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Motion of Positrons in Metals*

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Abstract. In this review we discuss the different aspects of positron annihilation in metals that involve the dynamics of positron motion before annihilation. The emphasis is on the theory, but also some experimental evidence is quoted. The topics covered are: slowing down and thermalization, effective mass, temperature dependence of positron vacancy trapping, positron channeling, and escape of low energy positrons from metal surfaces.

Index Headings: Positron annihilation – Metals

Some of the most tricky and recalcitrant problems in the field of positron annihilation are related to the motion of positrons before they annihilate. We believe that a few of these questions are of fundamental nature and thus of intrinsic interest and that even in the other cases a proper understanding is necessary to assure a correct interpretation of the experimental data. We limit ourselves to metals, but because the positron annihilation is becoming such a large field, we might be overlooking some important effects, something for which we wish to apologize.

In Section 1 we discuss the slowing down of positrons from the MeV energy region to thermal energies. The problem of the effective mass of the positron is discussed in Section 2, while the controversial question of the velocity dependence of the positron vacancy trapping rate is reviewed in Section 3. Section 4 contains a discussion of positron channeling, while Section 5 is concerned with the escape of low energy positrons from metal surfaces. The notation to be used frequently is defined in Table 1.

1. The Slowing Down and Thermalization

1.1. Slowing Down of Fast Positrons

When one considers the motion of positrons in metals, there are three main energy regions involved. In the range from a few MeV to, say, 10 keV the positron has enough energy to penetrate deeply into the metal. Nearly all the energy loss is then due to plasmon production and ionizing collisions and only at still higher energies does radiation loss become the dominant effect. There seems to be relatively little difference in this range between a fast electron and a positron. Rohrlich and Carlson [1]

Table 1. Some commonly used symbols. Units $\hbar = 1$ are used throughout

E_k	Energy of a positron with wave vector $\boldsymbol{k}$
ε_k	Energy of an electron with wave vector $\boldsymbol{k}$
$\varepsilon(\boldsymbol{q}, \omega)$	Dynamic dielectric function
m	Positron bare mass
$1/m^* = d^2E_k/dk^2\|_{k=0}$	Positron effective mass
$M(\boldsymbol{k}, \boldsymbol{k}')$	Transition probability per unit time between positron states indicated by the labels $\boldsymbol{k}$ and $\boldsymbol{k}'$
f_k	Conduction electron momentum distribution (Fermi-Dirac distribution at zero temperature)
g_q	Equilibrium positron distribution
$n(\boldsymbol{q}, t)$	Positron momentum distribution at time t after it has been inserted in the crystal
$v_q = 4\pi e^2/q^2$	Fourier transform of the Coulomb potential
k_B	Boltzmann's constant
Ω	Volume of the crystal
Ω_0	Volume of the unit cell
N	Number of lattice sites in the crystal
M	Ionic mass
S	Longitudinal sound velocity

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have estimated the positron-electron differencies in the average energy loss and penetration depth in Al and Pb. Their results indicate that, almost independent of Z, positrons lose energy more rapidly than electrons below about 350 keV, but less rapidly above that value. This effect increases percentagewise with the average ionization potential and is about a factor 1/6 to 1/3 larger in Pb than in Al. When experiments on the relative positron-electron penetration depth in metals are done, also the effect of the positron-electron difference in the multiple scattering has to be considered. This affects the penetration depth z_d at which the memory of the original direction of the particle beam has been essentially lost and this has to be taken into account in addition to the part describing the energy loss to give the theoretical estimate of the average penetration depth.

Seliger [2], Takhar [3, 4], and Rupaal and Patrick [5, 6] report experimental data on electron and positron transmission through thin metal foils. Above the energy 350 keV their values for the ratio of positron range to electron range and theoretical calculations agree within the experimental errors, giving e.g. 1.12 for Al and 1.35 for Pb, when monoenergetic positrons of energy 1.88 MeV are used. For the equivalent thickness t in units of $\mathrm{mg/cm^2} \cdot (Z/A)$, Z denoting the nuclear charge and A being the mass number, and for a given transmission T one can write the empirical formula

$$\ln[t^{\pm}(T)] = C(T) + B^{\pm} Z^{1/3}, \tag{1}$$

where the + and − signs refer to positrons and electrons, respectively, C depends on T, and B is a constant. The same experimental law with different values of C and B is obtained to hold in the lower energy region, too [2, 5, 6].

In metals of low Z-values there seems to be, in the energy region below 350 keV, a discrepancy between theory and experiment, when it comes to the difference between the electron and positron penetration depths. Whether this a genuine discrepancy or whether the experimental data are compared to the correct theoretical quantity is somewhat unclear ([5] compares the experimental results only with the ratio z_d^+/z_d^- of [1]).

The intermediate energy range from about 10 keV to a few eV has not been studied very much. For electrons, data on the 1–10 keV region are given by Feldman [7].

