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Resonance trapping of positrons

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Abstract. Trapping of positrons by defects has been investigated by replacing the defects by a complex potential: the real part describes the average potential energy felt by the positron within the defect and the imaginary part indicates the strength of the processes giving rise to the exchange of energy between the incoming positron and the medium. It is shown that not only the positron s-wave resonance but also p and d resonances make substantial contributions to the trapping rate of positrons in the thermal energy region. Because of the resonance effect, the specific trapping rate is very sensitive to the trapping potential and does not increase monotonically with the defect size. Furthermore, in the neighbourhood of a resonance, the specific trapping rate depends strongly on the incoming positron energy. This resonance model can consistently account for many long-standing problems in the study of positron trapping.

It has been well established that positrons entering metals are thermalised in a very short time ($\sim 10^{-12}$ s), tend to be trapped by lattice defects such as vacancies, vacancy clusters, voids and dislocations, and are annihilated with observable characteristics which directly reflect the electronic structure of the type of defect in which they are trapped (West 1979). Considerable efforts have been made to treat theoretically the positron-trapping rate at defects in metals. Most of the previous approaches were made using the Fermi Golden Rule (Hodges 1970) or the continuum theory of nuclear reactions (Brandt 1974) and have predicted little or no temperature dependence of the specific trapping rate for monovacancies, small vacancy clusters and dislocations in metals (Nieminen and Manninen 1979). Recently, however, some groups (Hautojärvi *et al* 1981, Hashimoto *et al* 1985, Shirai *et al* 1987) observed a strong temperature dependence of the positron trapping rate which cannot satisfactorily be interpreted on the basis of existing theories.

It seems that both the Golden Rule (or the Born approximation) and the continuum theory are not such good approximations when the incident energy is small compared with the potential energy as in the case of thermal positrons interacting with defects in metals. Alternatively the trapping rate ν can be calculated (Shirai and Takamura 1980, 1987, Shirai 1983) using the 'cloudy-crystal-ball' model (Feshbach *et al* 1954) which is more applicable to the case of lower incident energy than the continuum theory: one of the main consequences is the appearance of resonance in the trapping cross section, which has been precluded in calculations using the previous theories. Very recently, McMullen and Stott (1986) and Puska and Manninen (1987) have also pointed out the substantial role of positron resonance trapping by vacancies and their small clusters. In

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this paper, we show by using the cloudy-crystal-ball model that not only s- but also p- and d-wave resonances considerably enhance the trapping even in the thermal energy region. This model provides explanations not only for the strong temperature dependence of the specific trapping rate observed but also for existing problems such as the pre-vacancy effect (Smedskjaer 1983) and trap–non-trap and saturation–non-saturation behaviour of a annihilation parameters for thermal vacancies in various metals.

In the cloudy-crystal-ball model, a positron, once entering a defect, has a finite chance of leaving without being trapped, i.e. without exchanging energy or momentum with the medium, which is neglected in previous approaches. In this case, actual trapping of a positron that has entered the defect occurs only with a probability smaller than unity, and the defect acts upon the incoming positron as a potential well. Hence the effect of the defect on the incident positron can be described as the effect of a potential well with absorption. Thus, the defect can be replaced by a complex potential which acts on the incoming positron.

For simplicity, we employ a square-well potential given by

$$\begin{aligned} V &= -V_0(1+\mathrm{i}\zeta) \qquad & r<R \\ V &= 0 \qquad & r>R \end{aligned} \tag{1}$$

at radius r where ζ is the absorption coefficient and R is the defect radius. The real part V_0 describes the average potential energy felt by the positron within the defect. The trapping is brought about by the imaginary part ζV_0, which indicates the strength of the processes giving rise to the energy exchange between the incoming positron and the medium. The value of ζ is to be determined from the specific energy absorption mechanism. Usually, a binding energy of the order of 1 eV for trapping of the positron is liberated and then consumed by the electron–hole excitation in metals (West 1979, Nieminen and Manninen 1979, Nieminen 1983). Then, the value of ζ may turn out to be dependent on the binding energy as was shown by Hodges (1970). However, we simply use a constant value of ζ which would not affect the general qualitative features, since the purpose of the present approach is to show some salient features of resonance trapping.

