

A Theory of the Electrical Breakdown of Solid Dielectrics.

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§ 1. *Introduction.*

In the modern theory of metallic conduction initiated by Bloch, conductors, semi-conductors, and non-conducting crystals may be represented by the same model. In this model each electron is supposed to move freely in the periodic field of the lattice. Owing to this field, not all electronic energy levels are allowed; the allowed levels are grouped into bands, separated by energy intervals which are disallowed. If all the energy levels of a given band are occupied by electrons, then, according to the theory, these electrons can make no contribution to an electric current in the crystal. If all the bands are full, the crystal must be an insulator. Thus in an insulator there exist a number of energy bands which are completely full, and a number of bands of higher energy which, for a perfect crystal at the absolute zero of temperature, are empty.

In a real non-conducting crystal, however, there will be a few electrons in the first unfilled band, owing to thermal excitation, impurities, etc. Their number is, however, too small to give an appreciable current at ordinary field strengths. As the field strength is increased, the current due to these few electrons increases steadily, but it will not show the sudden rise observed in dielectric breakdown. For this sudden rise it is necessary that the number of electrons in an unfilled band should suddenly increase as the field strength passes a critical value. Two distinct mechanisms have been suggested for this sudden increase. Of these, the first† is a process analogous to the electrical breakdown of gases. In the absence of an external field, the few electrons in the upper band are in the lowest energy state of this band; under the action of an electric field, they are raised to higher levels. When one of these electrons reaches a sufficiently high level, it will give up energy to an electron in a lower (full) band, both electrons making a transition to a low level of the upper band. The process will then be repeated; the number of electrons in the

† Hippel, 'Z. Physik,' vol. 67, p. 707, vol. 68, p. 309 (1931); vol. 75, p. 145 (1932).

upper band will thus increase exponentially with time as long as the electric field is maintained.

When a constant electric field is present energy bands have significance only with reference to restricted regions of space, since such an electric field makes each energy band (defined for no external field) of a lattice of infinite extent degenerate with every other energy band, *cf.* fig. 1. Thus in the presence of a constant electric field an electron may pass from one "energy band" into another which, if the external field were absent, would lie above the first band. This second process of excitation is analogous† to the auto-ionization of free atoms by large electric fields. In a gas the effect of auto-ionization is of no practical importance, being masked by the first mechanism of dielectric breakdown. In a solid the analogous process is of more importance than in gases, both because the mean free path of the electrons is shorter than in gases, and because, as we shall show, the electric field can more readily *excite* an electron in a lattice than *ionize* an isolated atom.

The purpose of this paper is to examine this second method of dielectric breakdown. In § 2 the Bloch model of a metal is used to calculate the rate at which electrons escape from the lower into the upper energy bands under the influence of a constant electric field. In § 3 we show that both the magnitude of the breakdown field and the suddenness of the breakdown are obtained by this theory, assuming only the second mechanism to be operative.

§ 2. Theory.

The rate at which electrons pass from one band into another under the action of a constant electric field is independent of the thermal motion of the lattice, at least for not too high temperatures. The potential energy of an electron in the lattice will thus be considered a periodic function of the co-ordinates. Only a one-dimensional lattice will be treated, the potential energy of the electron being a function $V(x)$ with period a of the co-ordinate x of the electron.

We shall first determine approximately the motion of an electron in a lattice under the influence of a constant electric field by the method introduced by Bloch.‡ The wave equation with a periodic potential energy has solutions of the form

$$\psi_k(x) = e^{ikx} U_k(x), \quad (1)$$

† Rosenkewitsch and Sinelnikow, 'Z. Physik,' vol. 73, p. 118 (1932); Eisler, 'Z. Physik,' vol. 79, p. 266 (1932).

‡ 'Z. Physik,' vol. 52, p. 555 (1928).

where $U_k(x)$ has the same period as $V(x)$. The condition that ψ_k should remain finite for all values of x imposes the restriction that k be real. But only when E_k lies in the bands of allowed energy referred to in § 1 has the wave equation solutions of the type (1) with a real k . The first energy band lies within the interval $-\pi/a \leq k \leq \pi/a$ of k .

Bloch further showed that if, when an electric field F is present, the wave function $\psi(x, t)$ is expanded in terms of wave functions of the lowest energy band when $F = 0$, in the form

$$\psi(x, t) = \int_{-\pi/a}^{\pi/a} g(k, t) \psi_k(x) dk,$$

thus neglecting all energy bands except the first and so excluding from the calculation any possibility of a transition to these bands, then

$$\frac{\partial}{\partial t} |g|^2 = -\frac{2\pi eF}{h} \frac{\partial}{\partial k} |g|^2,$$

or

$$|g|^2 = G\left(k - \frac{2\pi eF}{h} t\right),$$

where G is an arbitrary function. When we remember that $\psi_{-\pi/a} = \psi_{\pi/a}$, we see that $|g|^2$ is a periodic function of t . Since the range of k is $2\pi/a$, and since $|g|^2$ moves in k space with the velocity $2\pi eF/h$, the period of the time variation of $|g|^2$ is $(2\pi/a)/(2\pi eF/h) = h/eFa$; its frequency is thus

