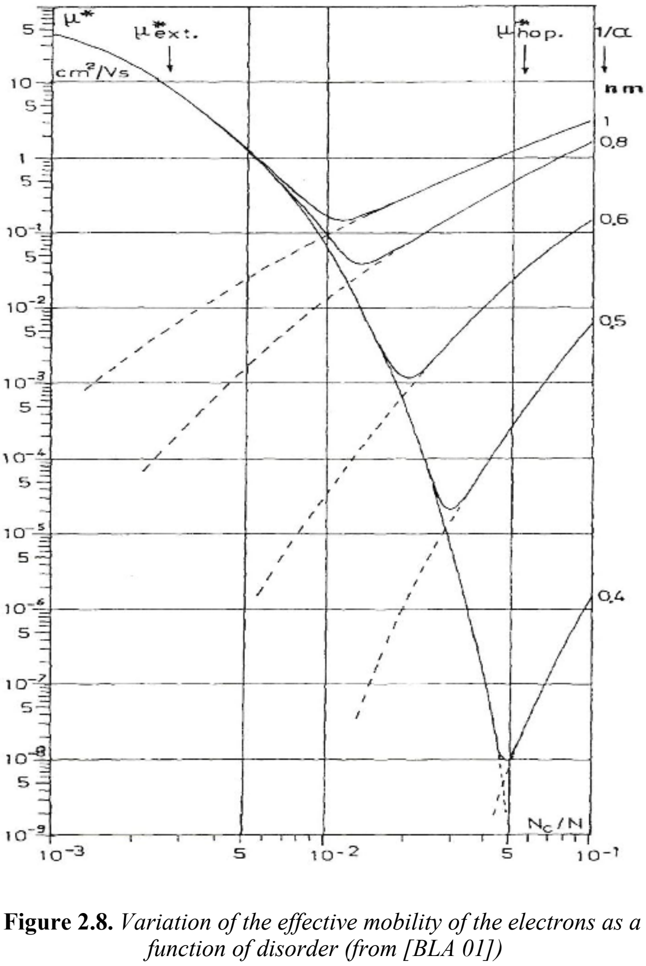


**Figure 2.8.** *Variation of the effective mobility of the electrons as a function of disorder (from [BLA 01])*

### 2.3.5. *Mechanical energy related to the trapping of one charge*

Trapping imposes a restructuring of the network around the localized polaron, creating a local distortion. Different calculations [RAM 97], [BLA 91] have shown that a trapped charge can result in the localization of a mechanical energy of 5eV or more, which is considerable, of the order of the energy of a defect formation. This energy localization leads to a metastable state which "weakens" the material and can trigger catastrophic effects (strain, fracture, wear, etc.) or, to say the least, results in an ageing of the material.

## 2.4. Detrapping

The trapped charges can be detrapped if a sufficient energy is brought to the system. Of particular mention are thermal detrapping and detrapping under the influence of an electric field, which lowers the trapped energy (the Poole-Frankel effect).

### 2.4.1. *Thermal detrapping*

In order to be detrapped, an electron trapped at a negative energy level $-E_a$ in the forbidden band, must reach the bottom of the conduction band (level 0). By applying Boltzman statistics, the detrapping probability is proportional to $\exp(-E_a/kT)$. We can then see that for shallow traps (< 0.1 eV) the detrapping probability is high at room temperature (300 K); conversely for deep traps (3eV), thermal detrapping at room temperature is not likely to occur.

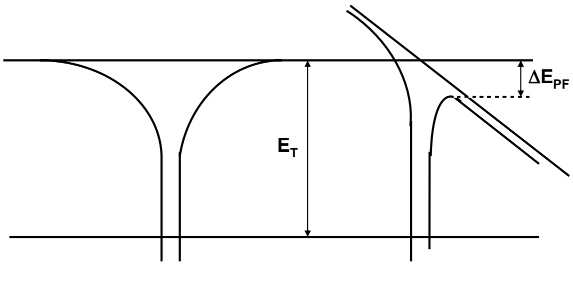
The phenomenon is, however, more complex than a simple mono-electronic transition. Indeed, calorimetric measurements show that trapping is endothermic whereas detrapping is exothermic. This shows that in a trapping situation, the lattice is constrained and forms a metastable state which releases its energy at the moment of detrapping; hence the observed exothermic effect and, in other experiments, a difference between the trapping temperature and that of detrapping. It appears then that trapping-detrapping phenomena are related to collective lattice distortion processes.

