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## LETTER TO THE EDITOR

# Electron–positron interaction in metals: momentum dependence of HMC and ionic core enhancement factors

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**Abstract.** The momentum dependence of an effective enhancement factor is investigated both for itinerant and core electrons. The local density approach is applied to describe electron–positron interaction.

The possibility of over-enhancement of HMC is predicted for the first time. The results obtained for core electrons are consistent with experimental data. It is shown that for some momenta electron–positron attraction can give not only enhancement, but also damping of the probability annihilation.

For a proper interpretation of the angular correlation of positron annihilation radiation (ACPAR) data, knowledge of the influence of the electron–positron ( $e-p$ ) interaction on the  $e-p$  momentum density  $\rho(\mathbf{p})$  is of vital importance.

The question of the enhancement (due to the  $e-p$  interaction) of the contribution of conduction electrons to the ACPAR spectra has been extensively investigated both theoretically and experimentally. However, most papers deal with positron annihilation with electrons inside the central Fermi surface (FS) (in the extended zone scheme). As regards the enhancement of higher-momentum components (HMC) only few papers have been devoted to this problem [1–5] (and references therein).

There is also a lack of information about the enhancement factor (EF) for ionic core electrons and its momentum dependence, except for some average values in low- and high-momentum regions [6–8]. It turns out that at the beginning of each series of metals (Na to Al, K to Zn and Rb to Cd) there is a large difference between these average values of core EFs in the high- and low-momentum regions. However, at the end of each series the difference between the two averages is still much smaller. Thus, a constant core EF is an acceptable approximation in e.g. Al [9] or Cu [10], but completely unsatisfactory in alkali metals. Two-dimensional ACPAR measurements in alkali metals for the [110] orientation are able to separate out the core annihilation in some momentum regions, and it was indeed verified that a constant EF for core electrons is not sufficient to describe the core contribution [1].

The local density approximation proposed by Daniuk and co-workers [11, 12] follows the Thomas–Fermi philosophy and is a generalisation of the corresponding approximation which is so efficient in determining the crystal potential. So, it seems to be

interesting to apply it to calculate the momentum of the EFS both for valence HMC and ionic core electrons (the problem of the EF for ionic core electrons seems to remain an enigma—c.f. [13]).

We discuss our results by using Na as an example.

We first make some basic assumptions. According to [11, 12], the momentum density of annihilation pairs (MDAP) may be expressed as

$$\rho(\mathbf{p}) = \sum_{k,n}^{\text{occ}} \left| \int \{ \varepsilon[X_{k,n}(\mathbf{r}), r_s(\mathbf{r})] \}^{1/2} \psi_{k,n}(\mathbf{r}) \varphi_+(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}} d\mathbf{r} \right|^2 \quad (1)$$

where  $\mathbf{p}$  represents the photon-pair momentum, and  $\psi_{k,n}(\mathbf{r})$  and  $\varphi_+(\mathbf{r})$  are the wavefunctions of the annihilating electron and the thermalised positron, respectively. The function  $\varepsilon[X_{k,n}(\mathbf{r}), r_s(\mathbf{r})]$  is the electron gas EF applied locally within the unit cell.  $X_{k,n}(\mathbf{r}) = (E_{k,n} - V(\mathbf{r})) / (E_F - V(\mathbf{r}))$  represents the ratio of local kinetic energies (here  $E_{k,n}$  is the electron energy,  $E_F$  the Fermi energy and  $V(\mathbf{r})$  is the crystal potential) and  $r_s(\mathbf{r})$  is the local electron density parameter. Setting  $\varepsilon = 1$  in (1), we obtain the MDAP within the independent particle model (IPM), hereafter denoted as  $\rho^{\text{IPM}}(\mathbf{p})$ .

The effective momentum-dependent EF [5] is defined as

$$\tilde{\varepsilon}(\mathbf{p}) = \rho(\mathbf{p}) / \rho^{\text{IPM}}(\mathbf{p}). \quad (2)$$

In both valence and ionic core MDAP calculations, the EF of Rubaszek and Stachowiak [14] and Rubaszek and co-workers [15] was used. The corresponding  $\tilde{\varepsilon}(\mathbf{p})$  will be denoted as  $\varepsilon_v(\mathbf{p})$  (valence) and  $\tilde{\varepsilon}_c(\mathbf{p})$  (core), respectively.

