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# The Temperature Dependence of the Diffusion Coefficient and of the Trapping Rate of Positrons in Metals

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**Abstract.** The paper explores the consequences of metastable self-trapping of positrons for the temperature variation of positron diffusion coefficients and trapping rates. It is shown that the diffusion coefficient is expected to decrease with increasing temperatures from a value determined by the scattering of positron Bloch waves by acoustic phonons to a much lower one governed by a hopping process. The temperature variation of the rate of trapping by small defects such as vacancies is more complicated since only at high temperatures can we expect it to be limited by the positron diffusion coefficient. At low temperatures the observed magnitude of the rate of trapping at monovacancies can only be understood if the trapping rate is controlled by the rate of capture of positrons that have arrived at the trap.

**Index Headings:** Positrons – Vacancies in metals – Positive muons

In recent years positron annihilation has become a widely used tool for the investigation of vacancy-type defects, dislocations, and voids in metals (for reviews see [1–7]). The quantitative analysis of such experiments is based on the so-called trapping model. In its simplest, original form [8–10] the trapping model compares the rate $\sigma$ at which thermalized positrons are trapped by a unit concentration of defects with the annihilation rate of the positrons. From this the product $\sigma C$, where $C$ is the concentration of the defects capable of trapping positrons, but not the individual quantities $\sigma$ and $C$ may be deduced.

According to the preceding discussion, positron annihilation measurements alone can at best give relative variations of the concentration of traps. When investigating trapping of positrons by monovacancies one often employs the temperature variation of the equilibrium concentration of monovacancies, $C_{1V}^{eq}$, which obeys the simple Arrhenius law

$$C_{1V}^{eq} = \exp(S_{1V}^F/k_B)\exp(-H_{1V}^F/k_BT). \tag{1}$$

In (1) $H_{1V}^F$ and $S_{1V}^F$ denote the enthalpy and the entropy of formation of monovacancies; as usual, $k_B$ is Boltzmann's constant and $T$ the absolute temperature. Fitting of (1) to positron annihilation measurements in order to determine $H_{1V}^F$ requires the knowledge of the temperature variation of the trapping rate $\sigma_{1V}$ of monovacancies. In 1972 the present author pointed out that in metals the diffusion coefficient $D_+$ of thermalized positrons in metals must be expected to depend on temperature, and that, as a consequence, $\sigma_{1V}$ may also be temperature dependent [11, 12]. Since then a considerable amount of theoretical [6, 13, 14] and experimental [15–17] work has been done in order to determine the temperature variation of the capture cross-sections of, say, monovacancies in metals. No clear and generally accepted picture has emerged from these studies.

The present paper intends to develop a more general view of the theoretical situation than has been given hitherto. It will be seen that the recently discovered possibility [18] of a self-trapped (polaron-like) positron state with *negative* binding energy adds unexpected new features to the problem. It is suggested that some of the difficulties in obtaining a well-defined temperature dependence of $\sigma_{1V}$ are associated with the existence of this metastable self-trapped state, which is thought [18] to be responsible for the "intermediate" temperature dependence in the temperature variation of positron annihilation in metals [19, 20]. While it will be possible to resolve some of the existing discrepancies, at least qualitatively, we shall see that difficulties remain, particularly in the determination of monovacancy formation enthalpies from high-temperature positron annihilation experiments. It appears likely that investigations using positive muons will help to solve some of these problems. Therefore, throughout this paper free reference will be made to muon experiments, the details of which will be discussed elsewhere [21].

## 1. Estimates of Diffusion Coefficients of Positrons in Metals

By analogy with positive holes in non-degenerate semiconductors, the notion of diffusion coefficient of thermalized positrons in metals is intuitively clear. Not so clear is the quantitative relationship between the positron diffusion coefficient $D_+$ and the capture rate per unit atomic concentration of traps. Brandt and Waung [22], as well as Seeger [11, 12], used Waite's formula [23]

$$\sigma = 4\pi D_+ r_0/\Omega_A \,. \tag{2}$$

In (2) the trap is characterized by a capture radius $r_0$; $\Omega_A$ denotes the atomic volume. The difference in energy between the lowest trapping state and the ground state of untrapped positrons will be denoted by $\Delta\varepsilon$.

