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Angular distribution of positrons emitted from metal surfaces

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The effect of inelastic scattering processes on the angular distribution of positrons spontaneously emitted from metal surfaces is investigated. Angular and energy spectra are calculated for positrons suffering energy loss due to electron-hole excitation in emission from materials with low (aluminum) and high (tungsten) positron work functions.

Positrons thermalized in bulk solids are spontaneously emitted from negative work function surfaces.[1] Upon emission, the positron may lose part of its kinetic energy to inelastic excitations at the surface. When the magnitude of the positron work function is of the order of an electron volt, the main inelastic mechanism at a metal surface is the creation of an electron-hole pair. Under some circumstances, the coupling to other local modes such as adsorbate vibrations can be large, as demonstrated by Fischer *et al.*[2] for CO on Ni. The acronym RE-PELS (reemitted positron energy loss spectroscopy) has been coined[2] for the technique which can complement the more familiar electron energy loss spectroscopy, particularly in the low-energy region.

For adsorbate studies, it is important to know the emission spectra for clean, well-characterized surfaces. We have recently[3] reported a calculation of the energy loss spectra for positrons spontaneously ejected from metal surfaces. Although the calculations show reasonable agreement with experiment,[4] the comparison is made difficult by the fact that measurements of the perpendicular energy cannot distinguish between an inelastic event and off-normal emission from faceted or rough surfaces. This paper reports an extension of Ref. 3 to full energy and angle dependent emission spectra. We show the characteristic angular shapes expected for electron-hole excitation. These should be useful in detailed studies of angle-resolved positron emission.

The model we use here is the same as in Ref. 3. The crystalline potential for the positron contains a simple step at the surface and a square well just outside, mimicking the image interaction which can support a bound state. The conduction electrons of the metal are confined in the metal by an infinite barrier, and the electron-positron interaction is statically screened. Thus the Hamiltonian reads

$$H = H_0 + U_{ep} , \qquad (1)$$

with

$$H_0 = T_e + T_p + V_e(z) + V_p(z) . \qquad (2)$$

Here T_e and T_p are the kinetic energy operators for electrons and positrons, respectively. The electron potential $V_e(z)$ has an infinite barrier at $z=0$, while the positron potential $V_p(z)$ is approximated by

$$V_p(z) = \begin{cases} |\phi_+| , & z \leq 0 , \\ -V_0, & 0 \leq z \leq d , \\ 0, & z \geq d , \end{cases} \qquad (3)$$

where ϕ_+ is the (negative) positron work function of the metal and V_0 and d the surface well parameters. The electron-positron interaction $U_{ep}(r)$ has the screened Thomas-Fermi form

$$U_{ep}(\mathbf{r}) = -\frac{1}{r} e^{-\mu r} , \qquad (4)$$

where μ is treated as an adjustable parameter.

The probability Λ_{fi} of a positron leaving the metal to scatter from a state of initial momentum $\mathbf{p}_i$ to a final state characterized by an outgoing momentum $\mathbf{p}_f$ is obtained from the Golden Rule formula

$$\Lambda_{fi}(\mathbf{p}_f, \mathbf{p}_i) = \frac{2\pi}{\hbar} \sum_{\substack{\mathbf{k},\mathbf{q} \\ |\mathbf{k}+\mathbf{q}| > k_F}} |M_{fi}(\mathbf{k},\mathbf{q})|^2$$

$$\times \delta \left[E_f - E_i + \hbar^2 \frac{(\mathbf{k}+\mathbf{q})^2}{2m} - \frac{\hbar^2 k^2}{2m} \right] , \qquad (5)$$

where E_f (E_i) is the final (initial) state energy and M_{fi} the matrix element of the interaction potential U_{ep} between the initial and final states. Following Ref. 3, we use box-normalized eigenfunctions of H_0, whereby

$$M_{fi}(\mathbf{k},\mathbf{q}) = \frac{4\pi}{L^3}\delta_{\mathbf{P}_f,\mathbf{P}_i+\mathbf{Q}}$$