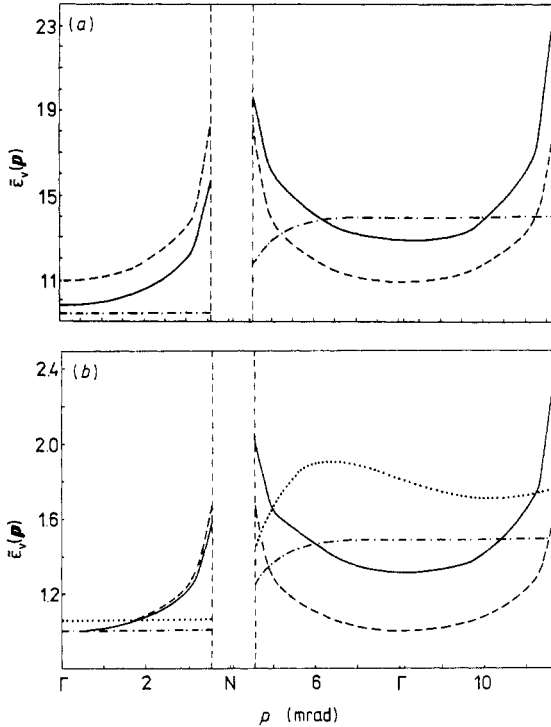
As concerns the study of the EFS for the HMC, we will use the notion of de-enhancement if  $\tilde{\varepsilon}_n(\mathbf{k} + \mathbf{G}) < \tilde{\varepsilon}_n(\mathbf{k})$  and the notion of over-enhancement if  $\tilde{\varepsilon}_n(\mathbf{k} + \mathbf{G}) > \tilde{\varepsilon}_n(\mathbf{k})$ , where  $\mathbf{G}$  denotes a reciprocal lattice vector.

We first present results for the valence electrons. The band structure of alkalis and their valence MDAP were calculated along the principal crystallographic directions by means of the linear-muffin-tin-orbitals (LMTO) method [16].

In figure 1(a) we present the results obtained for Na in the [110] direction. The  $\tilde{\varepsilon}_v(\mathbf{p})$  corresponding to  $\varepsilon[X_{k,n}(\mathbf{r}), r_s(\mathbf{r})]$  applied in equation (2) is represented by the full curve. It can be seen that  $\tilde{\varepsilon}_v(\mathbf{p})$  for HMC differs from that in the central FS. In order to understand such a behaviour of  $\tilde{\varepsilon}_v(\mathbf{p})$  in the region of HMC, we studied the influence of  $X_{k,n}(\mathbf{r})$  and  $r_s(\mathbf{r})$  separately on the shape of  $\tilde{\varepsilon}_v(\mathbf{p})$  by changing the variables in  $\varepsilon$  (in equation (2)). Taking  $\varepsilon = \varepsilon(E_{k,n}/E_F, r_s = 3.93)$  (i.e. using  $V(\mathbf{r}) = 0$  in  $X_{k,n}(\mathbf{r})$ ) and  $\varepsilon = \varepsilon(0, r_s(\mathbf{r}))$  we obtained the corresponding effective EFS denoted as  $\tilde{\varepsilon}_v^E(\mathbf{p})$  and  $\tilde{\varepsilon}_v^r(\mathbf{p})$ , respectively (figure 1(a)). In order to compare the momentum dependence of the above EFS we also present them after normalising their values (for  $\mathbf{p} = 0$ ) to unity (figure 1(b)).