The physical concept behind (2) is that any positron that has reached the trap during its diffusive motion falls immediately into the trap. However, by analogy to electron-hole recombination in semiconductors, the transition into the bound state may be a rather slow process if the energy $\Delta\varepsilon$ that the positron has to give up is large compared with the maximum phonon energies in the crystal. In positron studies of defects in thermal equilibrium this is always the case, since trapping can be observed only if [1]

$$\Delta\varepsilon > k_B T \ln(k_B T \tau_t/h)\,, \tag{3}$$

where $h$ denotes Planck's constant, and $\tau_t$ the lifetime of trapped positrons. In thermal equilibrium measurements $k_B T$ is comparable with or larger than the maximum phonon energies and the logarithm in (3) is large compared with unity, hence $\Delta\varepsilon$ is large compared to the phonon energies. Frank and Seeger [24] have, therefore, considered a more general situation, in which the positrons have to overcome a barrier before falling into the bound state at the trap. They obtain the following expression for the trapping rate

$$\sigma \approx \sigma(\infty) = \frac{4\pi r_0}{\Omega_A} \frac{1}{\dfrac{1}{D_+} + \dfrac{1}{k_0 r_0 \Delta r_0}} \,. \tag{4}$$

Here $\Delta r_0$ denotes the width of the barrier and $k_0$ the rate-constant for the capture by the trap. We see that the slower of the two processes (diffusion – characterized by the positron diffusion coefficient $D_+$ – or capture – characterized by the quantity $k_0 r_0 \Delta r_0$) determines the trapping rate $\sigma$ and hence its temperature variation [1].

In situations in which the main part of the positron energy to be given up during the capture process cannot be carried away by phonons, the most important process determining the positron capture rate in metals is presumably the excitation of electron-hole pairs. This process, which should be essentially independent of temperature, has been treated by Hodges [25], and by Bergersen and Taylor [26].

Seeger [11, 12] proposed that the mechanism limiting the mobility of thermalized positrons in metals is the scattering by acoustic phonons. This has recently been supported by Bergersen *et al.* [27], who considered the excitation of electron-hole pairs as an alternative mobility limiting process. For an elastically isotropic solid one finds for the scattering by acoustic phonons [6, 11, 12] [2]

$$D_{ph} = \frac{2}{3} \frac{(2\pi)^{1/2}\hbar^4 Y}{(m_+)^{5/2}(\varepsilon_d)^2(k_B T)^{1/2}} \cdot \frac{(1-\mu)}{(1-2\mu)(1+\mu)} \,, \tag{5}$$

where $m_+$ is the effective positron mass, $\varepsilon_d$ the positron deformation potential constant [11], $\hbar = h/2\pi$, $Y =$ Young's modulus and $\mu =$ Poisson's ratio. The mean

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[1] In the literature the nomenclature on "trapping" and "capture" is not uniform. We propose to distinguish between the *trapping* rate $\sigma$ and the *capture* rate $k_0$ or $k_0 r_0 \Delta r_0$.

[2] Equation (3.7) of [6] contains a printing error: $h^4$ should be replaced by $\hbar^4$.

free path of the positrons is given by [28]

$$l_{ph}=\frac{\pi\hbar^4 Y}{m_+^2\varepsilon_d^2 k_B T}\,\frac{1-\mu}{(1-2\mu)(1+\mu)}\,. \tag{6}$$

Equations (5) and (6) hold for temperatures [12, 13]

$$T\geqq T_0\equiv 12\,\frac{m_+ Y(1-\mu)}{k_B(1-2\mu)(1+\mu)\varrho}\,. \tag{7}$$

Below $T_0$ the positron diffusion coefficient, as limited by phonon scattering, increases exponentially with decreasing temperature ($\varrho$ = density of the solid).

