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LETTER TO THE EDITOR

Effective charge of slow ions in solids

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Abstract. The concept of effective charge for slow ions interacting with condensed matter is discussed. For slow ions ($v < v_F$, where v_F is the Fermi velocity) theories based on linear response are shown to be not fully adequate to describe the physical situation. A non-linear description using the density functional formalism to describe the scattering processes at the Fermi energies is presented and the results compared with those of earlier effective-charge theories.

When a charged particle penetrates through condensed matter it polarises the medium which in turn reacts back slowing down the penetrating particle. For fast enough incident particles the projectile charge state remains the same and the process of stopping is sometimes described in linear theory (Ritchie 1959) in terms of the induced electric field acting on the particle itself. Due to the quantum nature of the probe complicated processes of capture into (and loss from) the bound states of the probe might occur. A detailed account of all these processes is unnecessary, besides being clearly a cumbersome task, and what is required is an averaged picture. Brandt (1975, 1982) and Brandt and Kitagawa (1982, hereafter referred to as BK) have presented a theory of effective stopping-power charge describing the mean effect of all capture and loss processes.

In Brandt's approach an ion of charge Z_1 moves in a medium accompanied by a cloud of bound electrons consisting of $N_1(v_r)$ electrons extending over a radius $\Lambda(v_r)$ where v_r is the relative speed of the ion and electrons. Electrons in the medium at impact parameter greater than Λ encounter the ion as a point charge $Q_1(v_r) = Z_1 - N_1(v_r)$ in distant collisions, but as an ionic charge larger than Q_1 for smaller impact parameters. Brandt (1975, 1982) was able to condense a great amount of data by introducing the concept of effective charge which has provided much physical insight. When the speed of the incident charge Z_1 is much slower than the Fermi velocity of the electrons, non-linear processes not described, of course, in linear theory are important. In fact the mean ionic charge might be zero or even negative (Almbladh *et al* 1976) and one would not expect Brandt's theory to be able to describe the process. As we vary Z_1 new bound states will be filled and one would expect to find oscillations in the effective charge as a function of Z_1 which cannot be described in what is, essentially, a linear theory. To make these ideas more quantitative we have evaluated the effective charge as a function of Z_1 for slow ions incident on an electron gas both within Brandt and Kitagawa's formalism and using the density functional formalism to describe the

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scattering processes at the Fermi level as suggested by Echenique *et al* (1981). The local density functional formalism has also been applied to study static impurities in metals (Puska *et al* 1981, Norskov 1977, 1978, 1979). The effective charge is defined in terms of the stopping power of the charge $Z_1(S)$ and that of the proton moving in the same medium at the same velocity (S_p) by

$$Z_1^* = (S/S_p)^{1/2}. \tag{1}$$

In Brandt and Kitagawa's theory Z_1^* is obtained from equation (1) by using linear response theory to obtain S (we work in atomic units throughout):

$$S = \frac{2}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}|\rho(k)|^2 \int_0^{kv} \mathrm{d}\omega\, \omega\, \mathrm{Im}\left(\frac{-1}{\varepsilon(k,\omega)}\right) \tag{2}$$

where v is the particle velocity and $\varepsilon(k,\omega)$ is the longitudinal dielectric function for the stopping medium. The one-electron radius $r_s = (3/4\pi n)^{1/3}$; n is the electron density and $\rho(k)$ is the Fourier transform of $\rho(\boldsymbol{r}, t)$.

$$\rho(\boldsymbol{r}, t) = Z_1\delta(\boldsymbol{r}) - \rho_e(\boldsymbol{r}) \tag{3}$$

where $\rho_e(\boldsymbol{r})$, the bound-electron charge, is written in terms of the screening parameter $\Lambda(v_r)$ and is determined by minimising the internal energy of the ion.

When the ion is moving at very slow velocities ($v \ll v_F$) linear response theory does not describe adequately the interaction with the electrons of the medium. In table 1 we show the ratio of the induced electron density at the proton position, calculated in the non-linear theory, to the one in linear theory (Almbladh *et al* 1976, Mazarro *et al* 1983). This varies from 1.93 for $r_s = 1$ to 33.7 for $r_s = 6$, showing that linear theory does not describe adequately the electronic screening, as the non-linearity becomes more important as the density of the electron gas decreases, i.e. for bigger r_s. This is illustrated in figure 1 in which we show the induced charge density as a function of the distance to the static proton for several one-electron radii. The bound-state nature of the induced charge clearly appears as r_s increases.

Table 1. Ratio of the induced electron density at the proton position calculated in the non-linear theory (NL) to that calculated in linear theory (L) for different values of r_s.

r_s	$\rho_{NL}^{(0)}/\rho_L^{(0)}$
1	1.93
2	4.34
3	8.59
4	14.9
6	33.6

Recognising the importance of non-linearity, Echenique *et al* (1981) put forward a theory of stopping power for slow ions in which the stopping power is calculated from the scattering phaseshifts from the self-consistent potential of the ion in an electron gas.

