Charge States and Energy Loss of Ions in Solids

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Abstract

The interrelation between electronic energy loss and charge states of ions in solids is analyzed with particular attention to the cases of hydrogen and heavy ions. Different theoretical schemes and empirical evidences are discussed. Various approaches to describe the behavior of slow protons in metals are reviewed and compared with alternative experimental evidences obtained with other subatomic projectiles. Recent developments in theoretical evaluations of the energy loss of heavy ions using non-perturbative methods are compared with previous linear approaches using different ion charge models. Important differences in the ion charges assumed in previous models are explained by the influence of saturation effects which are absent in the linear and perturbative methods (and contained in the non-linear approach).

Contents

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1. Introduction

The question of the energy loss of light and heavy ions in solids is intimately connected with the question of the charge state of the ions inside the medium. The two problems have been present in the studies of ion penetration in matter for many years (Betz, 1972; Kumakhov and Komarov, 1981). The early developments based on classical and quantum perturbation theory provided close analytical expressions for the mean energy loss only for the case of bare ions, but nevertheless have served for qualitative analysis and applications in various fields. The recent books by Sigmund (2004, 2006) together with an ICRU Report (2005) provide a very complete coverage of the field.

In this context, it is also a nice opportunity to make a special recognition in these Proceedings to the masterful contribution done by Peter Sigmund along many years in almost all the fields of ion-matter interactions covered in this volume.

For many years, the problem of dressed ions was approached from the perspective of statistical atomic models (Firsov, 1959; Lindhard and Scharf, 1953; Yarlagadda et al., 1978) and also by the introduction of effective charge models, where the emphasis was more on providing phenomenological scaling properties than formulating a complete theory of the complicated process of electronic energy loss of partially stripped ions. The greatest difficulties appeared of course in the case of heavy ions. In particular, the range of low energies proved to be much more complex than the statistical models predicted as clearly evidenced by the discovery of the oscillatory Z_1 dependence of the stopping coefficients for different ions (Ormrod and Duckworth, 1963; Ormrod et al., 1965).

Important advances were made in more recent years with the development of non-perturbative methods that include in the calculations terms of all orders in the interaction strength (Briggs and Pathak, 1973, 1974; Echenique et al., 1981, 1986, 1990; Grande and Schiwietz, 1991, 1993, 2002; Maynard et al., 2000, 2002; Sigmund and Schinner, 2000, 2002; Lifschitz and Arista, 1998; Arista, 2002). In various ways, these non-perturbative approaches hinge on nearly exact calculations of the energy loss either by directly solving Schrödinger's equation or by using alternative methods of approximation. In these approaches, the charge state of the ion plays a determinant role as a relevant input parameter.

While these aspects have been studied for a long time, various fundamental issues are still not properly understood. Different approaches have been proposed, but problems still remain and discrepancies between different views are important; this situation affects both light and heavy ions. In this work I will discuss the current state of the knowledge on some relevant questions concerning the charge state of ions moving in solids and its relevance to the stopping power problem. Following a usual convention, I will distinguish between light (hydrogen and helium) and heavy ions (everything heavier than helium). The discussion of light ions, however, will be centered on the case of hydrogen, since helium does not present significant problems compared with the rest of the cases.

2. Light Ions: The Case of Hydrogen

In spite of being the simplest case of a free ion, the question of protons moving in solids is one of the most elusive ones. The existing pictures for slow hydrogen in metals go from the simplest view of the protons remaining as unbound point particles, strongly screened by the conduction electrons, to the opposite extreme of considering the proton binding two electrons and forming H^- as the stable system for low energies. To try to understand the difficulties and subtleties encountered in this area it is useful to review some of the ideas and discussions that took place in the last three decades.