1.2. Thermalization

Once the positron has been sufficiently slowed down so that the excitation of plasmons and ionizing collisions are energetically forbidden, the positron can lose energy only by creating conduction electron particle-hole pairs or exciting phonons. The simplest reasonably realistic theory for these processes is obtained by assuming that the rate of energy loss $R(\boldsymbol{k})$ of a positron with momentum $\boldsymbol{k}$ is equal to an average over the energy loss associated with a collision into a positron state with momentum $\boldsymbol{k}-\boldsymbol{q}$ weighted by the transition rate into this state

$$R(\boldsymbol{k}) = \sum_{\boldsymbol{q}} (E_{\boldsymbol{k}} - E_{\boldsymbol{k}-\boldsymbol{q}}) M(\boldsymbol{k}, \boldsymbol{k}-\boldsymbol{q}). \tag{2}$$

Carbotte and Arora [8] considered only collisions which excited electron-hole pairs and their theory is equivalent to the use of (2) with

$$M(\boldsymbol{k}, \boldsymbol{k}-\boldsymbol{q}) = \frac{4\pi}{\Omega^2} \sum_{\boldsymbol{p}} \left| \frac{v_{\boldsymbol{q}}}{\varepsilon(\boldsymbol{q}, E_{\boldsymbol{k}} - E_{\boldsymbol{k}-\boldsymbol{q}})} \right|^2 f_{\boldsymbol{p}}(1 - f_{\boldsymbol{p}+\boldsymbol{q}}) \cdot \delta(E_{\boldsymbol{k}} - E_{\boldsymbol{k}-\boldsymbol{q}} - \varepsilon_{\boldsymbol{p}} + \varepsilon_{\boldsymbol{p}+\boldsymbol{q}}). \tag{3}$$

By evaluating these expressions numerically they found that the time it takes for a positron to slow down from the Fermi energy to energies of the order 0.1 eV is insignificant compared to the later stages of the thermalization. In the case of Na they found that the time it takes for a positron to slow down to an energy corresponding to 110°K is about 10^{-10} sec, i.e. a factor 4 less than the lifetime. The corresponding number for Al is about $5 \cdot 10^{-10}$ sec or about 2.5 times the lifetime in that metal.

Majumdar [9] has given arguments (similar to those of Kohn *et al.* [10, 11] in the case of conduction electrons) that there will, in the idealized case of thermalized positrons annihilating at zero temperature, be a sharp break in the 2γ-angular correlation corresponding to the Fermi momentum. This should hold even when the positron interaction with the electrons and the lattice is taken into account. The result is based on perturbation theory and therefore needs not be true (Arponen [12]), although we know of no strong arguments that many-body perturbation theory actually breaks down for positrons. Carbotte and Kahana [13] have calculated the Fermi surface discontinuity due to electron gas interactions and found it to be about the same as in the non-interacting case. Hede and Carbotte [14] further found that the zero temperature positron-phonon interaction has essentially no effect on the angular correlation near the Fermi angle.

Table 2. Theoretical [17] and experimental [15] values of the minimum positron temperature in alkali metals. The experimental value is related to the assumed effective mass through $\Theta_{\min} \sim (m^*/m)^{-1}$, while for the theoretical value the relationship is $(m^*/m)^{-\frac{1}{2}}$

$\Theta_{\min}$[°K]			
Metal	Theory [17]	Exp. [15]	m^*/m
Rb	37.5	~ 60	2.3
K	39.2	~ 100	2.1
Na	49.0	160 ± 50	1.8
Li	64.3	~ 200	1.8

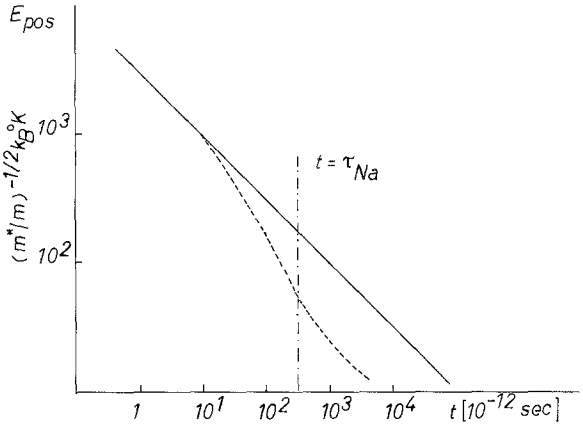

Fig. 1. Positron energy as a function of time from [16]. The full curve denotes the result, when only electron = hole pair excitations are taken into account as the thermalization mechanism for the positron. In the dashed curve also positron-phonon interaction is included. The calculation was done for Na and τ_{Na} is the positron mean lifetime in Na. (Note the logarithmic scales on both axes)

It might then be argued that any residual smearing of the Fermi surface discontinuity that remains at zero temperature must be due to incomplete thermalization. Experimentally Kim *et al.* [15] arrived at the conclusion that there is a minimum positron temperature, below which the positron will not have time to thermalize. Their estimate of this temperature is given in Table 2. These values are larger than those given by Carbotte and Arora [8], the discrepancy being clearest in the case of Na.