The validity of (5) has been discussed in detail [13]. The principal result is that above $T_0$ the $T^{-1/2}$-dependence of $D_{ph}$ (and hence also the $T^{-1}$-dependence of $l_{ph}$) should remain valid for thermalized positrons under quite general conditions.

In all the preceding considerations the assumption has been made that the positrons may be described by Bloch-type waves or by wave-packets formed from them. Of course, this picture is applicable only if the positron mean free path is larger than the interatomic distance. For a numerical example we use the elastic data of aluminum ($Y=7.142\cdot 10^{12}$ erg/cm$^3$, $\mu=0.34$ [29]), $\varepsilon_d=10$ eV and $T=600$ K. We then find that for a mean free path of $2.4\cdot 10^{-8}$ cm Eq. (6) gives us an effective mass $m_+=10\,m_e$, where $m_e$ is the free electron mass. Since the band-mass of positrons is unlikely to exceed $m_e$ by more than a factor of two, we may conclude that for free or quasi-free positrons the mean free path $l_{ph}$ is long enough for (5) and (6) to be applicable.

If the positron mobility is limited by the excitation of electron-hole pairs Bergersen *et al.* [27] estimated the diffusion coefficient

$$D_{eh}=\frac{4}{\pi}\,\frac{m_e}{(m_+)^2}\,\frac{\hbar\varepsilon_F}{k_B T}\,, \tag{8}$$

where $\varepsilon_F$ denotes the Fermi energy. It is true that $D_{eh}$ decreases more rapidly with increasing temperature than $D_{ph}$, but the temperature at which $D_{eh}=D_{ph}$, i.e., above which the excitation of electron-hole pairs rather than the phonon scattering would limit the positron mobility, lies so far above the melting point that we may completely disregard the effect of the electron-hole excitation on the positron diffusion coefficient. In conclusion, except for quite low temperatures where complete thermalization of positrons is not achieved anyway, phonon scattering must be considered the dominant mobility-limiting process in pure metals[3,4].

Using the same assumptions as in the above estimate of $l_{ph}$ together with $m_+=m_e$ we find $D_+=12.3$ cm$^2$/sec. The high-temperature experiments on aluminum give [30]

$$\sigma\exp(S^F_{1V}/k_B)=1.2\cdot 10^{15}\ \mathrm{sec}^{-1}\,. \tag{9}$$

If we insert $S^F_{1V}/k_B=0.6$ [5] and the atomic volume $\Omega_A$ of aluminum, we may tentatively use (2) to deduce a capture radius $r_0=0.71\times 10^{-10}$ cm. This value is unrealistically small. The numerical values of $m_+$ and $\varepsilon_d$ may be somewhat larger than assumed in our estimate, but hardly to the extent to bring $r_0$ into the range of $2\cdot 10^{-8}$ cm. It is tempting to conclude that for monovacancies in aluminum $k_0 r_0 \Delta r_0 \ll D_+$ and that in this case the capture of positrons in the bound state is rate-determining, i.e., that we may simplify (4) to give

$$\sigma=4\pi k_0 r_0^2 \Delta r_0/\Omega_A\,. \tag{10}$$

However, since the quantum mechanical transition rate is essentially temperature-independent, such a conclusion would mean that $\sigma$ should be temperature-independent over a wide temperature range. This is at variance with recent observations on Al [16] and Au [17], reporting a $T^{\alpha}$-dependence with $\alpha=1.2\pm 0.3$ [16] and $\alpha=0.9\pm 0.1$ [17].

We must therefore look for an alternative explanation for the numerical discrepancy found above. We recall that in the derivation of (5) and (6) the assumption has been made that the positrons are in Bloch states. There is the alternative possibility that they are self-trapped in polaron-like states giving rise to a displacement of neighbouring atoms. The consequences of this possibility for positron diffusion and trapping will be explored in Section 2.