About 30 years ago Brandt (1975) conjectured that a proton would not be able to bind an electron in a metal due to the strong screening conditions. This conjecture was based on theoretical evidences of the time (Friedel, 1952, 1954, 1958; Langer and Vosko, 1959; Payne, 1970; Rogers et al., 1970). In particular, exact calculations of the effects of screening on the bound states of hydrogenic systems by Rogers et al. (1970), showed that, for the typical screening distances in metals, a bound state of hydrogen would not be possible. While the analysis for protons at low energies was reasonably well supported on physical grounds, the extension of the same picture to protons at all energies was not obvious. These conclusions were then objected by Cross (1977) who analyzed the case of swift protons and gave arguments to support the view of collisional equilibrium between protons and neutral hydrogen, dynamically connected by capture and loss processes. It should be noted that the criticism by Cross in principle does not apply to slow protons, as it presumes a dynamical decoupling between projectile and target states (ignoring also screening effects that play a dominant role at low energies) using a picture that is appropriate for swift ions.

Later on, and from a different perspective, self energy calculations based on a dielectric model (Guinea et al., 1981, 1982) predicted that both hydrogen and

helium in metals would be neutralized at low energies. It may be noted however that one should take these results with caution since the use of perturbative models for velocities below one atomic unit is quite risky (Mann and Brandt, 1981).

A different view emerged in the following years (Peñalba et al., 1992), inspired by the new methods of density functional theory (Hohenberg and Kohn, 1964; Kohn and Sham, 1965). According to this view, the ground state of hydrogen in metals (represented by a jellium model) would be a state with two bound electrons, resembling H^-. This rather unexpected picture (considering the very low binding energy of H^- in vacuum, $E_0 \sim 0.75$ eV) emerged from the analysis of the eigenvalues of the Kohn-Sham equations which arise in the density functional theory when the wavefunction of the total system is represented by a Slater determinant, using an independent particle approach (but including exchange and correlation effects in the effective potential through a local approximation). In this representation, an eigenvalue corresponding to a doubly occupied Kohn–Sham state with an energy slightly below the bottom of the conduction band is obtained. The interpretation of this eigenvalue as an evidence of a real physical state of H^- is, however, a doubtful point, since, as is well known, the only physically meaningful quantity in density functional theory is the density itself. In particular, there is a specific mention that the KS eigenvalues do not represent the actual energies of the real system (Sham and Kohn, 1966).

One of the shortcomings of the jellium model is the failure of including lattice structure effects. While these effects may not be extremely important for the description of static interstitial ions, they may become of paramount importance for moving ions. A more complete picture that includes both band structure and lattice structure effects is the one given by the linear-muffin-tin-orbital (LMTO) or related formulations (Vargas et al., 1986; Vargas and Christensen, 1987). An illustrative picture emerging from these studies is shown in Figure 1. The figure illustrates the localized state around the proton, which is located in an interstitial position within the lattice. Here we should call the attention on two points. First, the density of states shown on the right-hand scale shows that the localized state is degenerate in energies with the unlocalized states of the conduction band. This is typically the case for screening of ionized impurities (or scattering resonances) rather than a bound state. The physical image that emerges from these calculations is that of a strongly screened, or overscreened, proton with a non-integer value of screening charge larger than 1 (note that the excess screening charge is compensated at larger distances by Friedel oscillations). Secondly, we note the shape of the effective lattice potential in this figure, which, although qualitative, is representative of the real behavior predicted by extensive calculations (Vargas and Christensen, 1987). It produces important energy barriers that break

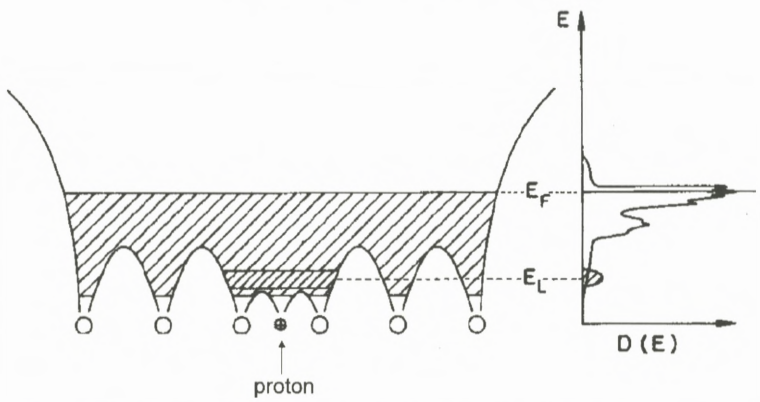

Figure 1. Illustrative picture of the properties of the localized states around protons in metals according to band structure calculations by (Vargas et al., 1986; Vargas and Christensen, 1987).

the translational symmetry assumed in the jellium model. Because of these potential barriers, the possibility of bound electrons following adiabatically the motion of the ion through the solid is ruled out. The wavefunction of the localized states will suffer scattering by the potential barriers and will be dispersed, leaving the proton as a single ion moving through the solid (subject to the strong screening by the free electrons).