Since we have only one band, the  $\tilde{\varepsilon}_v^E(\mathbf{p})$  represented by a broken curve in figures 1(a) and 1(b) is periodic according to the reciprocal lattice vectors (i.e. the enhancement of the central FS and HMC is the same) [5]. It may be treated as a reference for comparison with  $\tilde{\varepsilon}_v(\mathbf{p})$  and  $\tilde{\varepsilon}_v^r(\mathbf{p})$ . The shape of  $\tilde{\varepsilon}_v^r(\mathbf{p})$  is very similar to the ratio  $\gamma_v(\mathbf{p}) = \rho^{\text{IPM}}(\mathbf{p}) / \rho^e(\mathbf{p})$ , where  $\rho^e(\mathbf{p})$  denotes the electron momentum density. The  $\gamma_v(\mathbf{p})$  gives also the ‘over-enhancement’ of the first HMC for Na in the [110] direction (in the IPM approximation)—i.e. the influence of the positron wavefunction  $\varphi_+(\mathbf{r})$  with respect to  $\rho_e(\mathbf{p})$  is qualitatively similar to the effect of  $\varepsilon(\mathbf{r}) = \varepsilon(0, r_s(\mathbf{r}))$  with respect to  $\rho^{\text{IPM}}(\mathbf{p})$ .

For all calculated cases (Li, Na and K for the [100] and [110] directions) we obtained almost constant values of  $\tilde{\varepsilon}_v^r(\mathbf{p})$  inside FS and its rather strange behaviour for HMC: an over-enhancement or de-enhancement of HMC depending on crystallographic directions



**Figure 1.** (a) Effective enhancement factors for valence electrons in Na in the [110] direction: —,  $\tilde{\epsilon}_v(\mathbf{p})$ ; ----,  $\tilde{\epsilon}_v^E(\mathbf{p})$ ; - · - · - ·,  $\tilde{\epsilon}_v^S(\mathbf{p})$ . (b) The above  $\tilde{\epsilon}$  normalised to unity (for  $\mathbf{p} = 0$ ) where  $\gamma_v(\mathbf{p}) = \rho^{\text{IPM}}(\mathbf{p})/\rho^e(\mathbf{p})$  is also shown (· · · ·).

even in the same metal. One can see that the  $r$  dependence of  $\epsilon$  connected with the  $r_s$  dependence of EF applied in equation (2) has a strong influence on the shape of  $\tilde{\epsilon}_v(\mathbf{p})$  for HMC.

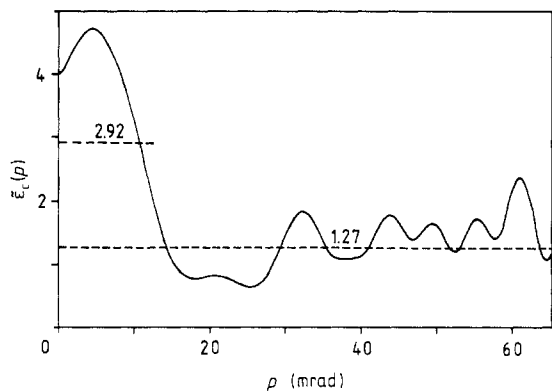
We now present results for the ionic core electrons.

The MDAP  $\rho_{c, nl}(\mathbf{p})$  corresponding to the  $n$ th ionic core shell was determined according to the formula:

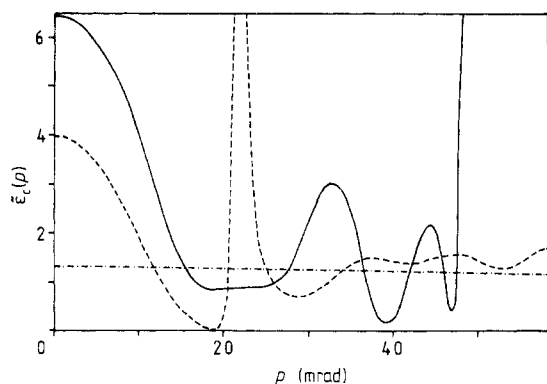
$$\rho_{c, nl}(\mathbf{p}) = 8\pi(2l + 1) \left| \int r^2 \{ \epsilon [X_{nl}(r), r_s(r)] \}^{1/2} R_{nl}(r) \varphi_+(r) j_l(pr) dr \right|^2 \quad (3)$$

where  $R_{nl}(r)$  is the radial electron wavefunction computed relativistically using the method given in [17] with the Hedin and Lundqvist exchange–correlation potential [18].