Since we know the value of the logarithmic derivative of the positron wavefunction u_l at the defect boundary for each angular momentum l,

$$f_l = R(u_l'/u_l)_{r=R} \tag{2}$$

the cross section σ for the positron trapping at the defect can be obtained from the expression due to Feshbach *et al* (1954)

$$\sigma_l/\pi R^2 = (4/x^2)(2l+1)s_l[-\operatorname{Im} f_l/(M_l^2+N_l^2)] \tag{3a}$$

$$\sigma = \sum_l \sigma_l \tag{3b}$$

where

$$\Delta_l + \mathrm{i}s_l = 1 + xh_l'(x)/h_l(x) \tag{4}$$

$M_l = s_l - \operatorname{Im} f_l$ and $N_l = -\Delta_l + \operatorname{Re} f_l$. Δ_l and s_l both have real magnitudes and are defined as the real and imaginary part of the expression on the right-hand side of equation (4). The function h_l is the spherical Hankel function, while x is kR. Here k is the wavenumber of the incoming positron. $h_l'(x)$ is the derivative of $h_l(x)$ with respect to x.

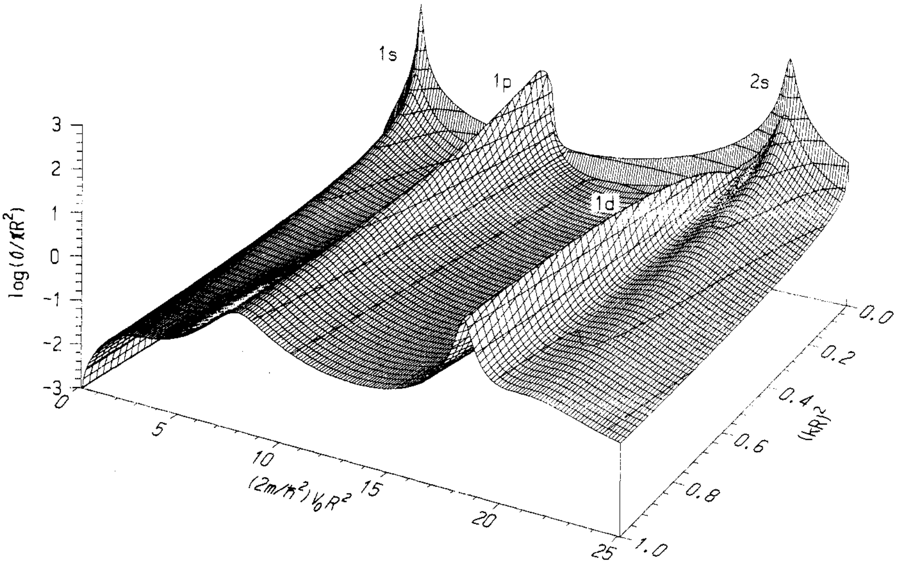

Figure 1. Normalised trapping cross section $\sigma/\pi R^2$, showing the resonance behaviour due to s, p and d waves, as a function of positron energy in units of $(kR)^2$ and the defect trapping potential in units of $X_0^2 = (2m/\hbar^2)V_0R^2$, for an absorption coefficient $\zeta = 5 \times 10^{-3}$.

For the potential (1), following Feshbach *et al* (1954), f_l is written down directly as

$$f_l = 1 + Xj_l'(X)/j_l(X) \tag{5}$$

where $X^2 = x^2 + X_0^2(1 + \mathrm{i}\zeta)$ and $X_0^2 = (2m^*/\hbar^2)V_0R^2$.

The function j_l is the spherical Bessel function and m^* is the positron effective mass. For $l = 0$, we get

$$f_0 = X \cot X \tag{6a}$$

$$\mathrm{Re} f_0 = \frac{X_1 \sin 2X_1 + X_2 \sinh 2X_2}{\cosh 2X_2 - \cos 2X_1} \tag{6b}$$

$$\mathrm{Im} f_0 = \frac{X_2 \sin 2X_1 - X_1 \sinh 2X_2}{\cosh 2X_2 - \cos 2X_1} \tag{6c}$$

where $X = X_1 + \mathrm{i}X_2$. The recurrence relations which follow from

$$f_l = X^2/(l - f_{l-1}) - l$$

are

$$\mathrm{Re} f_l = \frac{(X_1^2 - X_2^2)(l - \mathrm{Re} f_{l-1}) - 2X_1X_2 \,\mathrm{Im} f_{l-1}}{(l - \mathrm{Re} f_{l-1})^2 + (\mathrm{Im} f_{l-1})^2} - l \tag{7}$$

$$\mathrm{Im} f_l = \frac{(X_1^2 - X_2^2)\,\mathrm{Im} f_{l-1} + 2X_1X_2(l - \mathrm{Re} f_{l-1})}{(l - \mathrm{Re} f_{l-1})^2 + (\mathrm{Im} f_{l-1})^2}. \tag{8}$$

Figure 1 shows the normalised trapping cross section $\sigma/\pi R^2$ as a function of the positron energy in units of $(kR)^2$ and the defect trapping potential in units of