Going back to the historical summary, it should be mentioned that while some calculations have stressed the picture of three ionic components (H^+, H^0, H^-) most of the calculations have used the standard view of two charge states: H^0 and H^+ (Guinea et al., 1981, 1982; Lakits et al., 1990; Alducin et al., 2003); the most complete non-linear screening and stopping calculation for protons using the jellium model is the one made by Salin et al. (1999) including dynamical effects for slow ions.

While the intention of this paper is not to give a final conclusion on these intricate questions, it may be useful to perform a simplified but physically revealing analysis of the problem on the basis of recent approaches emerging from self consistent models of proton-solid interactions, including the relevant question of non-linear treatments of screening and scattering processes.

Following a previous proposal (Lifschitz and Arista, 1998), the interaction between the proton and the free electron gas will be approximated by an effective (self consistent) model potential $V(r)$ which, for analytical convenience, will take either of the following forms:

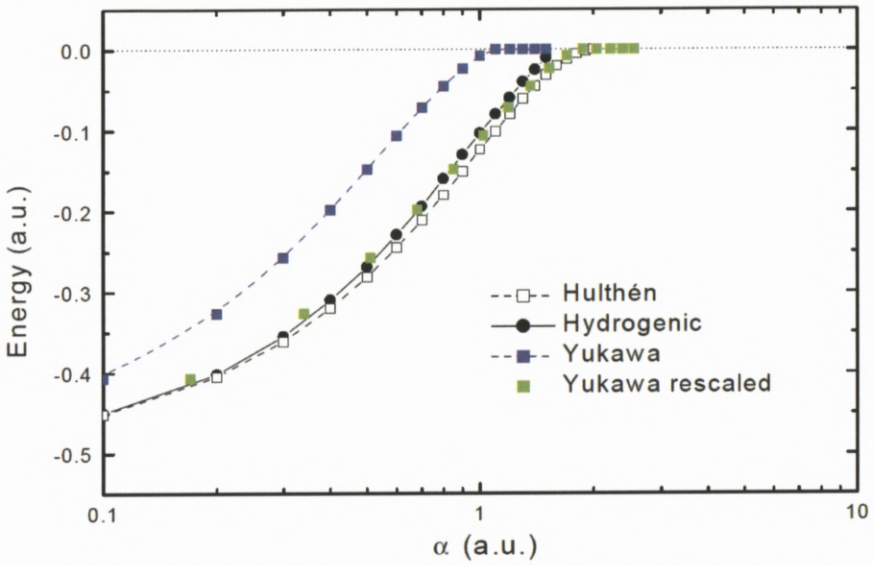

Figure 2. Energy eigenvalues, in atomic units, corresponding to the $1s$ state of three screened potentials: Hydrogenic, Hulthén and Yukawa, as a function of the screening parameter α, obtained by numerical solution of the Schrödinger equation. The rescaled points for the Yukawa potential are obtained by multiplying the corresponding α values by a fixed factor 1.7.

(a) Yukawa potential:

$$V(r) = -\frac{e^2}{r}\,\mathrm{e}^{-\alpha r},$$

(b) Hydrogenic potential,

$$V(r) = -\frac{e^2}{r}\left(1+\alpha\frac{r}{2}\right)\mathrm{e}^{-\alpha r},$$

(c) Hulthén potential

$$V(r) = -e^2\alpha\,\frac{\mathrm{e}^{-\alpha r}}{1-\mathrm{e}^{-\alpha r}}\,.$$