$$\times \int_{-\infty}^{\infty} dz\, \psi_f(z)\left[\frac{\cos q_z z}{Q^2+q_z^2+\mu^2}\right.$$

$$\left. -\frac{\cos(2k_z+q_z)z}{Q^2+(2k_z+q_z)^2+\mu^2}\right]$$

$$\times \psi_i(z) \ . \tag{6}$$

Above, L is size of the normalizing box in the z direction and $\mathbf{P},\mathbf{Q}$ denote the momentum components parallel to the surface. ψ_f and ψ_i are the positron initial and final wave functions, respectively. The analytic expressions corresponding to the potential (3) can be written down in straightforward way. We include temperature effects by introducing a thermal energy spread of $\frac{3}{2}k_B T$ in the kinetic energy of the initial state.

The expression for the differential probability of inelastic scattering per single encounter with the surface is given in terms of Λ_{fi} as

$$\frac{d\tilde{\Lambda}}{dE_{fz}d\theta} = \frac{L^3}{(2\pi)^3}\frac{2L}{\hbar p_{iz}}\frac{1}{\hbar^2 p_{fz}}2\pi p_{fz}^2$$

$$\times \tan\theta(1+\tan^2\theta)\Lambda_{fi}(\mathbf{p}_i,\mathbf{p}_f) \ , \tag{7}$$

where θ is the angle measured from the surface normal and p_{iz}, p_{fz}, and E_{fz} are the initial and final momenta in the z direction and the final perpendicular kinetic energy, respectively. It follows that

$$\tan\theta = \frac{P_f}{p_{fz}} \ . \tag{8}$$

The total angular distribution of the emitted positrons, irrespective of their kinetic energy, is obtained by integrating (7) over energy to the maximum $|\phi_+|$:

$$\frac{d\tilde{\Lambda}}{d\theta} = \int_0^{|\phi_+|} dE_{fz}\frac{d^2\tilde{\Lambda}}{dE_{fz}d\theta} \tag{9}$$

while the total rate of transmission is given by an additional integral over the angle as

$$\tilde{\Lambda} = \int_0^{\pi/2} d\theta \int_0^{|\phi_+|} dE_{fz}\frac{d^2\tilde{\Lambda}}{dE_{fz}d\theta} \ . \tag{10}$$

The algebraic details are discussed in Refs. 3 and 5. The integrals over the surface parallel momenta can be done analytically, but the remaining double integral over k_z and q_z must be carried out numerically.

In Figs. 1–5 we present numerical results for the energy and angular spectra for representative cases. We have chosen the parameters to mimic both a high ($\phi_+ = -3.1$ eV, tungsten) and a low ($\phi_+ = -0.3$ eV, aluminum) positron work function material.[1] The well parameters V_0 and d are chosen to give an image-potential bound state at an energy $E_b = 3.0$ eV below the vacuum level in both cases. The conduction electron system in the infinite barrier model is represented by its density (in terms of the usual density parameter r_s), and the screening parameter is chosen to be $\mu = 0.3\mu_{TF}$, where μ_{TF} is the Thomas-
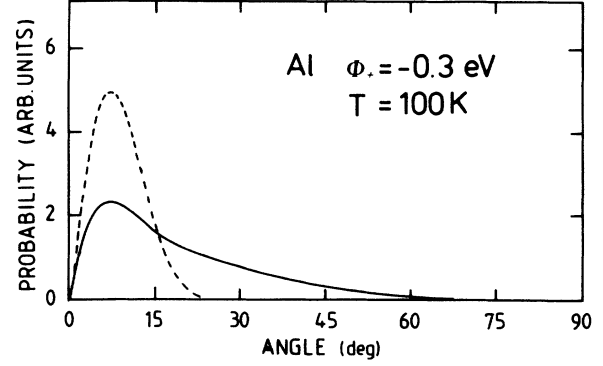