## 2. The Effects of Self-Trapping

The fact that the diffusion of both protons (see, e.g., [31]) and positive muons [32] in metals proceeds by

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[3] Estimates based on the theory of scattering of electrons by lattice imperfections show that this statement also holds if the scattering of positrons by impurities or dislocations is taken into account. See also Brandt [7].

[4] We use the opportunity to point out that the assumption $D_{eh}\sim T^{1/2}$ made in Ref. [6], Fig. 3, is in error. This error arose from an erroneous statement in a preprint of [14], which has been corrected in the printed version. It is regretted that because of the overlap of the production schedules of [6] and [14] this error could not be eliminated from [6]. In view of what has been said above, the reference to electron-hole pair creation should be completely eliminated from Ref. [6], Fig. 3.

thermal activation indicates that positively charged elementary particles may be localized on interstitial sites in metals. This "self-trapping", which is accompagnied by a distorsion of the matrix surrounding the positively charged particle, has recently been treated semi-quantitatively [18] following the work of Toyozawa and Sumi [33] on self-trapping of positive holes in semiconductors. In the present context the most important result is that a particle with mass $m_+$ and elementary positive electric charge may be self-trapped in a metal if

$$2\pi \frac{K}{\varepsilon_d^2} \frac{\hbar^2}{m_+} \equiv \kappa_{\max} < \kappa_0 . \tag{11}$$

Here $K$ is an elastic constant of the matrix and $\kappa_0$ of the order of magnitude $2 \cdot 10^{+7}\,\mathrm{cm}^{-1}$. If the stronger condition

$$\kappa_{\max} < 2\kappa_0/3 \tag{12}$$

is satisfied, the binding energy in the self-trapped state is positive, i.e., the self-trapped configuration is stable relative to a free or quasi-free ("Bloch-wave type") particle. For muons, protons, and deuterons (11) and (12) are fulfilled for any reasonable choice of the deformation potential constant $\varepsilon_d$ and of $K$. If, however,

$$2\kappa_0/3 < \kappa_{\max} < \kappa_0 , \tag{13}$$

the self-trapped state lies above the Bloch-wave state by an energy

$$\varepsilon_0 \equiv \varepsilon_0(\kappa_0) = \frac{3\pi\hbar^2}{2m_+} \kappa_0^2 \left(1 - \frac{2\kappa_0}{3\kappa_{\max}}\right) > 0 . \tag{14}$$

In this situation, which may be realized for positrons in metals, the self-trapped positron state is metastable with respect to the Bloch-wave state. It is virtually unpopulated at temperatures $T \ll \varepsilon_0/k_B$. At temperatures $T \gg \varepsilon_0/k_B$ practically all positrons are in the self-trapped state.

At intermediate temperatures the diffusion coefficients of "free" (Bloch-wave) positrons, $D_f$, and of self-trapped positrons, $D_{st}$, have to be weighted according to the probabilities

$$f_f = \frac{1}{1 + AT^{-3/2} \exp(-\varepsilon_0/k_B T)} \tag{15a}$$

and

$$f_{st} = 1 - f_f = \frac{1}{1 + A^{-1} T^{3/2} \exp(\varepsilon_0/k_B T)} \tag{15b}$$

that a positron is "free" or self-trapped. The numerical parameter $A$ is such that $AT^{-3/2}$ is large compared with unity. The average positron diffusion coefficient is thus given by

$$\bar{D}_+ = D_f f_f + D_{st} f_{st} = D_{st} + (D_f - D_{st}) f_f . \tag{16}$$

$D_f$ has been estimated earlier [11–13], comp. (5). For the estimation of $D_{st}$ different physical pictures may be used. These have recently been reviewed by Stoneham [34], and we may therefore be rather brief.