First I consider the question of determining the conditions for the existence of bound states in the indicated potentials, taking as a parameter the screening constant α. To this end, I have solved by numerical methods the corresponding Schrödinger equation, obtaining the energy eigenvalue for the ground ($1s$) state as a function of α. Note that only for the Hulthén potential there are exact analytical solutions, both for the wavefunctions and energies (Hulthén, 1942). The results

of the calculations are shown in Figure 2. It is observed that as the equivalent screening distance, $\Lambda = 1/\alpha$, decreases (α increases) the state becomes more loosely bound and finally disappears. This occurs for values of α close to one atomic unit, and hence in the range of screening conditions in real metals. As a guide, a first approximation to the value of the screening constant for fixed impurities in a free electron gas is given by the Thomas–Fermi (or RPA) approximation as $\alpha_{\mathrm{RPA}} = \sqrt{3}\,\omega_{\mathrm{P}}/v_F$, where ω_{P} and v_F are the plasma frequency and Fermi velocity of the electron gas. Introducing the usual r_{s} parameter of the electron gas by $(4\pi/3)r_{\mathrm{s}}^3 n = 1$, in terms of the electron density n, the value of α_{RPA} is given by $\alpha_{\mathrm{RPA}} = 1.563/\sqrt{r_{\mathrm{s}}}$ a.u. (in the following the values indicated by a.u. refer to atomic units).

However, this value is not a very good one from the point of view of a non-linear representation of impurity screening in solids. A more appropriate value of α is the one that may be obtained in a self-consistent way by applying the Friedel sum rule (Friedel, 1952). This rule expresses the condition of overall charge neutrality when an impurity is immersed in a metal. The mathematical condition is expressed in terms of the scattering phase shifts δ_l (corresponding to the scattering of electrons at the Fermi surface) by

$$\frac{2}{\pi}\sum_{l=0}^{\ell_{\max}}(2l+1)\delta_\ell(k_{\mathrm{F}}) = 1, \tag{1}$$

where $k_{\mathrm{F}} = 1.919/r_{\mathrm{s}}$ is the Fermi wavenumber.

In a full non-linear representation of the screening problem the phase shifts are calculated by numerical integration of the Schrödinger equation corresponding to the scattering of partial waves with angular momentum l in the self-consistent potential $V(r)$. The maximum value of ℓ required in this sum ($\ell_{\max}$) depends on the value of r_{s}, and it has been numerically determined for each r_{s} so as to obtain an accuracy better than 10^{-5} in the total sum.

The resulting values of α obtained from this procedure for each of the indicated potentials are plotted in Figure 3 as a function of r_{s}. In the case of the hydrogenic potential the present result coincides with calculations by Apagyi and Nagy (1987).

By combining the results of the two previous figures we obtain the expected values of binding energy for static protons, as a function of r_{s}; the results are shown in Figure 4. In the case of the Hydrogenic potential this procedure yields no bound states for any value of r_{s}. Moreover, the figure shows a very restricted window of possible r_{s} values, and also, the values of binding energies are so small that they almost preclude the possibility of bound states at any density. These results, although mathematically correct, are physically misleading, as it

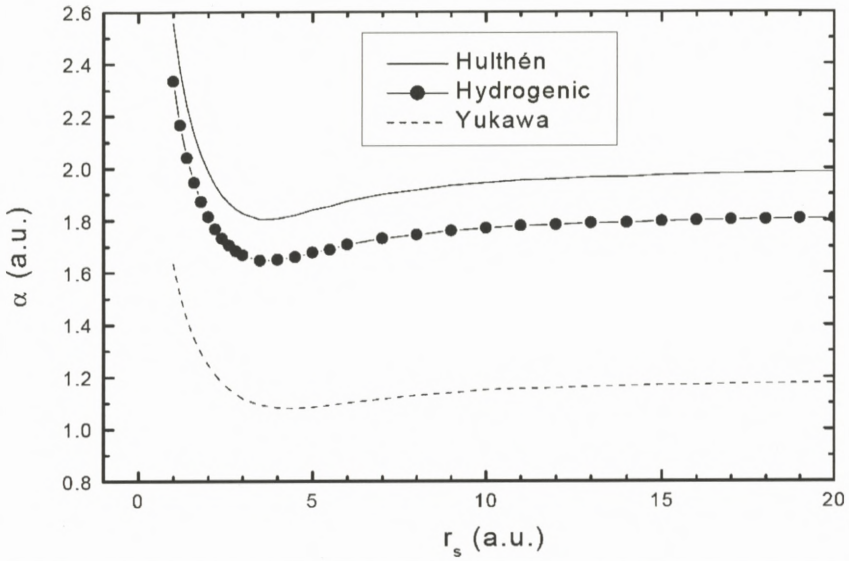

Figure 3. Values of the screening constant α calculated from the Friedel sum rule as described in the text, for the three model potentials: Hydrogenic, Hulthén and Yukawa *versus* the electron gas parameter r_S.