This discrepancy becomes larger when the effect of the positron-phonon interaction is included within the framework of a theory based on (2). Such a theory has been developed by Perkins and Carbotte [16]. In our notation their treatment is equivalent to putting

$$M(\boldsymbol{k}, \boldsymbol{k}-\boldsymbol{q}) = 2\pi\gamma_{\boldsymbol{q}}\gamma_{-\boldsymbol{q}}\delta(E_{\boldsymbol{k}} - E_{\boldsymbol{k}-\boldsymbol{q}} - Sq)\,, \tag{4}$$

where the positron-phonon matrix element $\gamma_{\bar{q}}$ is given by

$$\gamma_{\boldsymbol{q}} = -i(N/2SqM)^{1/2} v_{\boldsymbol{q}} |U_0|^2/[\Omega\varepsilon(\boldsymbol{q}, 0)]\,. \tag{5}$$

Here $|U_0|^2$ is a numerical factor which is calculated from the positron wave function, and is unity when plane waves are used. The factor arises from the repulsion of the positron from regions close to the ion cores. Figure 1 summarizes the results of [8] and [16]. For large positron energies the creation of particle-hole pairs is the most efficient mechanism when it comes to slowing down positrons, while for lower energies the phonon effects dominate. In the case of Na the cross-over point where both mechanisms are equally important comes at the positron energy of $190\,k_B$°K if $m^*/m = 1$. For larger effective masses the cross-over occurs at higher energies, e.g. when $m^*/m = 2$ it would be at $380\,k_B$°K, corresponding to a positron temperature of 253°K.

The approach expressed by (3) might be too crude if the individual collisions typically involve large fractional energy losses. The Boltzmann equation will in such a case give a more accurate treatment of the problem and detailed calculations based on this approach were made by Woll and Carbotte [17]. The Boltzmann equation can be written as

$$\dot{n}(\boldsymbol{k}, t) = \sum_{\boldsymbol{k}'} [M(\boldsymbol{k}, \boldsymbol{k}')n(\boldsymbol{k}', t) - M(\boldsymbol{k}', \boldsymbol{k})n(\boldsymbol{k}, t)] - \frac{1}{\tau_A} n(\boldsymbol{k}, t)\,. \tag{6}$$

The last term comes from the loss of positrons due to annihilation. Woll and Carbotte [17] solved (6) numerically from different starting distributions considering only electron gas correlations and substituting thermal electron momentum distributions in (3). They found that when the positron is being slowed down in a medium where the temperature is not too low it will have time to reach an approximate equilibrium Boltzmann distribution. At lower temperatures the positron will not have time to do so and there will be a minimum effective temperature which the positron can reach. The calculated minimum effective temperature of [17] are listed in Table 1 together with the assumed effective masses (these are the same effective masses as were used by Kim *et al.* [15]). If a different effective mass value were more appropriate (see Section 2),

one can correct for this by noting that the minimum temperature obtained from experiment is inversely proportional to the assumed effective mass, while the theoretical value scales approximately as the inverse square root of m^*. When the same values of the parameters are used, and the minimum values of the temperature are obtained by the Boltzmann equation approach of [17] and the simpler approach of [8] using (2) and (3), it is found that the latter one overestimates the minimum temperature by a factor 1.64.

In conclusion, we note that the calculation of [17] gives values for the minimum temperature which are of the same order of magnitude as the experimental values, but the theoretical ones are consistently lower. It might be argued that since [17] presents an electron gas calculation the authors should have used the electron gas effective masses which are lower than the values they used. Even so one would obtain a minimum temperature which is lower than the experimental one. We recall further that at the temperatures we are considering the phonon energy loss mechanism actually is more effective than that associated with the conduction electrons. One could therefore conclude that a Boltzmann equation approach, including the phonons, would result in a considerable lowering of the minimum temperature and thus increase the discrepancy even more. A possible complication is that in analogy with the hot electron work of Thornber [18] the Boltzmann equation may not be valid for the phonon contribution and it might therefore be tempting to use the path integral method or a related formalism for this problem. The calculation becomes then more difficult and perhaps before such a major computational task is undertaken more experimental results should be available.

2. Effective Mass

To our knowledge there has not been more experimental work on this problem since the papers of Kim *et al.* [19–22]. What they did was to measure the 2γ-angular correlation in the alkali metals at different temperatures and then to extract the effective masses by fitting the temperature dependence of the curves to a simple model described in detail by Kim [22]. The high values thus obtained for the ratio between the effective and bare masses ($m^*/m = 1.8 \pm 0.3$; 1.8 ± 0.2; 2.1 ± 0.3 and 2.3 ± 0.3 for, respectively, Li, Na, K, and Rb) have represented somewhat of a puzzle. The early works in this field were reviewed by Majumdar [23]. In the independent particle model the momentum distribution of the annihilating pair will be proportional to

$$E(\boldsymbol{K}) = \sum_{\boldsymbol{q}} g_{\boldsymbol{q}} f_{\boldsymbol{K}-\boldsymbol{q}} . \tag{7}$$

It is easy to see [20] that the temperature dependence of the electron distribution $f_{\boldsymbol{q}}$ is insignificant compared to that of the positron distribution $g_{\boldsymbol{q}}$. Assuming that a positron with a momentum $\boldsymbol{q}$ has the energy $q^2/2m^*$ and that the Boltzmann momentum distribution is applicable, one gets at temperature T

$$E(\boldsymbol{K}) = (2\pi m^* k_B T)^{-3/2} \int d^3q E_0(\boldsymbol{K}-\boldsymbol{q}) e^{-q^2/2m^* k_B T}, \tag{8}$$

where $E_0(\boldsymbol{K})$ is the zero-temperature momentum distribution of the annihilating pair. In a real metal there will, of course, be correlation effects which modify (7). It is assumed, however, in the model used to analyze the experimental data that (8) would still be valid even if the true zero temperature result, instead of the independent particle result, is substituted for $E_0(\boldsymbol{K})$.

