Comment on the plasmon model for image-potential-induced surface states

N. Barberán and P. M. Echenique
Departamento de Física, Universidad de Barcelona, Spain
(Received 22 November 1978)

Calculations of the binding energy of bound positron states in metal surfaces, with explicit inclusion of plasmon dispersion and single-particle effects, are presented. The binding energy is greatly reduced with respect to the undispersed case.

It is well known that a charged particle can be localized by its own image force at a vacuum-medium interface. States of this kind were first suggested on theoretical grounds by Cole and Cohen[1] who noted that liquid helium showed total reflectivity to electrons near the vacuum zero in energy and therefore should trap electrons. The existence of trapped positron states at a void-metal interface has also been suggested.[2,3] In a recent paper Nieminen and Hodges[4] have estimated the dynamic corrections to the image potential of a charged particle at a metal-vacuum interface and hence calculated the binding energy of bound positron states in metal surfaces. They predict that binding should occur for positrons trapped in Al, Ga, Zn, Cd, and possibly other high-density metals. The main contribution to the binding (see Table II of Nieminen and Hodges' paper) comes from the real part of the surface self-energy of the positron state.

Inclusion of surface-plasmon dispersion, and, in an approximate manner, of single-particle effects will reduce the binding energy calculated by Nieminen and Hodges. It is our purpose to estimate by how much. In the specular-reflection model[5] the response of the surface can be expressed in terms of a surface dielectric function $\epsilon(\vec{Q}, \omega)$ related to the bulk dielectric function through

$$\epsilon(\vec{Q}, \omega) = \frac{Q}{\pi} \int_{-\infty}^{\infty} dq_z \frac{1}{(Q^2+q_z^2)\epsilon(\vec{q}, \omega)} , \tag{1}$$

where $q^2 = Q^2 + q_z^2$.

We could take any of the well-known dielectric functions for the bulk and solve Eq. (1) to get $\epsilon_{\vec{Q}}(\omega)$. Instead, and in the spirit of the Lundqvist plasmon-pole approximation to the bulk dielectric constant,[6] we introduce directly a kind of surface-plasmon-pole approximation for $\epsilon_{\vec{Q}}(\omega)$ given by[7]

$$\epsilon_{\vec{Q}}(\omega) = 1 + \frac{\omega_p^2}{[\omega(\omega+i\gamma) - \omega_p^2 - \alpha Q - \frac{1}{4}Q^4]} , \tag{2}$$

where ω_p is the bulk plasma frequency, γ a positive infinitesimal constant, and α is given by

$$\alpha = \sqrt{\tfrac{3}{5}}\, v_F \omega_s , \tag{3}$$

where v_F is the Fermi velocity and $\omega_s = \omega_p/\sqrt{2}$ is the surface-plasmon frequency. This dielectric constant reproduces Ritchie and Marusak's[5] surface-plasmon dispersion for small Q and takes into account in an approximate manner the individual character of the response throughout the Q^4 term. The coefficient $\frac{1}{4}$ is chosen to reproduce the long-Q-limit solution of Eq. (1).

We have calculated the binding energies of positrons trapped at metal surfaces using $\epsilon_{\vec{Q}}(\omega)$ given in Eq. (2) as our surface dielectric constant. The rest of the calculation is analogous to that of Nieminen and Hodges. Table I shows the positron binding energies as a function of the parameter r_s for both Nieminen and Hodges' prescription and for our prescription. As can be seen, inclusion of plasmon dispersion and single-particle effects reduces the binding energy of positron bound states by about 40% with respect to the values of Nieminen and Hodges. According to this calculation positrons would only be trapped in Al and Zn. However, a word of caution about the reliability of this calculation should be said. On the one hand, as pointed out by Nieminen and Hodges the positron states are fairly localized so details of atomic and electronic structure may be important. On the other hand, in our calculation the dielectric response of the metal is only described

TABLE I. Positron binding energies for both Nieminen and Hodges and our results. If $E_B > \phi_B$ (work function) there is a trapped state. All energies are in eV; ϕ_B is the positron work function.

	r_s	$-E_B$ (eV) Nieminen and Hodges	Ours	ϕ_B (eV)
Al	2.07	2.1	1.13	0.7
Ga	2.19	2.3	1.39	2.0
Zn	2.31	2.0	1.11	0.9
Cd	2.59	2.1	1.2	1.8

by the random-phase approximation (RPA). It is well known that the RPA underestimates the electron-positron bulk correlation energy. This could lower the binding energy of the surface state by, perhaps, 1 eV.[8] At the energies where trapping occurs, most of the positron wave function will be inside the metal, hence experiencing the bulk value of the correlation energy.

[1]M. W. Cole and M. H. Cohen, Phys. Rev. Lett. 23, 1238 (1969).
[2]C. H. Hodges and M. J. Stott, Solid State Commun. 12, 1153 (1973).
[3]R. M. Nieminen and M. Manninen, Solid State Commun. 15, 403 (1974).
[4]R. M. Nieminen and C. H. Hodges, Phys. Rev. B 18, 2568 (1978).
[5]R. H. Ritchie and R. Marusak, Surf. Sci. 4, 234 (1966).
[6]B. I. Lundqvist, Phys. Konden. Mater. 6, 206 (1967).
[7]P. M. Echenique, R. H. Ritchie, N. Barberán, and J. C. Inkson (unpublished).
[8]C. H. Hodges and M. J. Stott, Phys. Rev. B 7, 73 (1973).