The self-trapped positively charged particles may be considered as "quasi-particles". In an unbounded crystal we may form "Bloch states" for these quasi-particles; the energy eigenvalues associated with these Bloch states form a band structure[5]. The general ideas of conductivity theory may then be used to calculate mean free paths, mobilities and diffusion coefficients of the quasi-particles, as limited by the scattering by phonons (see, e.g., [35]). Even if the self-trapping of a positron leads to a change in the interatomic distances by only a few percent, the effective mass of the particles will be much larger than the free positron mass. The estimate at the end of Section 1 indicates that this will reduce the positron diffusion coefficient and the positron mean free path so much that the Bloch-wave picture becomes inapplicable.

The alternative description is to consider the self-trapped positrons as *localized* on individual interstitial sites, and to treat their motion from one interstitial site to an adjacent one as a hopping process. Since the positron (and also positive muons and protons) are light compared with the lattice atoms, they are able to follow the lattice vibrations almost instantaneously. The theory of rate processes in such situations has been developed by Flynn and Stoneham [34, 36] and by Kagan and Klingler [37]; it has been shown to be fairly successful for hydrogen in metals [34]. For temperatures above the Debye temperature and for so-called "direct" processes, in which the energy barrier $\Delta E$ for the hopping process comes entirely from the need to "shift" the lattice displacement

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[5] The formation of Bloch states out of the self-trapped configurations localized at different lattice sites (which are indeed degenerate in an unbounded crystal) may lead to a lowering of the energy. However, because of the large effective mass of the quasi-particles the band-width is small compared with the free positron band width. The treatment introduced elsewhere [18, 33] and used above, in which the self-trapped state is characterized by one energy parameter $\varepsilon_0$ to be eventually determined by fitting experimental data, appears completely adequate. Therefore, we continue to speak of "self-trapped" particles on the one hand, and Bloch-type particles on the other hand, in the latter case referring to positrons without appreciable lattice distorsions.

associated with self-trapping from one interstitial site to the next, one finds for the diffusion coefficient

$$D_{st}=\frac{a^2}{2\hbar}\sqrt{\frac{\pi}{\Delta E k_B T}}\,|J|^2\exp(-\Delta E/k_B T)\,. \tag{17}$$

In (17) is has been assumed that the lattice sites form a simple, body-centred, or face-centred cubic lattice with edge-length $a$ of the elementary cube. $J$ denotes the matrix element between wave-functions located at two adjacent interstitial sites, and $\Delta E$ is the activation energy needed to take the lattice from its configuration with the charged particle on the initial site to that with the particle on the final site. If the jump geometry is such that the jumping charged particle has to open up a window formed by neighbouring atoms, the activation energy contains an additional term, and the pre-exponential $T^{-1/2}$-factor is replaced by a temperature-independent term [36].

## 3. Discussion

In contrast to the positron case, in many metals the diffusion coefficient of positive muons may be measured without recourse to trapping phenomena. The diffusion coefficient of positive muons in copper may be represented by an Arrhenius-type temperature dependence with an activation energy of $\Delta E = 0.047$ eV [32]. We may conclude from this that the positive muon *is* self-trapped, in agreement with the theoretical estimates [18], and that it moves by a hopping process, again in agreement with our estimate of Section 3. (The mass of a free muon is $m_\mu = 207\ m_e$.)

For positrons there is considerable experimental evidence [19, 20] that in many metals the self-trapped state is metastable, with $\varepsilon_0$ being of the order of magnitude of a few tenth of an eV [18]. This means that at low temperatures (but above $T_0$)[6] the positron diffusion coefficient is given by (5). At intermediate and high temperatures $\bar{D}_+$ has to be calculated from (16). On account of the large effective mass associated with self-trapped positrons[7] in this temperature range $D_{st}$ is given by (17) or its generalization. $D_f$ decreases with increasing temperature and is large compared to $D_{st}$, which increases with increasing temperature except for $T > \Delta E/k_B$. Taken together with (15) this results in a complicated temperature dependence of $\bar{D}_+$, particularly if $\Delta E$ is comparable in magnitude with $\varepsilon_0$.