The theoretical validity of (8) was discussed in some detail by Bergersen and Pajanne [24]. It was found that (8) is indeed correct in the idealized case of a positron annihilating in an interacting electron gas, and the m^* which then enters the formula is the same as the effective mass defined by the energy momentum dispersion relation. As was pointed out earlier by Mikeska [25, 26] the situation changes, when the positron-phonon interaction is included. Then the momentum distribution of the (quasi)positrons is no longer completely Boltzmann-like and (8) has to be replaced by the more general formula

$$E(\boldsymbol{K}) = (2\pi m^* k_B T)^{-3/2} \int d^3q E_0(\boldsymbol{K}-\boldsymbol{q}) \sigma(\boldsymbol{q}, T) \tag{9}$$

with the resolution function $\sigma(\overline{\boldsymbol{q}}, T)$ given by

$$\sigma(\boldsymbol{q}, T) = \int d\omega A(\boldsymbol{q}, \omega) e^{-\omega/k_B T}, \tag{10}$$

where $A(\boldsymbol{q}, \omega)$ is the positron spectral function (essentially the imaginary part of the single positron Green's function). In the non-interacting case $A(\boldsymbol{q}, \omega)$ is a delta-function centered at $\omega = q^2/2m^*$. When the electron-positron interaction is included the quasi-positron peak will, in the formalism of [24], get a width which, however, vanishes in the limit of zero momentum. Furthermore, this happens sufficiently

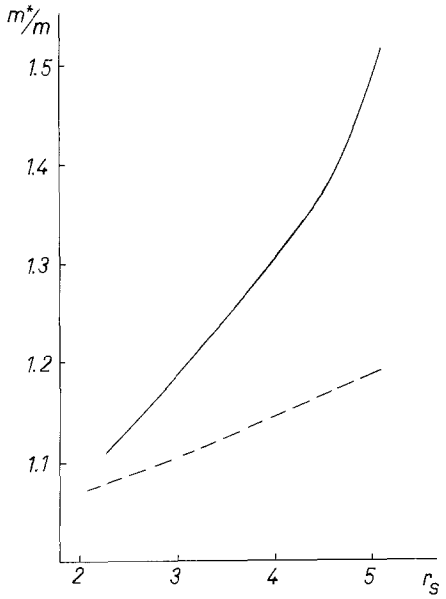

Fig. 2. The contribution to the positron effective mass from conduction electron correlations. The fulldrawn curve is taken from [33] while the dotted curve is taken from [29]

fast so that for moderate temperatures the quasi-positron momentum distribution will still be Boltzmann-like. This is a major reason that (8) remains applicable even when the interacting electron-positron system is studied. If, on the other hand, the positron-phonon interaction is included, the width of the spectrum becomes broad enough to cause a significant change in the momentum distribution. Indeed, when (9) is used to fit the data the apparent effective mass obtained will differ from the effective mass m^* defined from the dispersion relation by an amount which was estimated in [24] to be between 15 and 30%. This is significant, but not in itself a large enough effect to explain the high reported values of the apparent effective masses.

The positron-phonon [14] and band [22, 27, 28] contributions to the effective mass have been evaluated for the alkali metals and found to be small. The value of the contribution to m^* from positron conduction electron correlation is more difficult to calculate accurately. Hamann [29] evaluated the effective mass from the positron self-energy in the random phase approximation. It appears doubtful to us whether such a simple approximation remains quantitatively valid in low density metals such as the alkalis. Bergersen and Pajanne [30] calculated the effective mass from a ladder approximation to the self-energy with a potential adjusted to satisfy the displaced-charge sum rule. It can also be argued against this procedure [31] that the correlations included in [30] are not the most important ones at low density. Baldo and Pucci [32, 33] have performed a more detailed calculations including estimates of vertex correction effects in lowest order. At the sodium density they obtain the value $m^*/m = 1.3$ and somewhat smaller values for larger densities (see Fig. 2). Considering the difference between the apparent and true effective mass values and the uncertainties involved, we feel that the discrepancies between the calculated and observed values need not be significant.

3. Temperature Dependence of Positron Trapping at Vacancies

The many important applications of positron annihilation to the study of defects in solids will be discussed by others during this conference. We will here instead concentrate on the somewhat controversial question of how the different models for the motion of the positron before it annihilates will affect the trapping rate. We also make some comments on the validity of the different models.