The radial positron wavefunction has been obtained using the same potential as for electrons but with opposite sign while the exchange–correlation part has been subtracted. As concerns the EFS used for core electrons, the negative values of  $X_{nl}(r)$  (whenever they occur) were substituted by zero as the electron gas EF is defined only for non-negative  $X_{nl}$ . Negative kinetic energies are due to tunnelling, which is a quantum effect neglected in the Thomas–Fermi approach, this last forming the basis of the local density approximation expression by equation (1) (c.f. equation (3)). Note that these results are in principle the same as those obtained by using  $\epsilon = \epsilon[X_{nl}(r) = 0, r_s(r)]$  in equation (3). Moreover, as follows from the analysis of the experimental data [12, 19], the momentum dependence of the EF for high electronic densities ( $r_s \leq 2$ ) obtained on the basis of the Kahana theory [15] is overestimated. For those reasons it was assumed (as an experimental fact) that for these densities the EF does not depend on momentum.



**Figure 2.** —, effective enhancement factors  $\bar{\epsilon}_c(p)$  for ionic core electrons in Na. ----, average values of  $\bar{\epsilon}_c$  in the low- and high-momentum regions [6, 7].



**Figure 3.** The partial effective  $\bar{\epsilon}_{c,n}(p)$  in Na: - · - · - ·, 1s; ----, 2s; —, 2p states.

The above procedure was applied to alkali metals. In figure 2 we present the momentum-dependent total effective core EF  $\bar{\epsilon}_c(p)$  for Na and in figure 3 the partial EF  $\bar{\epsilon}_{c,n}(p)$  for 1s, 2s and 2p states in Na. As can be seen, after increasing to a maximum at about 6 mrad the  $\bar{\epsilon}_c(p)$  decreases, even reaching values less than one in the interval between 16 and 27 mrad. Such a behaviour (i.e.  $\bar{\epsilon} < 1$ ) will be called 'damping' in contrast to 'enhancement' (i.e.  $\bar{\epsilon} > 1$ ).

In the high-momentum region the  $\bar{\epsilon}_c(p)$  oscillates around some value which is not very far from the corresponding average value (1.27) calculated in [6]. Also the average of  $\bar{\epsilon}_c$  in the low-momentum region determined previously by the comparison of theoretical IPM and experimental ACPAR results (equal to 2.92 in [6]) corresponds quite well with the present  $\bar{\epsilon}_c$ . A similar agreement of the averages [6] with the present momentum-dependent results has been found in K, Rb and Cs.

Note that in some particular cases the EF diverges when  $\rho^{\text{IPM}}(p) \rightarrow 0$  and  $\rho(p) \neq 0$ , and is equal to zero when  $\rho(p) = 0$  (see figure 3). This situation takes place quite often as the employment of  $\epsilon$  in equation (1) shifts the zeros of  $\rho(p)$  relative to the zeros of  $\rho^{\text{IPM}}(p)$ . In that case wild oscillations take place. Such a behaviour of  $\bar{\epsilon}_c(p)$ , i.e. strong oscillations of  $\bar{\epsilon}_c(p)$  for momenta greater than 40 mrad was also obtained for Li, K, Rb and Cs.

It is worth emphasising that the application of the momentum-independent EF leads (for a given state) to strongly momentum-dependent  $\bar{\epsilon}_c(p)$ .

To conclude, the core EFS obtained for alkali metals are consistent with the average values obtained earlier by comparison of theoretical and experimental results [6, 7]. It is shown that in some momentum regions the e-p attraction may lead not only to the enhancement of the annihilation probability, but also to damping (i.e., the attraction decreases the annihilation probability).

At present we are not able to answer the question as to whether for higher momenta ( $p > 40$  mrad) the core EFS increase with increasing momentum (as is suggested in [20, 21]) or whether they tend asymptotically to a constant value [6, 7]. However, in this momentum region the densities are very small and it is difficult to obtain reliable values of  $\bar{\epsilon}_c(p)$ .