Positron diffusion coefficients are usually deduced from trapping experiments [7, 38]. If there are no long-range forces between positrons and traps, (4) should be a fairly good approximation to the relationship between trapping rate $\sigma$ and positron diffusion coefficient $D_+$. We have already indicated that Bloch-type positrons have presumably difficulties in getting rid of their energy at small traps such as monovacancies[8]. In such a situation $k_0 r_0 \Delta r_0$ is likely to be small compared with $D_+$ and temperature-independent, giving us the essentially temperature-independent trapping rate (10).

The existence of self-trapping changes the situation of the preceding paragraph in two ways: (i) $\bar{D}_+$ is smaller than $D_{ph}$ as given by (5), and may in fact – at least in a certain temperature range – become so small that it falls below the capture coefficient $k_0 r_0 \Delta r_0$ calculated from the electron-hole excitation mechanism. (ii) The coupling of a self-trapped particle with the lattice is likely to be so strong that a positron that has arrived at the trap has no difficulty in giving up to the lattice the energy difference $(\Delta\varepsilon + \varepsilon_0)$ between a self-trapped and a defect-trapped positron. At temperatures larger than $T^* \equiv \varepsilon_0/\ln(A T^{*\,-3/2})k_B$, where diffusing positrons spend more than half their time in the self-trapped state [18], $k_0 r_0 \Delta r_0$ is thus expected to increase rapidly with increasing temperature, until (4) may eventually be replaced by (2). For positive muons, protons, deuterons etc. this simple situation is likely to obtain over the entire temperature range accessible to experiments because of $\varepsilon_0 < 0$.

For positrons, however, we have to expect a more complicated temperature dependence $\sigma(T)$ if self-trapping occurs with $\varepsilon_0 > 0$, as appears to be the case for many metals. It is therefore not surprising that the attempts to deduce $\sigma(T)$ from rather limited experiments [15–17, 39] have not been successful. In particular, the comparison between low-temperature experiments on quenched-in vacancies and high-temperature experiments on the equilibrium vacancy concentration should be considered with utmost caution, since in the low-temperature experiments the positron diffusion coefficient may be given by (5)

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[6] With $m_+ = m_e$ Eq. (7) yields for aluminum $T_0 = 21$ K.

[7] Note that the transition between the self-trapped and the Bloch-type positron configuration is discontinuous [18]; hence in the self-trapped state $m_+$ may always be expected to exceed $m_e$ by a large factor.

[8] In this context "small" means small compared with the de Broglie wavelength of thermalized positrons. The wavelength of thermalized positrons is indeed large compared with the interatomic distance, particularly at low temperatures, i.e., in that temperature range in which for $\varepsilon_0 > 0$ diffusing positrons spend most of their time in Bloch-type states.

whereas at high temperatures the positron behaviour is dominated by self-trapped positrons.

Simple results for the temperature variation of $\sigma$ can only be expected in temperature ranges where one and the same mechanism dominates. This condition is likely to be fulfilled in the experiments of McKee *et al.* [15], who compared the differences in the mean positron lifetimes between 100 K and 275 K of annealed gold and of gold that had been quenched from 923 K. Within their experimental error they find that $\sigma$ is independent of temperature. Since the observations of Triftshäuser and McGervey [40] indicate that in gold $T^*$ lies well above room temperature, this is in agreement with the idea that $(k_0 r_0 \Delta r_0)^{-1}$ is the dominant term in gold at low temperatures. It must be said, however, that Hall *et al.* [17] have determined the temperature variation of $\sigma$ between 115 K and 298 K on one gold specimen quenched from 1073 K, and that they report a $T^{1/2}$ temperature variation. Further experiments are clearly necessary.