The current theory of vacancy trapping is based on the rate equation approach of Brandt [34] which was applied to the trapping in metals by Bergersen and Stott [35] and Connors and West [36]. The basic equations are

$$\left.\begin{aligned} \dot{n}_f &= -\lambda_f n_f - \nu c_t n_f \\ \dot{n}_t &= -\lambda_t n_t + \nu c_t n_f \end{aligned}\right\} \tag{11}$$

Here n_t and n_f are, respectively, the probabilities that the positron is trapped and free at time τ after it is injected, λ_t and λ_f are the trapped and free annihilation rates, c_t is the trap concentration and ν the average trapping rate per unit vacancy concentration. We have in (11) neglected the possibility that once trapped, the positron can escape. This is certainly justified in a metal such as Al if one considers the estimated binding energy of a positron to a vacancy (Arponen *et al.* [37] found the value 2.6 eV, while Hodges [38] obtained 2.0 and 3.8 eV with and without electron-electron correlations taken into account). In most other metals the binding energy is expected to be somewhat smaller, but it seems reasonable to assume that it is in almost all cases much larger than the thermal energy $k_B T$.

As demonstrated by MacKenzie *et al.* [39] the angular correlation differ markedly in the free and trapped states. The rate equation approach predicts that the observed angular correlation curves should be linear combinations of curves associated with the pure free and trapped states. The weighting factors are proportional to the respective probabilities R_f and R_t of annihilation from these states

$$R_t/R_f = \nu c_t/\lambda_f . \tag{12}$$

The equilibrium vacancy concentration at temperature T is given by

$$c_t = A e^{-E_v/k_B T} \tag{13}$$

with A an entropy factor and E_v the vacancy formation energy. MacKee *et al.* [40] obtained accurate vacancy formation energies from angular correlation data taken at different temperatures, using an Arrhenius plot based on (12) and (13). In principle, the accuracy of the method depends on the extent to which one knows the temperature dependence of the trapping rate ν, although in practice other uncertain factors are probably more or equally important. In any case the temperature dependence of ν is a question which has been much discussed recently.

The conventional way to calculate transition probabilities in quantum mechanics is to use the "golden rule" expression. This approach was used by Hodges [38] and is further discussed by Bergersen and Taylor [41]. The trapping rate $\nu_{\boldsymbol{p}}$ for a positron with wave vector $\boldsymbol{p}$ is, in such a model, given by the expression

$$\nu_{\boldsymbol{p}} = 4\pi \sum_{\boldsymbol{k},\boldsymbol{q}} |M(\boldsymbol{p},\boldsymbol{k},\boldsymbol{q})|^2 \delta(E_t - E_{\boldsymbol{p}} + \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}}) . \tag{14}$$

The binding energy liberated in the trapping process is of the order of an electron volt and therefore the process involves creation of particle-hole pairs which absorb at least most of the excess energy. For this reason it was assumed in [38] and [41] that the matrix element has the following form

$$M(\boldsymbol{p},\boldsymbol{k},\boldsymbol{q}) = \frac{4\pi e^2}{\Omega q^2 \, \varepsilon(\boldsymbol{q},0)} \langle \boldsymbol{p}-\boldsymbol{q} | \boldsymbol{l} \rangle f_{\boldsymbol{k}}(1 - f_{\boldsymbol{k}+\boldsymbol{q}}) . \tag{15}$$

Here $|\boldsymbol{p}\rangle$ represents a positron Bloch state and $|\boldsymbol{l}\rangle$ the state vector for a trapped positron at site $\boldsymbol{l}$.

From the discussion in Section 1 one can assume the positrons to be approximately thermalized. Neglecting the small deviations discussed in Section 2, we assume a Boltzmann-type positron momentum distribution. This gives for the mean trapping rate per unit vacancy concentration

$$\nu = \frac{1}{\Omega_0} \sum_{\boldsymbol{p}} \left(\frac{2\pi}{m^* k_B T} \right)^{3/2} e^{-p^2/2m^* k_B T} \nu_{\boldsymbol{p}} . \tag{16}$$

Since the positron trapping energy is large compared to $k_B T$, the Bohr radius of the trapped state will be short compared to typical thermal de Broglie wave lengths. The matrix element in (15) will then be approximately independent of the $\boldsymbol{p}$-vector, i.e. of the temperature. The same holds for the phase space factor in (14). The "golden rule" model thus predicts an essentially temperature independent trapping rate, as was confirmed by explicit numerical calculations in [41].

Connors and West [36] and Connors *et al.* [42] predict a different behaviour by assuming that the positron follows a collision-free path to the trap. They too assume a Boltzmann-type positron velocity distribution resulting in a mean velocity given by

$$v = (8 k_B T/\pi m)^{1/2} . \tag{17}$$

By treating the positron as a classical particle they get

$$\nu = \sigma v/\Omega_0 = \pi a^2 v/\Omega_0 , \tag{18}$$

where a is a trapping radius which was approximately given by the Thomas-Fermi screening length, and σ is the trapping cross-section. This model results in a $T^{-\frac{1}{2}}$-law for the trapping rate ν.