$$v = eFa/h. \quad (2)$$

We thus conclude that the velocity of the electron, *i.e.*,

$$\frac{\partial}{\partial t} \int \psi x \psi^* dx,$$

is also a periodic function of time with the frequency v , since the identity

$$\frac{\partial}{\partial t} \int \psi x \psi^* dx = \int v_k |g|^2 dk$$

may be readily established when v_k is the velocity of an electron in state k . Thus if we represent the electron by a wave packet confined to the first energy band, the electron moves in the direction of the field until it is reflected by the lattice, then moves in the opposite direction until it is stopped by the field, whereupon the motion is repeated.

We must now calculate the probability per unit time that the electron will make a transition to an excited band. If we take the wave function $\psi(x, t)$ to be a wave packet, then each time the wave packet is reflected by the lattice, a small fraction of the wave packet will pass through into the upper zone, giving the probability p that the electron escapes into the upper zone (cf. fig. 1). The probability, γ , per unit time is obtained by multiplying p by the

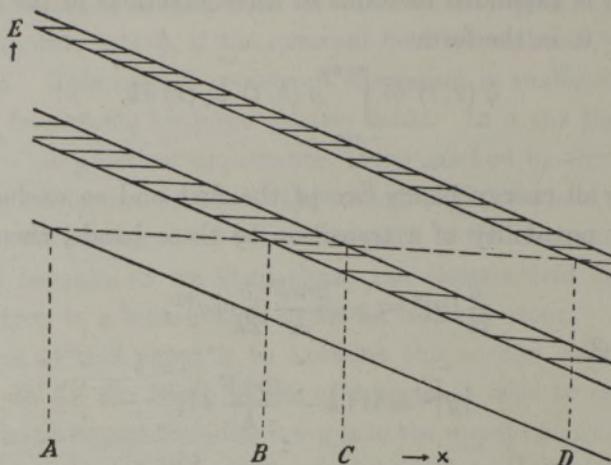


FIG. 1.—“Potential barrier” diagram. The shaded regions represent zones of forbidden energy in the presence of an electric field.

number of times per second that the wave packet is reflected by the lattice, namely, ν , so that

$$\gamma = \nu p.$$

We have now to calculate p . This is most simply done by taking for $\psi(x, t)$ a wave function *periodic* (in time), not a wave packet. The wave equation for an electron with energy E when an external electric field F is present is

$$\left\{ \frac{\hbar^2}{8\pi^2m} \frac{\partial^2}{\partial x^2} - V(x) + (E - eFx) \right\} \psi(E : x) = 0.$$

An approximate solution of this equation may at once be obtained if we observe that the term eFx changes only slightly in the distance of a single lattice constant. Such a solution is

$$\psi(E : x) = e^{i \int K dx} U_K(x),$$

where K is the same function of $(E - eFx)$ as it is of E alone when F is zero, and U_K is identical to the U_k of (1) with $k = K$. With a given E our K will now be real *only for certain values* of x , as shown in fig. 1. In the regions

where K is complex, $\psi(E : x)$ will decrease, or increase, exponentially. On either side of such a region $\psi(E : x)$ is nearly identical with the wave functions in the absence of a field which belong to two adjacent energy bands. Thus in fig. 1, $\psi(E : x)$ is similar to a wave function belonging to the first energy band in the interval AB, while in the interval CD it is similar to a wave function belonging to the second band. If we take the wave function ψ which *decreases* in the range BC, then we know that the transition probability p is given by†

$$p = |\psi(x_C)/\psi(x_B)|^2.$$

If we write, for values of x in the interval BC,

$$K = \xi(x) + i\eta(x) \quad (4)$$

then we have

$$|\psi(x_C)/\psi(x_B)| \approx e^{-\int_B^C \eta(x) dx} \quad (4a)$$

and hence, by (2) and (3)

$$\gamma = \frac{eFa}{h} e^{-2\int_B^C \eta dx}.$$

In order to obtain an explicit expression for $K(x)$, we write our wave equation in the standard form of Hill's equation,

$$\frac{d^2\psi}{ds^2} + (\theta_0 + 2\sum_{n=1}^{\infty} \theta_n \cos 2ns) \psi = 0.$$

Here

$$s = \pi x/a,$$

$$\theta_0 = 8ma^2(E - eFz)/h^2,$$

and θ_n is $4ma^2/h^2$ times the coefficient of $\cos 2\pi nx/a$ in the Fourier expansion of $V(x)$. When θ_1 is small in comparison with unity (with $a = 3 \times 10^{-8}$ cm, this condition means that the first Fourier coefficient must be small in comparison with 4 electron volts), and when the higher coefficients are still smaller, K is determined as a function only of θ_0 and θ_1 by the equation‡

$$\sin^2(aK/2) = \sin^2(\frac{1}{2}\pi\theta_0^{\frac{1}{2}}) \left\{ 1 + \frac{\pi\theta_1^2}{4\theta_0^{\frac{1}{2}}(1-\theta_0)} \cot(\pi\theta_0^{\frac{1}{2}}/2) \right\} + O(\theta_1^4). \quad (5)$$

In the first energy band in which K is complex, θ_0 is seen from (5) to differ

† Gamow, "Atomic Nuclei and Radioactivity," chap. 2, Oxford (1931); v. Laue, 'Z. Physik,' vol. 52, p. 726 (1928). Houtermans, 'Ergebn. exakt. Naturw.,' vol. 9, p. 133 (1930).