FIG. 1. The total angular distribution of positrons inelastically emitted from a low work function surface (Al, $\phi_+ = -0.3$ eV) at $T = 100$ K (solid curve) as compared to the distribution of elastically emitted positrons (dotted curve).
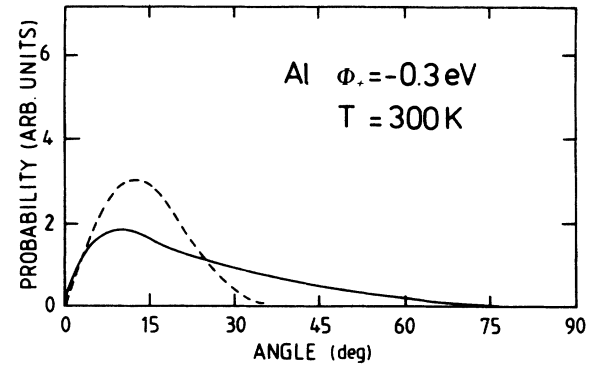

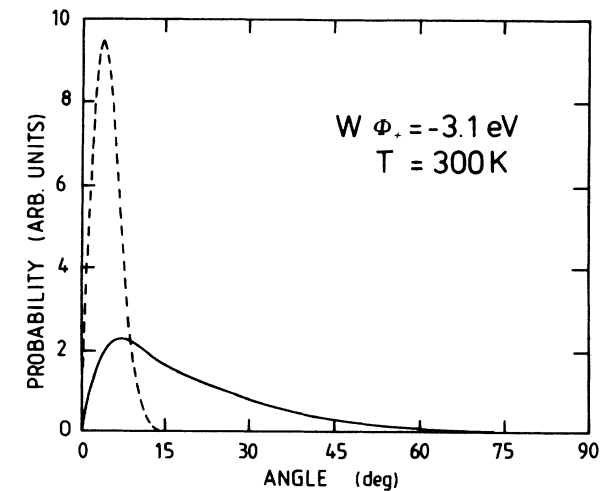FIG. 2. The same as Fig. 1, but for $T = 300$ K.

FIG. 3. The total angular distribution of inelastically emitted positrons from a high work function surface (W, $\phi_+ = -3.1$ eV) at $T = 300$ K.
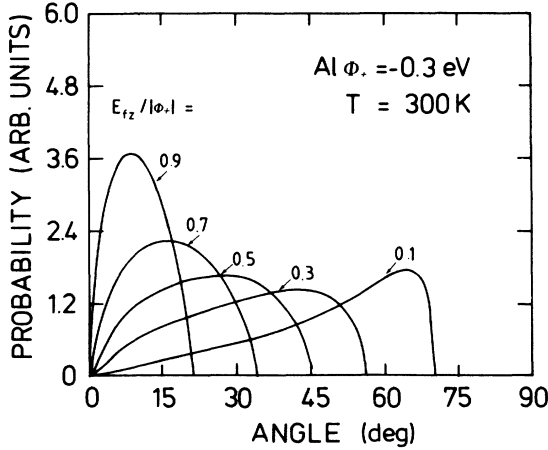
FIG. 4. The angular distributions of positrons with fixed final kinetic energy E_{fz} emitted from Al at $T=300$ K.
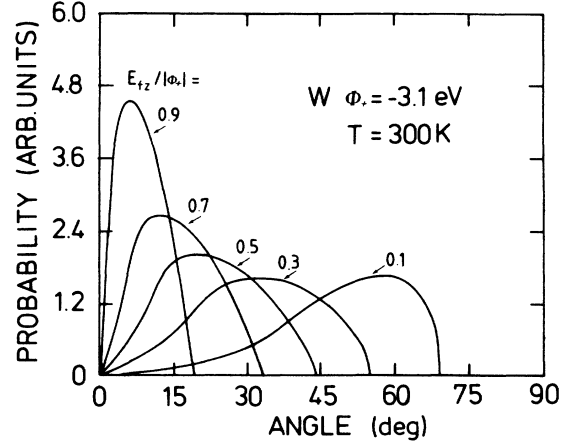

FIG. 5. The angular distributions of positrons with fixed final kinetic energy E_{fz} emitted from W at $T=300$ K.

Fermi screening constant of the bulk metal.[3] The value of the screening parameter is not critical to the shapes of the angular distributions. It does have an effect on the absolute values of the emission probabilities, as discussed in Ref. 3.

