energies, is not likely to be instrumental since at 1 eV the resolution of the spectrometer is very much smaller than the measured width. One can deduce a width of this magnitude if one assumes that the positrons leave an oscillating platform with a mass near that of the electron and with an energy near 1/40 eV. Then in the laboratory frame, the energy of the positrons would be $\sim 1 \pm 2\,(1 \times 0.025)^{1/2}$ eV. Accurate measurements of this width, the angular distribution, and the energy as functions of the source temperature and film thickness are needed. Since the negative work function is largely a surface effect, extreme care with surface conditions will have to be taken.

The yield of positrons was between 1 and 10 positrons/sec, or between 10^{-7} and 10^{-6} of the total positron yield from the source. This is in essential agreement with the unpublished results of Cherry.[3]

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*All enquiries or correspondence to be addressed to the above.

[1]D. E. Groce, D. G. Costello, J. Wm. McGowan, and D. F. Herring, Bull. Am. Phys. Soc. 13, 1397 (1968); *Proceedings of the VIth International Conference on the Physics of Electronic and Atomic Collisions* (MIT Press, Cambridge, Mass., 1969), p. 757.

[2]L. Madanski and F. Rasetti, Phys. Rev. 79, 397 (1950).

[3]W. H. Cherry, Ph.D. thesis (Princeton University, 1958) (unpublished).

[4]J. M. J. Madey, Phys. Rev. Letters 22, 784 (1969).

[5]W. H. Wilkie and R. D. Birkhoff, Phys. Rev. 135, A1133 (1964).

[6]L. V. Spencer and U. Fano, Phys. Rev. 93, 1172 (1954).

[7]D. A. L. Paul, P. W. Hietala, G. F. Celitans, P. G. Stangeby, and J. Maksimov, Bull. Am. Phys. Soc. 13, 1474 (1968).

[8]W. Kohn (private communication).

[9]J. Callaway (private communication).

[10]B. Y. Tong, following paper, Phys. Rev. B 5, 1436 (1971).

[11]B. Y. Jaduszliwer, T. J. Bowden, and D. A. L. Paul, Bull. Am. Phys. Soc. 15, 785 (1970).

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Negative Work Function of Thermal Positrons in Metals

B. Y. Tong
Department of Physics, University of Western Ontario, London, Ontario
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Theoretical study shows that thermalized positrons are thrown out of a metal with an energy of the order of several eV. This phenomenon is shown to be closely related to the electron work function of metals. Since energy is emitted when positrons leave the metal surface, it is named "negative work function." The negative work function of thermal positrons is $\Phi^p \simeq \Delta\phi^e - \mu_c^p + O(N_p/N)$, where N_p and N are the total number of positrons and electrons, respectively, in the metal. $\Delta\phi^e$ is the electrostatic potential across the metal surface due to the double layer taken from the electron work-function calculation, and μ_c^p is the correlation contribution to the positron chemical potential at the mean electrostatic potential.

Recently observations of low-energy positrons of several eV emitted from metallic surfaces when a high-energy positron source is directed onto the other side of the slab were reported.[1,2] Up to now the accuracy of such experiments[2] only allows us to take these results as qualitative indications of the existence of such low-energy positron sources. Metals and dielectrics like mica or polyethylene were used. Without realizing that such emission is mainly a surface phenomenon, in nearly all cases the material has been coated with a layer of metal, usually gold or chromium. The only quantitative measurement is reported in Ref. 1.

It is well known that high-energy positrons are easily thermalized in metals after a few collisions.[3] The low-energy emission of several eV, which is much larger than the kinetic energy of thermal positron (~0.025 eV), must therefore be related to the energy that a positron receives when it leaves the metallic surface. We call this the negative work function of the thermal positrons in metals. It is qualified by the word "negative" because unlike the electrons, energy is emitted on leaving the metal.

Let us first return to our understanding of the ordinary work function of a metal. The jellium model used in such theory says that the positive ions are replaced by a rigid uniform positive jelly. The electron cloud fills up the whole interior of the metal but it spills over a little near the edge [Fig. 1 (a)]. This leakage of electrons and the excess positive background form a double layer [Fig. 1(b)] first suggested by Frenkel[4] and used by Wigner and

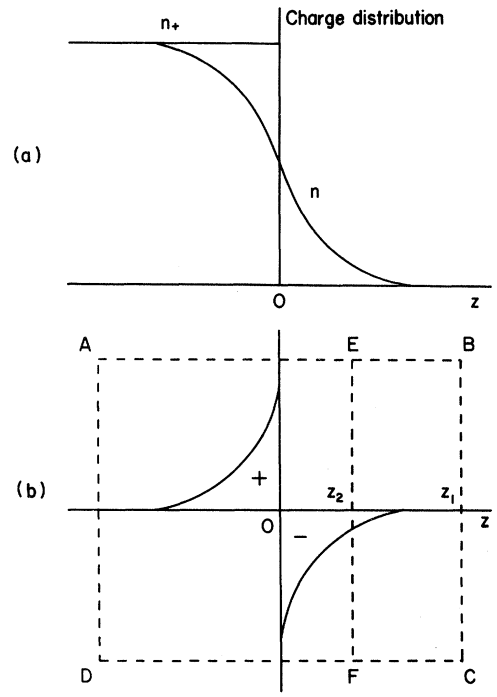

FIG. 1. (a) Charge distribution of a semi-infinite metal with surface at $z=0$ in the jellium model. $n+$ is the positive background and n is the electron density. (b) Double layer. The field at z_1 is zero because there is no net charge inside the box ABCD when $z_1 \gg 0$. At a point z_2 close to the surface the net charge in the box AEFD is positive. The double layer attracts an electron but repels a positron.