Seeger [43] has recently proposed a third model for the vacancy trapping of positrons. He also works with a velocity independent trapping radius. Seeger makes the additional observation that at realistic temperatures the positron must be expected to suffer many collisions with a mean free path which is short compared to a typical intertrap separation. The reaction should therefore be considered as diffusion controlled (Waite [44]) and one has

$$\nu = 4\pi a D/\Omega_0 , \tag{19}$$

where the diffusion coefficient D is given by the Nernst-Einstein relation

$$D = k_B T \mu , \tag{20}$$

μ being the positron mobility. Seeger [43] assumed that the mobility is limited by scattering with acoustical phonons and, at least qualitatively describable, by deformation-potential theory (see e.g.

Conwell [45]). We thus have (Bergersen and McMullen [46])

$$\mu = \frac{2eS\varrho}{3E_1^2}\left[\frac{2\pi}{m^5 k_B^3 T^2 T_p}\right]^{\frac{1}{2}}. \tag{21}$$

Here ϱ is the mass density and E_1 the deformation potential parameter (rate of change of the energy of the bottom of the positron band per unit dilation of the crystal). The effective positron temperature T_p will be equal to the crystal temperature T if the positron is completely thermalized and essentially independent of T if the thermalization is incomplete. Seeger [43] only considered the former case and thus arrived at a trapping rate which was proportional to $T^{-1/2}$.

From the discussion in Section 1 one would expect that the mobility is phonon-limited only for low temperatures. At higher temperatures the positron is most effeciently slowed down by excitation of particle-hole pairs. In that case the mobility should be proportional to T^{-2} instead of the $T^{-3/2}$ behaviour obtained from (21), and then the above model would give a trapping rate proportional to T^{-1}. We plan to present elsewhere estimates of the positron diffusion constants in some simple metals taking both the phonon and electron-hole contributions into account.

Returning to the framework of the theory based upon the "golden rule" we note that the positron-phonon interactions (which limit the positron mobility) enter in two distinct ways [24]. The first way is in vertex corrections to the trapping matrix element, but if the traps are deep compared to the Debye energy, this effect must be insignificant. The interactions contribute also to the positron self-energy and what they do is to modify the quasi-positron momentum distribution, which is the quantity that enters in (16). But as discussed in connection with this equation the modification will not be important in the present context if the traps are deep compared to $k_B T$. Thus the mobility, which is the critical quantity within the framework of diffusion controlled reactions, does not enter in the "golden rule" model as a very significant parameter. (Note, however, that the same factors which control the mobility also affect the "apparent effective mass" discussed in Section 2.)

The model of Connors and West and that of Seeger are both tied to the classical concept of a capture radius. Once the positron gets close enough, it is assumed to become always trapped – the problem is to get it there. In order to feel confident about the "golden rule", however, in a situation where a large fraction of the positrons are trapped, one would like to imagine a situation where the positron normally samples many vacancies before it gets trapped. In that case (15) gives a trapping cross section inversely proportional to the positron velocity. The fact that the fast positron samples more traps would then be compensated by the slow ones lingering longer. This means that the validity of the respective models is tied to the strength of the potential, or to be more specific, the validity is tied to the importance of multiple scattering terms in the t-matrix for trapping.

Bergersen and Taylor [41] estimated numerically the importance of these terms in a simple model and found them to be small. What would happen if in a more realistic calculation the correction terms turned out not to be so small? If mobility-limiting collisions can be neglected the only effect of this would be that the true trapping cross section would replace the "golden rule" result in the formula relating the trapping rate to the cross section. It seem, however, unlikely that the fundamental v^{-1}-dependence of the cross section will change, unless it should happen that an s-wave resonance lies near the thermal energy range for free positrons. When, in addition, the collisions are taken into account diffusion aspects will also, in principle, modify the result. It is, however, not expected [41] that such effects will modify the temperature dependence of the trapping rate. We therefore feel that of the proposed models the "golden rule" approach of Hodges [38] gives the most satisfactory description of the trapping process when the trapping potential is weak, while models that work with a velocity independent trapping radius probably never give a quantum mechanically consistent description.

Several conflicting opinions have been expressed also regarding the experimental situation. Seeger [47] quotes results by Connors *et al.* [48] from quenching experiments on Cd which indicate a trapping rate proportional to $T^{-1/2}$ in agreement to his model. This is, however, not confirmed by later work by Connors and Bowler [49]. Recent experiments by McKee *et al.* [50] in Au give results which are compatible with a T^0 behaviour i.e. the Hodges model [38], while Hall *et al.* [51] interprete their Au data in terms of a T^α-law, where $0.5 < \alpha < 1.0$. As pointed out by Cotterill *et al.* [52] it is quite hard to sort out the possible role of dislocations and va-

cancy clusters in these experiments. We do not know whether this is the reason for the discrepancies.