### 2.4.2. *Detrapping under an electric field by the Poole-Frankel effect*

This phenomenon describes the lowering of a trapped charge's potential barrier to cross in a potential well, in the presence of an electric field F: the energy to supply in order to detrap the charge will then be weaker. The activation energy is then $E_a = E_T - \Delta E_{PF}$ where $E_T$ is the activation energy in the absence of field (see Figure 2.9). To determine $\Delta E_{PF}$, we seek the local maximum of the potential in $r_0$. We find $\Delta E_{PF} = \beta_{PF} F^{1/2}$ where F is the applied electric field and $\beta_{PF}$ the Poole-Frankel constant:

$$\beta_{PF} = 2\frac{e^{3/2}}{(4\pi\varepsilon_0\varepsilon_r)^{1/2}} \qquad [2.18]$$

where $\varepsilon_r$ is the static dielectric constant of the material.



**Without electric field** **With electric field**

**Figure 2.9.** *Potential well model for a coulomb trapping site, with and without its applied electric field on the trap. In the presence of the field, the energy to supply is lowered by* $\Delta E_{PF}$

This effect, well known for gases, is open to criticism for solids on account of their strong atomic density. However, transport simulations by hops [MAD 02] in a medium with coulomb traps bring out behaviour of Poole-Frenkel type with a coefficient β very slightly less than the coefficient $\beta_{PF}$ calculated from expression [2.18].

The drop in the potential barrier is even stronger since the permittivity is weak and, if the activation energy of the trap is less than the drop in the potential barrier, the charge can immediately be trapped. Thus, for MgO, the calculations show that, at room temperature, the detrapping probability for an activation energy of 0.5 eV is about $10^{-9}$, and it becomes greater than 0.65 for a field of 4MV/cm because such a field lowers the barrier by 0.49eV. Consequently, the detrapping process of a charge distribution will occur preferentially in the zones where the field is strong, i.e. alongside the distribution of the trapped charges. Knowing that a trapped charge corresponds to a stored internal mechanical energy of over 5eV, when the density of trapped charges reaches a critical value causing detrapping, we see an energy liberation which, according to the ability of the material to evacuate it, will be transformed into thermal agitation which itself might lead (as we have already indicated) to an ageing of the material, i.e. the formation of shockwaves which are the cause of catastrophic phenomena (dielectric strain, mechanical rupture, or wear, etc.).

## 2.5. Bibliography

[AND 58] ANDERSON P.W., "Absence of diffusion in certain randol lattice", *Physics Review,* vol. 109, p. 1492–1505, 1958.

[AUS 69] AUSTIN I.G., MOTT N.F., "Polarons in crystalline and non crystalline materials", *Advances in Physics*, vol. 18, no. 71, p.41–102, 1969.

[BLA 91] BLAISE G., LE GRESSUS C., "Charging and flashover induced by surface polarization relaxation process", *Journal of Applied Physics,* vol. 69, p. 6334–6339, 1991.

[BLA 01] BLAISE G., "Charge localization and transport in disordered dielectric materials", *Journal of Electrostatics*, 50, p. 69–89, 2001.

[FRÖ 54] FRÖLICH H., *Adv. Phys*. 3, p. 325, 1954.

[FRÖ 62] FRÖLICH H., *Polarons and Excitons*, in C.G. Kuper, G.D. Whitfield, (eds), Oliver & Boyd, Edinburgh & London, p. 1–32, 1962.

[LAN 69] LANDAU L., LIFCHITZ E., *Electrodynamique des milieux continus*, éditions MIR, 1969.

[MAD 02] MADY F., Modélisation des phénomènes de transport et des effets de charge dans les matériaux isolants, Doctoral thesis, Nantes University (France), 2002.

[MOT 74] MOTT N.F., *Metal Insulator Transition*, Taylor & Francis, London, 1974.

[RAM 97] RAMBAUT C., OH K.H., JAFFREZIC H., KPHANNOF J., FAYEULLE S., "Molecular dynamics simulation of electron trapping in the sapphire lattice", *International Atomic Energy Agency. International Centre for Theoretical Physics*, IC/95/330, *Journal of Applied Physics,* 81, p. 3263, 1997.

[VAL 99] VALLAYER B., BLAISE G., TREHEUX D., "Space charge measurement in a dielectric material after irradiation with a 30 kV electron beam: Application to single-crystal's oxide trapping properties", *Review of Scientific Instruments*, vol. 70 no. 7, p. 3102–3112, 1999.