Bardeen.[5] The thickness of the double layer is only a few Å.

The double layer attracts an electron when the electron is very close to the surface. This can be seen if we use Gauss's theorem [Fig. 1(b)]. This attractive potential of the double layer is only one of the contributions to the work function of an electron. Fermi statistics and exchange and correlation effects must be included in a good self-consistent calculation. Only in recent years have techniques been developed to successfully calculate the work function.[6–9] Values obtained from a full theoretical calculation and from experiment are in good agreement (5–10%).

A positron, on the other hand, is repelled by the double layer near the surface. There is no exchange effect of the positron with the electron. Of course, Fermi statistics and exchange and correlation effects among the electrons are still the major contributors in determining the true electron-density distribution in the metal.

Let us now examine the above statements more quantitatively. We refer to Lang and Kohn[9] for the proof of an exact expression of the work function Φ^e of an electron in a metal:

$$\Phi^e = \Delta\phi^e - \mu^e, \tag{1}$$

where $\Delta\phi^e$ is the rise in mean electrostatic potential across the metal surface (double layer), and $\mu^e(n)$ is the bulk chemical potential of the electrons at the mean electron density n of the metal interior relative to the mean electrostatic potential. μ^e consists of three terms: the Fermi energy $k_F^2/2m$, the exchange $\mu_x^e(n)$, and the correlation $\mu_c^e(n)$ contributions. In all metals, the work function Φ^e is positive.

We can derive a similar expression for the positron work function:

$$\Phi^p = \Delta\phi^p - \mu^p, \tag{2}$$

where $\Delta\phi^p$ is the lowering of the mean electrostatic potential across the metal surface as described above, and μ^p is the chemical potential of the positron in the metal interior relative to the mean electrostatic potential. This is valid in the small (n_p/n) limit, where n_p and n are the positron and electron densities, respectively.

It should be emphasized here that in these expressions, all many-body effects including the image forces have been taken into account.[9]

In the evaluation[6–9] of $\Delta\Phi^e$, the only parameter entering the calculation is the mean electron density n in the bulk. In the positron case, n is not changed much since the mean density of positrons, n_p, is of the order $n_p/n \simeq 1/N$. We can talk of mean density of positrons, because we know both from experiments and from theory that at metallic densities positrons do not form bound states with electrons.[10–13] It is quite true that electrons crowd around a positron locally, but this does not affect the "mean" electron density in the bulk. Neglecting all contributions coming from terms proportional to n_p as compared to those containing n, we find $\Delta\phi^p(n) \simeq -\Delta\phi^e(n)$. Another way of saying the same

TABLE I. Negative work functions for thermalized positrons in metals. For the sake of reference, we give here a list of common metals and their r_s values: Al (2.1); Mg(2.7); Cu(2.7); Au(3.0)[a]; Na(4.0); K(4.9); Cs (5.6).

r_s	$\Delta\phi^p$[b] (eV)	μ^p (eV)	Φ^p (eV)
2.0	−6.80	−1.89	−4.91
2.5	−3.83	−1.69	−2.14
3.0	−2.32	−1.55	−0.77
3.5	−1.43	−1.43	0
4.0	−0.91	−1.34	0.43
4.5	−0.56	−1.26	0.70
5.0	−0.35	−1.20	0.85

[a] Φ^p for gold is −2.26 eV. If we use Smith's value for $\Delta\phi^e$, then $\Phi^p \sim -1.93$ eV. It may be of interest to compare these theoretical values with the measured value reported in Ref. 1.

[b] From Table I in Ref. 9.

thing is that neglecting corrections of $O(1/N)$, the chemical potential of an electron $\mu^e(n)$ is not changed.[14] Since $\mu^e(n)$ is a unique functional of the density n, it means that to $O(1/N)$, n is not changed, implying

$$\Delta\phi^p(n) = \Delta\phi^e(n) + O(1/N).$$

$\Lambda\phi^e(n)$ have been calculated by various authors[7-9]; a listing of values calculated by Lange and Kohn[9] are shown in Table I. They are of the order of several eV.