4. Positron Channeling

When energetic charged particles penetrate a crystal lattice in certain crystallographic low-index directions they will experience a strong steering effect caused by succesive correlated small angle scattering events with a large number of lattice atoms. This phenomen is called particle channeling and has been demonstrated experimentally with a wide variety of heavy ions and target materials (for a review see e.g. Datz *et al.* [53]). Channeling experiments have also been conducted with electrons and positrons in Si by Walker *et al.* [54] and Morokhovskii *et al.* [55], in alkali halides by Didenko *et al.* [56], and in Si and anthracene by Armağan Ok [57]. However, only few results on electrons and positrons channeling in thin metal single-crystal foils have been reported in the literature. Uggerhøj [58], Uggerhøj and Andersen [59] have studied the phenomenon in copper doped with Cu^{64} and Uggerhøj and Frandsen [60], Andersen *et al.* [61] in gold.

We will here discuss changes observed in the Rutherford scattering yield in the low-index direction in thin gold crystal foils. The results are essentially equivalent in the case of copper, where the Cu^{64} positron source was part of the material and directional effects of emission also were observed [58, 59].

For the scattering measurements a beam of positrons must be obtained. A well-collimated positron beam can be produced by accelerating positrons from a Co^{58} source in a 1-MeV electron Van der Graaff [61]. This method has the advantage of increasing the total intensity within a fixed solid angle and reducing the relative energy spread of the original positron spectrum. The dips for positrons and peaks for electrons in the Rutherford scattering yield are then studied by mounting the fcc gold single-crystals on a suitable goniometer set-up, allowing various tilts of the incoming beam to crystallographic axial or planar directions. Pronounced dips in the normalized scattering yield were found experimentally [61] in thin gold single crystals for various directions ($\langle 110\rangle$, $\langle 111\rangle$, $\langle 112\rangle$). Outside the minimum the dip has marked compensating shoulders, the size of which depends strongly on the azimuthal angle of the axial scan, indicating the importance of various planar channeling effects [59].

Lindhard [62] has presented a classical theory of the directional effects and according to him the observed half-widths for channeling along a crystallographic axis should be proportional to the critical angle ψ_1 defined as

$$\psi_1 = \{2Z_1 Z_2 e^2/\tfrac{1}{2}pvd\}^{\frac{1}{2}}, \quad \text{when} \quad \psi_1 < a/d\,. \tag{22}$$

Here Z_1 and Z_2 are the atomic numers of the incoming particle and the lattice ion, respectively, a is a screening distance of the string of atoms in the chosen direction, obtained in a continuum approximation for the scattering potential, d is the lattice spacing along the string and p the momentum and v the velocity of the penetrating particle. In the same continuum approximation the minimum yield $X_{\min}$ is expressible as

$$X_{\min} = \frac{Nd}{\Omega}\pi(\varrho_\perp^2 + a^2)\,, \tag{23}$$

where $\varrho_\perp^2$ is the mean-square thermal displacement perpendicular to the string of atoms. A recent modification has been proposed by Kubota and Ohtsuki [63] by taking into account the temperature and energy dependence in a more complicated way.

The proportionality constant between the half-width of the dip and ψ_1 includes the effect of thermal vibrations of atoms in crystal lattice. According to Andersen [64] the value for the proportionality constant in the case of gold is about 0.8. This means e.g. that the theoretical value for the half-width from (22) is about 20% larger than the experimental value in the $\langle 110\rangle$ direction. Since discrepancies of this magnitude are not unusual for heavy particle channeling, a more decisive test as to the applicability of classical channeling theory to the case of positrons would be a comparison with protons channeling with the same value for $1/2\,pv$. This has been done in [61] and the agreement obtained is very good both for the half-width and the minimum yield. From the results it can be concluded that in the axial case quantum corrections are not essential.

Lervig *et al.* [65] have given a thorough discussion of the possible quantum corrections to the classical channeling theory for positrons. They find that electrons and positrons are expected to behave more in a non-classical way than would a heavy

particle (e.g. wave interference due to inelastic collisions with atoms of the string and tunneling into classically forbidden potential regions). One way to estimate the relative importance of quantum effects in the axial and planar channeling is to look at phase space estimates for the respective transitions. When this is done, the above conclusions for the applicability of the classical theory for the axial case seem reasonable. For the planar channeling, say for the {111} plane, the number of bound states in the transverse phase space is so small that one might expect the planar dips to exhibit more structure due to quantum effects. The measurements in [61] had not, however, enough accuracy to resolve the interference "wiggles" in planar channeling. Pedersen *et al.* [66] have lately observed this fine structure in thin Si crystals for the planar dips.

It should finally be mentioned that Kudrin *et al.* [67] have simulated the positron scattering in single crystals as a series of classical binary collisions with the lattice atoms. The results of such a calculation compares well with the experimental curve for the ⟨110⟩-axial dip in gold of [61]. This fact gives further confidence to the conclusion that relativistic positrons follow essentially the classical theory of channeling.

5. Escape of Low Energy Positrons from Metal Surfaces

The main interest in the study of the escape of low energy positrons from the surface of different materials arose from the possibility of obtaining positron beams with a small energy spread for atomic collision experiments (for a review of this aspect of the problem see Keever *et al.* [68]).

The conceptually simplest way to obtain such a beam is to slow down a fraction of the randomly directed fast positrons that escape from a β^+-active source. A positron gun with an energy spread of a few keV that is based on this principle was described by Lohnert and Schneider [69]. The difficulty with this method is that the yield, necessarily, would become very small if a much better energy resolution were required.