‡ Hill, 'Acta Math.,' vol. 8, p. 27 (1886); M. J. O. Strutt, "Lame'sche-Mathieusche Funktionen," p. 25, Berlin (1932). In the latter reference $2\theta_1$ is erroneously used in place of θ_1 . This mistake is easy to make, since θ_1 is defined in Hill's memoir in two ways differing by a factor of two.

only slightly from unity, and K is seen to differ only slightly from $\pi\theta_0^{\frac{3}{2}}$, i.e., only slightly from π/a . Hence if we set

$$\left. \begin{aligned} \theta_0 &= 1 + \alpha \\ K &= \pi/a + \beta \end{aligned} \right\} \quad (6)$$

α and β , together with θ_1 , may be regarded as small quantities. Substituting (6) in (5), and neglecting powers of α , β , and θ_1 greater than the second, we obtain

$$K = \pi/a \pm i(\pi/a)(\theta_1^2 - \alpha^2)^{\frac{1}{2}}.$$

If we now choose the origin $x = 0$ to lie midway between B and C, we have, using (6),

$$K = \frac{\pi}{a} \left[1 \pm i \frac{8ma^2}{h^2} \left\{ V_0^2 - (eFx)^2 \right\}^{\frac{1}{2}} \right]. \quad (7)$$

The points B and C are now given by $x = -V_0/eE$ and $x = V_0/eF$, respectively, so that the energy gap ε between the two bands of allowed energy is $2V_0$. Performing the integration of (4a), we obtain for the rate γ with which an electron passes from the region AB into CD

$$\gamma = \frac{eFa}{h} \exp - \left\{ \frac{\pi^2 ma\varepsilon^2}{h^2 |eF|} \right\}. \quad (8)$$

§ 3. Discussion.

We have obtained in (8) the rate with which an electron escapes from one energy band into the next energy band. In the derivation of (8) we assumed the system to be one-dimensional, and the first Fourier coefficient of the potential energy of an electron in the lattice to be sufficiently small (considerably less than 4 electron volts when $a = 3 \times 10^{-8}$ cm). It is to be expected that the results obtained for a one-dimensional lattice are true in general for a three-dimensional lattice. Although the Fourier coefficients of most crystals are larger than allowed in the above derivation, it is nevertheless to be expected that the general dependence, given by (8), of the transition rate upon the energy gap ε will still be valid.

When we take the reasonable magnitudes $a = 3 \times 10^{-8}$ cm, $\varepsilon = 2$ electron volts, and let F^* be the electric field in volts cm^{-1} , (8) becomes

$$\gamma = 10^7 F^* 10^{-2 \times 10^7 / F^*}.$$

The dielectric breakdown is thus not to be expected until F^* reaches the order of magnitude of 10^6 , as is observed. Further, the breakdown will occur

suddenly as F^* is increased, γ being increased by a factor of 100 (in our example) when F^* changes from 1.0×10^6 to 1.1×10^6 .

It is to be particularly stressed that for field strengths obtainable in metals, equation (8) shows the transition between different energy bands to be altogether negligible. Thus for $a = 3 \times 10^{-8}$ cm, and $F^* = 1$, an electron will pass an energy gap as small as 2×10^{-3} electron volts only after a period of years.

§ 4. *Summary.*

A theory of the electrical breakdown of solid dielectrics is developed. The breakdown is assumed to be due to the direct excitation of electrons by the electric field. Agreement with experiment is obtained both for the magnitude of the breakdown field and for the suddenness with which the breakdown occurs as the electric field is increased.

Some Peculiarities in the Physical Properties of Iron-Aluminium Alloys.

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The thermal equilibrium diagram of alloys consisting of iron and aluminium has been the subject of several investigations from which it appears that solid iron forms a solid solution with aluminium up to 30% by weight of aluminium.* Whilst carrying out an examination of the change in physical properties of iron with increasing aluminium content, from 0% to 17%, it was noticed that certain physical properties, notably thermal expansion and electrical resistivity, exhibited certain peculiarities not to be expected from a range of solid solutions. It was thought worth while to examine these effects in greater detail and the results are recorded in this paper.

EXPERIMENTAL.

Production of Alloys.

The specimens were made from Swedish iron or conductor rail and high grade aluminium, and melted in a high frequency furnace in air. They were

* Gwyer and Philips, 'J. Inst. Met.', vol. 38, p. 29 (1927).