We shall now estimate the chemical potential μ^p of positron. The kinetic energy of the thermal positron is taken to be zero. Again neglecting terms proportional to n_p, we have $\mu^p(n) \sim \mu_c^p(n)$. To get a rough estimate of μ_c^p, let us evaluate the ring diagram (Fig. 2) with screened potential

$$v = -(e^2/r)\, e^{-\alpha r}\,, \tag{3}$$

where the screening constant α can be chosen[15] as either the Thomas-Fermi value $\alpha \sim 0.81\, r_s^{1/2}\, k_F$ or the random-phase-approximation (RPA) value $\alpha \sim 0.353\, r_s^{1/2} k_F$. We shall use the former to get an estimate of the magnitude. In addition to the small-momentum-transfer approximation, we shall assume n_p approach zero. This gives the correlation energy

$$\epsilon_c^p(\mathrm{RPA}) \sim -\frac{13.6}{2\pi}\,\frac{k_F}{\alpha} = -2.68 r_s^{-1/2}(\mathrm{eV}), \tag{4}$$

where r_s is the dimensionless parameter $a_B^{-1}(3V/4\pi N)^{1/3}$ and a_B is the Bohr radius. Now

$$\mu_c^p = \frac{d}{dn_p}(n_p \epsilon_c^p) \sim \epsilon_c^p$$

for small n_p. The RPA (static) estimates are listed in Table I. In real situations as compared to the jellium model, there is a local concentration of electrons near a positron.

Even if we suppose this local concentration in electron density is as high as 100 times greater, the above estimates in the static contribution to μ_c^p cannot be off by a factor more than 3. The small-momentum-transfer approximation, however, overestimates the value. A more accurately calculation of μ^p has been made by Bergersen and Carbotte,[16] and their values are close to these estimates. Because of the arbitrariness in both estimates of μ^p and $\Delta\phi^p$, the values in Table I should only be taken as an indication of the existence of negative work function for thermal positrons in some high electron density metals.

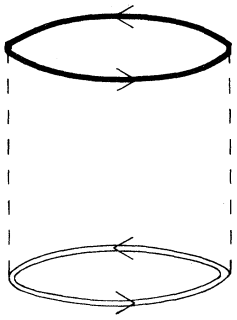

FIG. 2. Ring diagram. The double lines are positron and positron-hole lines, the solid lines are the electron and electron-hole lines, and the broken lines represent the screened interaction [Eq. (2)].

To this date, experiments yielding definite results were carried out at room temperature and pressure.[1,2] As has been indicated in this theoretical study, such observed low-energy positrons of several eV are most likely to be related to the "negative work function." It is a surface phenomenon. We learn from the work-function physicists that surface phenomena are very sensitive to the surface condition, to the purity of the metal, as well as to the presence of absorbed impurities and gases. High vacuum and low temperature are required. Measurements by Pendyala, Orth, Zitzewitz, and McGowan are being carried out under conditions closer to these requirements.[17]

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[1]D. E. Groce, D. G. Costello, J. W. McGowan, and D. F. Herring, *Proceedings of the VIth International Conference on the Physics of Electronic and Atomic Collisions* (MIT Press, Cambridge, Mass., 1969), pp. 757–759.

[2]Qualitative observations were reported by L. Madansky and F. Rasetti, Phys. Rev. 79, 397 (1950); W. H. Cherry, Ph. D. dissertation (Princeton University, 1958) (unpublished); J. M. J. Madey, Phys. Rev. Letters 22, 784 (1969); and D. Paul (private communication).

[3]G. E. Lee-Whiting, Phys. Rev. 97, 1157 (1955); E. J. Woll, Jr. and J. P. Carbotte, *ibid.* 164, 985 (1967); and J. P. Carbotte and H. L. Arora, Can. J. Phys. 45, 387 (1967).

[4]J. Frenkel, Z. Physik 51, 232 (1928).

[5]E. Wigner and J. Bardeen, Phys. Rev. 48, 84 (1935); J. Bardeen, *ibid.* 49, 653 (1936).

[6]A. J. Bennett and C. B. Duke, in *Structure and Chemistry of Solid Surfaces*, edited by G. Somorjai (Wiley, New York, 1969).

[7]J. R. Smith, Phys. Rev. 181, 522 (1969); B 1, 2363 (E) (1970).

[8]N. D. Lang, Solid State Commun. 7, 1047 (1969); N. D. Lang and W. Kohn, Phys. Rev. B 1, 4555 (1970).

[9]N. D. Lang and W. Kohn, Phys. Rev. B 3, 1215 (1971).

[10]J. Callaway, Phys. Rev. 116, 1140 (1959).

[11]A. Held and S. Kahana, Can. J. Phys. 42, 1908 (1964).

[12]H. Kanagawa, Y. H. Ohtsuki, and S. Yanagawa, Phys. Rev. 138, A1155 (1965).

[13]C. K. Majumdar and A. K. Rajagopal, Progr. Theoret. Phys. (Kyoto) 44, 26 (1970).

[14]C. K. Majumdar, Ph. D. thesis (University of California, San Diego, 1965) (unpublished).

[15]D. Pines, Solid State Phys. 1, 373 (1955).

[16]B. Bergersen and J. Carbotte (private communication).

[17]S. Pendyala, R. Orth, P. Zitzewitz, and J. W. McGowan (private communication).