We may ask the question whether it is possible to perform low-temperature trapping experiments on traps which are large enough for the capture at the trap to determine no longer the trapping rate. Cheng and Swanson [41] have measured the lifetimes of positrons in quenched Al+0.09 at.-% Mn single crystals between 77 K and 300 K. They found two lifetimes, a short temperature-independent one, which they consider as the average lifetime of positrons annihilating in the bulk and in small vacancy defects (monovacancies, divacancies etc.), and a longer lifetime $\tau_2$, which they attribute to the annihilation of positrons trapped in voids. The authors give arguments why under their quenching and annealing conditions voids may have formed in a concentration detectable by positron annihilation. The temperature dependence of the trapping cross-section associated with $\tau_2$ is found to be proportional to $T^{-\beta}$ with $\beta = 0.3 < \beta < 0.8$ and thus compatible with a $T^{-1/2}$-law. The authors interpret this as evidence for the $T^{-1/2}$ temperature dependence of the positron diffusion coefficient, Eq. (5), in a situation in which the capture barrier is negligible because of the large size of the traps. The observed increase of $\tau_2$ with increasing temperature is accounted for by the Hodges-Stott-Nieminen-Manninen model of surface trapping of positrons in aluminum [42, 43].

The interpretation of Cheng and Swanson may be tested by extending the measurements to lower temperatures. The $T^{-1/2}$-law cannot hold at very low temperatures; it must either be replaced by a faster rise below $T_0$ (which, according to (7), depends on the effective positron mass) or by a cut-off associated with the finite capture rate $k_0$. If the interpretation proves to be correct it verifies the predicted $T^{-1/2}$-dependence of the positron diffusion coefficient [11, 12] and offers the possibility, through a determination of void sizes and number densities by electron microscopy and X-ray or neutron small-angle scattering, to deduce the absolute value of $D_{ph}$.

Paulin *et al.* [44] have recently made an attempt to measure $D_+$ on fine-grained metal powders, making use of surface trapping. From experiments on Ni, Fe, Co, and NiFe-alloys they deduced $D_+ = (1.0 \pm 0.5)$ $10^{-2}$ cm$^2$ sec$^{-1}$ at 300 K. This value is clearly much too low to be compatible with (5). There are several possibilities that might account for this discrepancy: The assumption of no capture barrier at the surfaces may be in error; there may be additional trapping in the matrix, making $D_+$ an apparent diffusion coefficient; or $T^*$ may be so low that the self-trapping mechanism is operative already at 300 K.

Positrons are also trapped by dislocations, which are extended defects, too. They might, therefore, provide a possibility for determining $D_{ph}$ experimentally. However, long-range drift terms may become significant [6], and this introduces an additional temperature dependence into the trapping rate. Also, the nature of the bound state at dislocations is at present not too well known. It appears that additional work is needed before dislocation trapping can be used as a tool to measure positron diffusion coefficients.

The discrepancy, mentioned at the end of Section 1, between the capture cross-section determined from high-temperature experiments and that calculated from (2) and (5) with reasonable assumptions on the capture radius $r_0$ of monovacancies, appears to be a general phenomenon for metals [1]. It is qualitatively accounted for by the concept of metastable self-trapping discussed in Section 3, which leads to a considerable reduction of the positron diffusion coefficient relative to that of Bloch-type positrons[9]. Quantitative comparisons between experiment and theory require the evaluation of the matrix element $J$ appearing in (17).

The theoretical prediction that the diffusion coefficient of self-trapped positrons contains an Arrhenius-type temperature dependence interferes with the accurate

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[9] The empirical reasons why we consider it unlikely that in the case of the high-temperature experiments the discrepancy could be explained entirely in terms of a low *capture* rate at monovacancies have been given at the end of Section 1.

determination of $H^F_{1V}$ from high-temperature equilibrium experiments, since an Arrhenius-type temperature variation of $\sigma$ will be indistinguishable from the temperature variation of $C^{eq}_{1V}$. The values of $H^F_{1V}$ obtained sofar from positron annihilation must be considered as upper limits, requiring more detailed discussion. It is obvious that in this area much further work is needed. Experiments with positive muons, for which the theoretical situation is much clearer [21], should prove helpful.

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