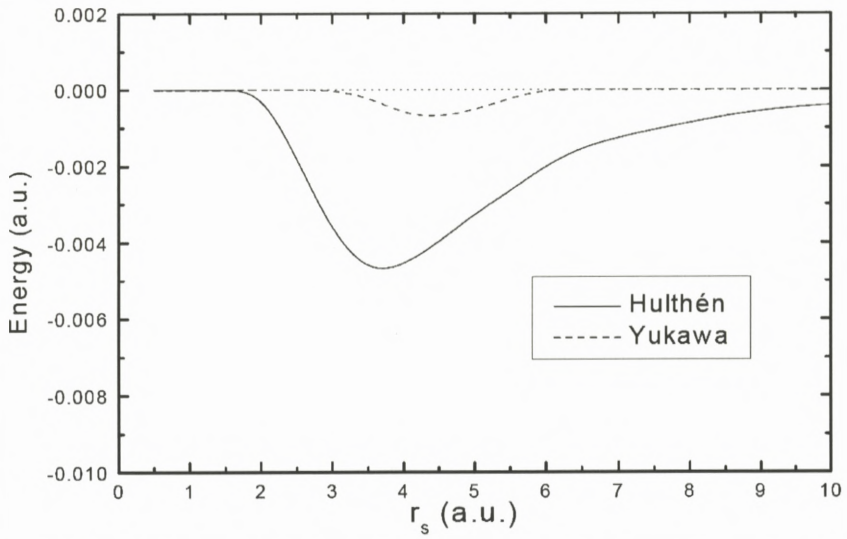

Figure 4. Binding energy of 1*s* state around protons in a jellium taking into account the values of the screening constant α that satisfies the Friedel sum rule (Figure 3) and the energy of the bound state for the corresponding values of α (Figure 2). No bound states are obtained in the case of the Hydrogenic potential (note also the very small values of binding energies obtained here).

becomes obvious when considering the high r_s limit. It is physically clear that for a dilute electron gas the ground state of the system should be that with one electron captured by the proton in a hydrogenic bound state. However this limit is not obtained with the present approach. A nice physical discussion of the problem was given some time ago by Ferrell and Ritchie (1977). They identify the origin of the problem in the absence of an important many-body effect that comes from a self interaction of the electron mediated by the polarization induced in the electron gas by the same individual electron. In order to take into account this effect they formulated a simple model, using still a one-electron Hamiltonian, and showing that the new result reproduces the bound state with the correct binding energy of the free hydrogen atom when $r_s \to \infty$. (The original calculations by Ferrell and Ritchie were made for helium ions but it is easy to check using their analytical expressions that the same property applies to protons).

Nevertheless, in the range of metallic densities the Ferrell–Ritchie approach would not guarantee a bound state for protons since one should add a correction term to the energy due to the difference between the Fermi and the vacuum level (i.e., the work function value) (Ferrell and Ritchie, 1977).

As indicated, the calculations mentioned so far were restricted to the case of ions at rest. Therefore, the possibility arises that by considering the relaxation of the screening conditions due to dynamical effects on moving ions, new conditions for the existence of bound states may arise.

To study this possibility I have extended the analysis to the case of moving ions, applying in this case the extended Friedel sum rule (Lifschitz and Arista, 1998) as a new constraining condition to determine in a self-consistent way the values of α for each type of potential, as a function of the proton velocity v, i.e. $\alpha = \alpha(v)$.