An alternative approach is based on the experimental observation that low energy positrons with energy of the order of eV are emitted from certain metals or metal coated surfaces of different materials [68, 70–75]. The simplest way to explain this phenomenon is to assume a negative positron work function. The most thorough theoretical evaluation of the positron work function, up till now, is that of Hodges and Stott [76] who analyzed it in terms of three contributions:

1. The Band Structure or Zero Point Energy E_0

The origin of this term is the repulsive positron-ion interaction, and E_0 can be identified with the bottom of the positron band in a band structure calculation. Hodges and Stott [76] tabulated values of E_0 for a large number of metals. The calculations were performed in the Wigner-Seitz approximation. The ions are described by a Hartree potential obtained from atomic structure calculations with special provisions for the *d*-electrons in the noble metals. In all metals (except for the alkalis and magnesium where it is smaller) E_0 was found to be positive and of the order of 1/3 Ry.

2. The Electron-Positron Correlation Energy E_{corr}

This is the energy associated with the attractive interaction between the positron and the conduction electrons. We expect it to approach -0.5 Ry, the free positronium value, for low densities. For higher densities E_{corr} will be still lower. Hodges and Stott [76] compute E_{corr} for an electron gas of the same densities as in the metals of interest from the electron positron correlation function $g^{+-}(r, Z)$. Here $Ng^{+-}(r, Z)/\Omega$ is the average electron density at a distance r from a "positron" of charge Z,

$$E_{\text{corr}} = \frac{-3e^2}{r_s^3} \int_0^1 dZ \int_0^\infty dr r[g^{+-}(r, Z) - 1] . \qquad (24)$$

The pair correlation function was in turn computed by the method of Sjölander and Stott [77, 78] which leads to a simple integral equation. The method diverges for low electron densities. Bhattacharyya and Singwi [79] eliminated this difficulty (at least for metallic densities) by including a density gradient term in the integral equation for the Fourier transformed pair correlation functions. This gives rise to a nonlinear integro-differential equation with one adjustable parameter, which was fitted to give the expected positron lifetime for low densities. Bhattacharyya and Singwi [80] then proceed to compute the positron correlation energy from the pair correlation function of [79]. Other authors [31, 33] have attempted to calculate the correlation energy from the positron self-energy by using diagrammatic methods.

3. The Surface Contribution E_s

The origin of this term is the dipole layer at the metal surface giving a negative contribution to the conduction electron energy. This energy will change sign for positrons, i.e. give a negative contribution to the positron work function. In his calculation of the positron work function Tong [81] made use of the jellium-model calculation of Lang and Kohn [82] for the surface contribution. Hodges and Stott [76] objected against this, because Heine and Hodges [83] have shown that for simple metals other than the alkalis and alkaline earths the ion pseudopotential is considerably more attractive than the jellium potential, thus reducing the electron "spill-over" into the vacuum. The electron work function might still be relatively insensitive to the strength of the pseudopotential because the reduction in the dipole layer is compensated for by the lowering of the band structure energy. The authors of [76] argue that the effect is important in the positron case and they try to take it into account in their calculation.

In the case of Au [76] obtains a negative work function in agreement with experiment, while in most other metals the work function is expected to be positive. The work function for positronium is in all cases lower than for free positrons and is expected to be negative in several metals.

Orth [84] and Pendyala *et al.* [85] have attempted to discuss the low-energy positron yield (number of emitted low energy positrons/number of positrons stopped in the moderator) which for gold surfaces is typically of the order of 10^{-7}. It is difficult to understand the observed spectrum [73] without assuming that the escaping low-energy positrons have first been approximately thermalized in the moderating material. The factors which influence the yield are expected to be [84]:

a. The Distribution of Stopped Positrons throughout the Volume of the Metal

This distribution can be taken to be fairly uniform, if the thickness t of the metal is not large compared to the positron range in the material.

b. The Positron Diffusion Length L

It can be expressed in the form

$$L = (lv/3\lambda_R)^{\frac{1}{2}},$$

where v is the average velocity, l the mean free path and λ_R the rate at which positrons are removed from the distribution of free positrons. Neglecting trapping mechanisms the diffusion length has been estimated [85, 86] to be about 500 Å. Vacancy trapping will reduce the positron diffusion length, but probably not more than by an order of magnitude.

c. The Probability of Escape

If positrons would always escape whenever they approach the surface layer, the yield would be approximately equal to L/t, leading to considerably higher yields than have been observed [84]. Hodges and Stott [87] have pointed out that the image potential when a positron is close to the metal surface leads to a deep potential "gutter" just outside the metal. Although no estimate has been made of this, it is plausible that a very large fraction of the positrons will be trapped by this potential. This is supported by the fact that the yield is very sensitive to surface treatment. Keever *et al.* [68] report that marked increases in the yield was obtained when the surfaces were not too clean and a slight leak maintained in the vacuum system. It should be mentioned that Canter *et al.* [88] obtained a remarkably high yield of 10^{-5} from a gold moderator covered with a layer of powdered MgO.

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