As concerns the EFS for HMC, one may obtain over-enhancement or de-enhancement (depending on crystallographic directions) even in the case of the same metal. The effect of the over-enhancement was obtained theoretically in Mg, in agreement with experimental data [19].

It may be concluded that the local density enhancement treatment of Daniuk and co-workers [11, 12] leads not only to a selective enhancement of different electronic states but is also capable of yielding momentum-dependent EF both for HMC of itinerant electrons and for ionic core electrons. Note here that such an approach has been successfully applied to positron annihilation in metals [22, 23], and metal vacancies [24], and also to ACPAR spectra for positrons trapped at an Al surface [25] giving, for the first time, the change of the anisotropy direction in the shape of theoretical ACPAR spectra in agreement with experimental data. Of course, only a detailed comparison of theoretical and experimental results for different metals could verify the correctness of such a treatment and of the corresponding results.

We are very grateful to the authors of the paper [16] for making available their crystal potentials for alkali metals.

## References

- [1] Oberli L, Manuel A A, Sachot R, Descouts P and Peter M 1985 *Phys. Rev. B* **31** 6104
- [2] Hede B B J and Carbotte J P 1972 *J. Phys. Chem. Solids* **33** 727
- [3] Fujiwara K, Hyodo T and Ohyama J 1972 *J. Phys. Soc. Japan* **33** 1047
- [4] Sormann H 1989 *Positron Annihilation* ed. L Dorikens-Vanpraet, M Dorikens and D Segers (Singapore: World Scientific) p 272
- [5] Kontrym-Sznajd G and Šob M 1988 *J. Phys. F: Met. Phys.* **18** 1317
- [6] Šob M 1985 *Solid State Commun.* **53** 249
- [7] Šob M 1985 *Solid State Commun.* **53** 255
- [8] Bonderup E, Andersen J U and Lowy D N 1979 *Phys. Rev. B* **20** 883
- [9] Gupta R P and Siegel R W 1979 *J. Phys. F: Met. Phys.* **9** 2353; 1980 *Phys. Rev. B* **22** 4572
- [10] Mijnders P E and Singru R M 1979 *Phys. Rev. B* **19** 6038
- [11] Daniuk S, Kontrym-Sznajd G, Mayers J, Rubaszek A, Stachowiak H, Walters P A and West R N 1985 *Positron Annihilation* ed. P C Jain, R M Singru and K P Gopinathan (Singapore: World Scientific) pp 43, 279
- [12] Daniuk S, Kontrym-Sznajd G, Mayers J, Rubaszek A, Stachowiak H, Walters P A and West R N 1987 *J. Phys. F: Met. Phys.* **17** 1365
- [13] We refer to the discussion after the talk of M Šob at the 8th Int. Conf. on Positron Annihilation, Gent, 29 August–3 September, 1988
- [14] Rubaszek A and Stachowiak H 1984 *Phys. Status Solidi b* **124** 159
- [15] Rubaszek A, Stachowiak H, Boronski E and Szotek Z 1984 *Phys. Rev. B* **30** 2490
- [16] Singh A K and Jarlborg T 1985 *J. Phys. F: Met. Phys.* **15** 727

- [17] Liberman D, Waber J T and Cromer D T 1965 *Phys. Rev.* **137** A27
- [18] Hedin L and Lundqvist B I 1971 *J. Phys. C: Solid State Phys.* **4** 2064
- [19] Kontrym-Sznajd G and Majsnerowski J unpublished
- [20] Osadchiev V M, Tazertdinov O M and Shiskin A V 1989 *Positron Annihilation* ed. L Dorikens-Vanpraet, M Dorikens and D Segers (Singapore: World Scientific) p 383
- [21] Osadchiev V M private communication
- [22] Jarlborg T and Singh A K 1987 *Phys. Rev. B* **36** 4660
- [23] Daniuk S 1988 *Proc. 18th Ann. Int. Symp. Electronic Structure of Solids* ed. P Ziesche (Dresden: Technische Universität) p 27
- [24] Boronski E 1987 *Cryst. Res. Technol.* **22** 1505
- [25] Rubaszek A and Lach J 1989 *Surf. Sci.* **211–2** 227