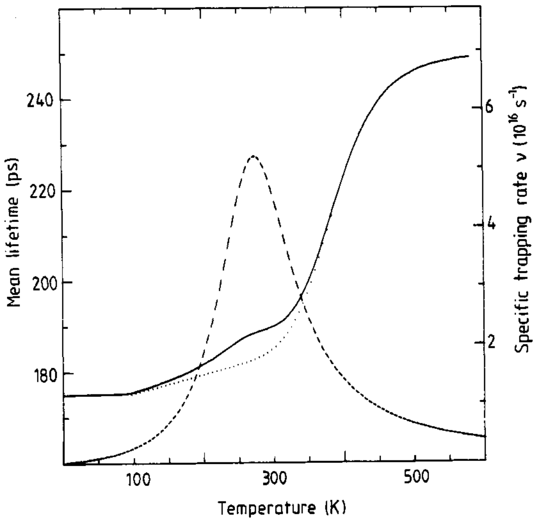

Figure 2. Positron mean lifetime, and specific trapping rate ν for vacancies in Cd. Full curve: lifetime simulated using likely parameter values $\zeta = 1 \times 10^{-3}$, $n = 4.64 \times 10^{22}$ cm^{-3}, $R =$ 1.73 Å, $V_0 = 12.5$ eV, vacancy formation enthalpy $H_v^F = 0.54$ eV and entropy $S_v^F = k_B$, and residual vacancy concentration $C_v^{res} = 1 \times 10^{-8}$. Dotted curve as full curve, but neglecting residual vacancies. Broken curve, specific trapping rate calculated using the present model.

$X_0^2 = (2m/\hbar^2)V_0R^2$ calculated on the basis of the potential represented by equation (1). In the numerical calculation, the rest mass was used since the positron effective mass m^* is not accurately known, and also the value of the parameter ζ was chosen as 5×10^{-3} in order to yield specific trapping rates in the range experimentally obtainable, i.e. 10^{12}–10^{16} s^{-1}. As the value of ζ is increased the resonance becomes less pronounced. Since we know the positron trapping cross section σ, the specific trapping rate ν is determined by $\nu = nv\sigma$, where n is the atomic density of the metal and v the velocity of positrons. For thermal positrons $v = (3k_BT/m^*)^{1/2}$ with effective mass m^* and Boltzmann's constant k_B and the thermal positron wavenumber $k = (3m^*k_BT/\hbar^2)^{1/2}$.

The most notable features of this model are as follows.

(i) The specific trapping rate ν gives maxima as a function of the defect radius R and the potential depth V_0.

(ii) On resonance, surprisingly high values of ν are attainable, particularly for small values of $(kR)^2$, i.e. at low energies.

(iii) In the vicinity of an s resonance, the trapping rate ν sharply increases toward the zero positron energy due to the zero-energy resonance of the positron s wave.

(iv) In contrast to the s-resonance case, a p or d resonance gives a maximum of ν at an intermediate positron energy as a consequence of the centrifugal force.

(v) For cases in which the resonance conditions are not satisfied, the trapping cross section σ displays a v^{-1} cross section behaviour, leading to a temperature-independent trapping rate as has been shown by previous investigators (Brandt 1974, Hodges 1974).

The above results have several implications. Firstly, trap–non-trap, and saturation–non-saturation problems can be well understood, since the specific trapping rate for vacancies in metals can extend over several orders of magnitude, i.e. 10^{12}–10^{16} s^{-1}, depending on whether or not the resonance condition is satisfied. Secondly, the zero-energy resonance effect of positron s waves provides a plausible explanation for the anomalous rise of the positron trapping rate recently observed at low temperatures (Shirai *et al* 1987, Hashimoto *et al* 1985, Linderoth *et al* 1985, Bentzon *et al* 1985, de Diego *et al* 1985, Smedskjaer 1983). Thirdly, the pre-vacancy effect observed in some metals (Smedskjaer 1983) can be explained as a manifestation of p-resonance trapping by vacancies as shown in figure 2. The strongly temperature-dependent trapping observed by Hautojärvi *et al* (1981) can also be explained as a p or d resonance by some vacancy clusters.

A square-well trapping potential was used in the present calculations, but in reality the potential would have a diffuse boundary, not the sharp one used here. A realistic potential would dampen the resonance behaviour. Furthermore, the value of ζ should be dependent on the binding energy and may differ somewhat from metal to metal. However, even if a value of ζ an order of magnitude higher is adopted, the general features of the results, such as the resonance position and the energy dependence, do not vary significantly (Shirai and Takamura 1987).

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