Figures 1 and 2 show the total angular distribution of positrons inelastically emitted from a low work function (Al) surface as compared to the elastic emission at two representative temperatures, $T=100$ and 300 K. The elastic current is characterized by the most probable half-angle for emission, $\theta_{1/2}$,

$$\theta_{1/2}=\frac{k_B T}{|\phi_+|} \ . \tag{11}$$

As expected, the inelastic distribution is wider, but the difference diminishes at higher temperatures because of thermal smearing of the initial positron energy. The

effect of inelastic scattering in broadening the angular distribution can be used to distinguish between elastically and inelastically emitted positrons. Even for a small work function material, such as Al, pronounced inelastic broadening is obtained by lowering the temperature to 100 K.

Figures 4 and 5 show the angular distributions for fixed final kinetic energies E_{fz} for the motion in the z direction in the case of Al and W, respectively. Those positrons suffering the largest inelastic losses have the widest angular distributions, and the angular distribution eventually starts to peak near the maximum angle allowed by kinematics. Note that for the low work function material the elastic curve (Fig. 2) is actually wider, as the tail comes from positrons having excess (thermal) energy in the surface parallel direction.

If one assumes a constant matrix element M_{fi} in Eq. (5), it can easily be converted into energy space as

$$\Lambda_{fi}(E_f,E_i)=\frac{2\pi}{\hbar}\int_0^\infty dE\, \rho_-(E)\rho_-(E+E_i-E_f)\rho_+(E_f)f(E)[1-f(E+E_i-E_f)]\,|M_{fi}|^2 \ , \tag{12}$$

where ρ_- (ρ_+) is the density of electron (positron) states and f the Fermi function. Taking the free-particle formula for the latter and assuming the electron density of states to be a constant near the Fermi level one obtains

$$\Lambda_{fi}(E_f,E_i\approx\phi_+)=\mathrm{const}(\phi_+-E_f)\sqrt{E_f} \ . \tag{13}$$

The current of transmitted positrons above perpendicular energy E_{fz} is

$$T(E_{fz})=\int_{E_{fz}}^{|\phi_+|} dE\, \Lambda_{fi}(E,\phi_+)$$

$$=\mathrm{const}\,|\phi_+|^{5/2}\left[\frac{4}{15}+2x^{3/2}\left[\frac{1}{3}-\frac{x}{5}\right]\right] \ , \tag{14}$$

where $x=E_{fz}/|\phi_+|$. Equation (14) is exactly the result of Pendry,[6] who derived it from the concept of positroni-

um formation and subsequent breakup at the surface region. We see that Pendry's result for the energy distribution is simply the constant-matrix-element limit of the Golden Rule formula (5), and as such analogous to the Berglund-Spicer[7] model of photoemission. In contrast, the full energy and momentum dependence of the matrix element and the phase-space limitations are considered here.

In summary, in Ref. 3 and here we have presented results for the energy and angular distributions of positrons inelastically scattered off electron-hole pair excitations when leaving a planar metallic surface. We have not included phonon excitations as their effect in blurring the angular spectra is expected to be small: the maximum energy loss in a single phonon event is small compared to the work function. The spectra should prove useful in analyzing in detail positron energy loss spectra. The calculations are based on the Golden Rule formula for the

transition rate. The characteristic shapes of the inelastic spectra are largely model independent and we conclude that angular distributions should allow experiments to distinguish positrons elastically emitted from the surface from those undergone inelastic scattering. It should be noted that the absolute values for the total inelastic rates do depend on the model parameters, and consequently accurate branching ratios are difficult to calculate. More-over, the role of dynamic corrections[8] on the branching ratios is not clear.

[1]For a general review of positron surface physics, see A. P. Mills, Jr., in Proceedings of the International School "Enrico Fermi," Course LXXXIII, edited by W. Brandt and A. Du-pasquier (North-Holland, Amsterdam, 1983); P. J. Schultz and K. G. Lynn, Rev. Mod. Phys. (to be published).

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