The stopping power is then (Echenique *et al* 1981)

$$S = \frac{3v}{k_F^2 r_s^3}\sum_{l=0}^{\infty}(l+1)\sin^2(\delta_l(E_F) - \delta_{l+1}(E_F)) \tag{4}$$

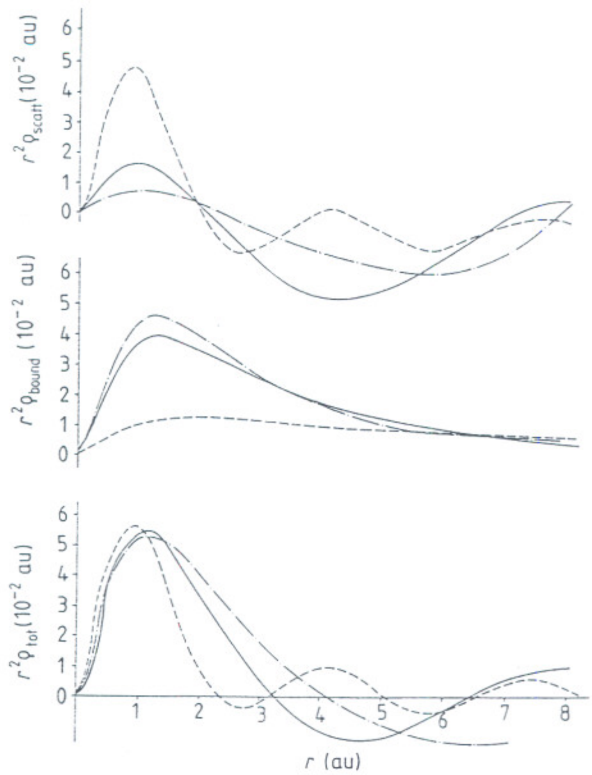

Figure 1. Distribution of induced electronic charge density $r^2\rho_e(r)$ as a function of the distance r from the ion. Calculations were performed in a density functional formalism. Different curves for $r_s = 2$ (broken curve), 4 (full curve) and 6 (chain curve) are plotted.

where k_F is the Fermi momentum, v the ion velocity and $\delta_l(E_F)$ are the scattering phaseshifts at the Fermi energy.

We have used the density functional formalism of Hohenberg and Kohn (1964) and Kohn and Sham (1965) to calculate the self-consistent potential and thus the phaseshifts for several values of the ion charge Z_1. The effective charge is given by

$$Z_1^* = (S(Z_1)/S(Z_1 = 1))^{1/2} \tag{5}$$

where S is given by equation (4). The local-density approximation for exchange and correlation has been used with the parametrisation given by Gunnarson and Lundqvist (1976). The Friedel sum rule is satisfied for all energies to a good accuracy, usually within 0.02 electrons.

In figures 2 and 3 we plot the effective charge Z_1^* against Z_1 obtained from the BK theory and from equations (4) and (5). As expected from the preceding discussion the curve labelled BK does not show any oscillations with Z_1, while the non-linear result does. The non-linear theory takes into account, in a natural way, the filling up of the bound states of the ion and is therefore able to reproduce the experimental oscillations of the stopping power with Z_1 (Echenique *et al* 1985). Each minimum is correlated with a filled shell of the incident particle which is closely related to the atomic structure; this cannot be reflected in any linear theory. For smaller values of r_s (Echenique *et al* 1985) or larger values of the projectile velocity (Pathak 1982) the peaks are shifted towards higher values of Z_1 because a higher nucleus charge is necessary for a filled shell of bound electrons.

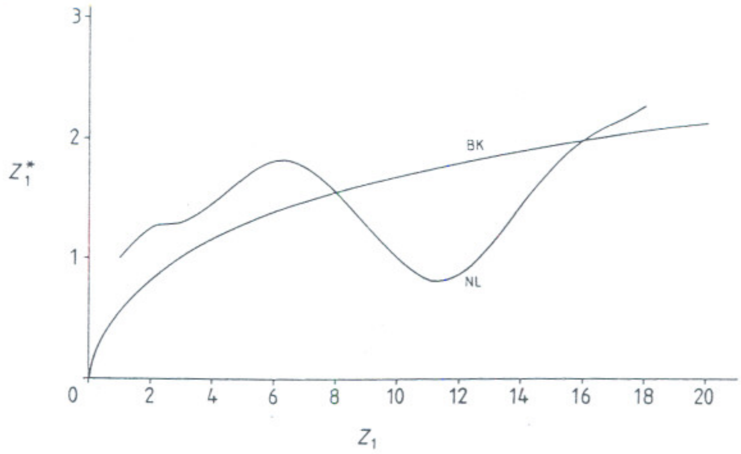

Figure 2. Effective charge Z_1^* plotted against the atomic number of the ion, Z_1, for $r_s = 2$. BK, theory of Brandt and Kitagawa; NL, non-linear result.

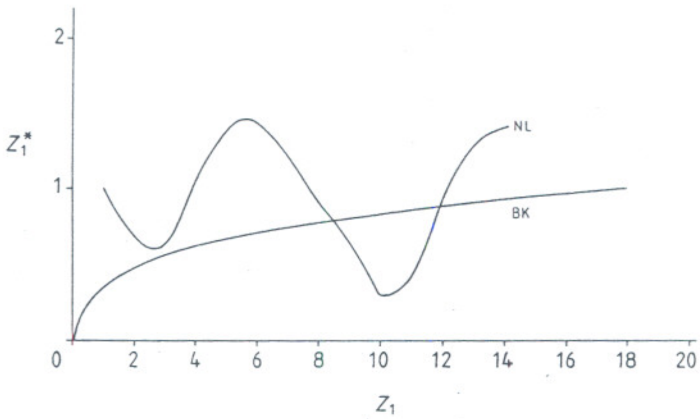

Figure 3. Effective charge Z_1^* plotted against the atomic number of the ion, Z_1, for $r_s = 4$. Curves as in figure 2.

In conclusion, the effective-charge theory of Brandt and Kitagawa is a useful concept and provides much physical insight. However for slow ions a non-linear theory, taking into account the bound states of the probe, is clearly necessary.

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