The values of α obtained from these adjustments are shown in Figure 5, for $r_s = 2$, corresponding to typical electron densities in metals. The results show two clear regimes: a low-energy range ($v < v_F$) where α is basically constant, and a high-velocity range where it drops quite rapidly (dynamical screening regime); the asymptotic behavior for the Yukawa potential is of the form $\alpha \sim \omega_P/v$. Using the values of $\alpha(v)$ so determined, and the previous results for the binding energy as a function of α (Figure 2) we finally determine the binding energies as a function of velocity for the three potential models. The results are shown in Figure 6. We note that, in spite of the *a priori* independence of the three potential models (note in particular the differences in the values in Figure 5) the final results for the binding energies show a remarkably close agreement. The reason for this agreement lies in the use of the Friedel sum rule to adjust in a self-consistent way the three potentials.

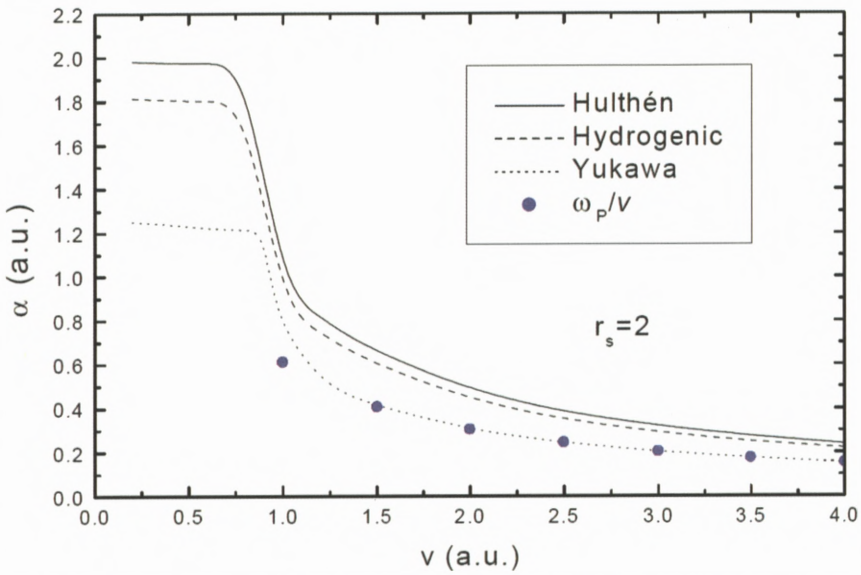

Figure 5. Values of the screening constant α *versus* proton velocity v for the three model potentials considered in the text, for a typical electron density in metals corresponding to $r_S = 2$. The solid symbols show the values of ω_P/v.

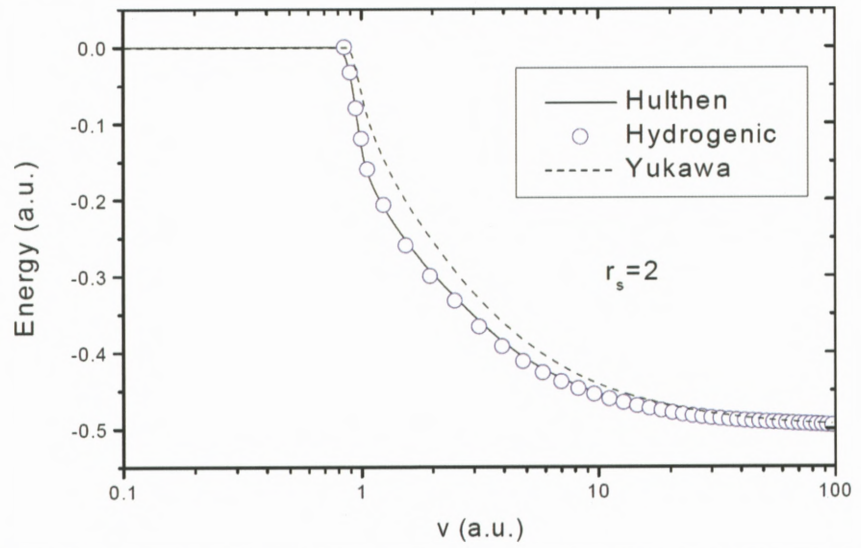

Figure 6. Binding energy of an electron state around a moving proton as a function of proton velocity v for the three potential models indicated in the text, for an electron density corresponding to $r_S = 2$. Bound states appear for velocities larger than about 1 a.u. For high velocities the binding energy converges to the normal value for the hydrogen atom, $E_0 = -0.5$ a.u.

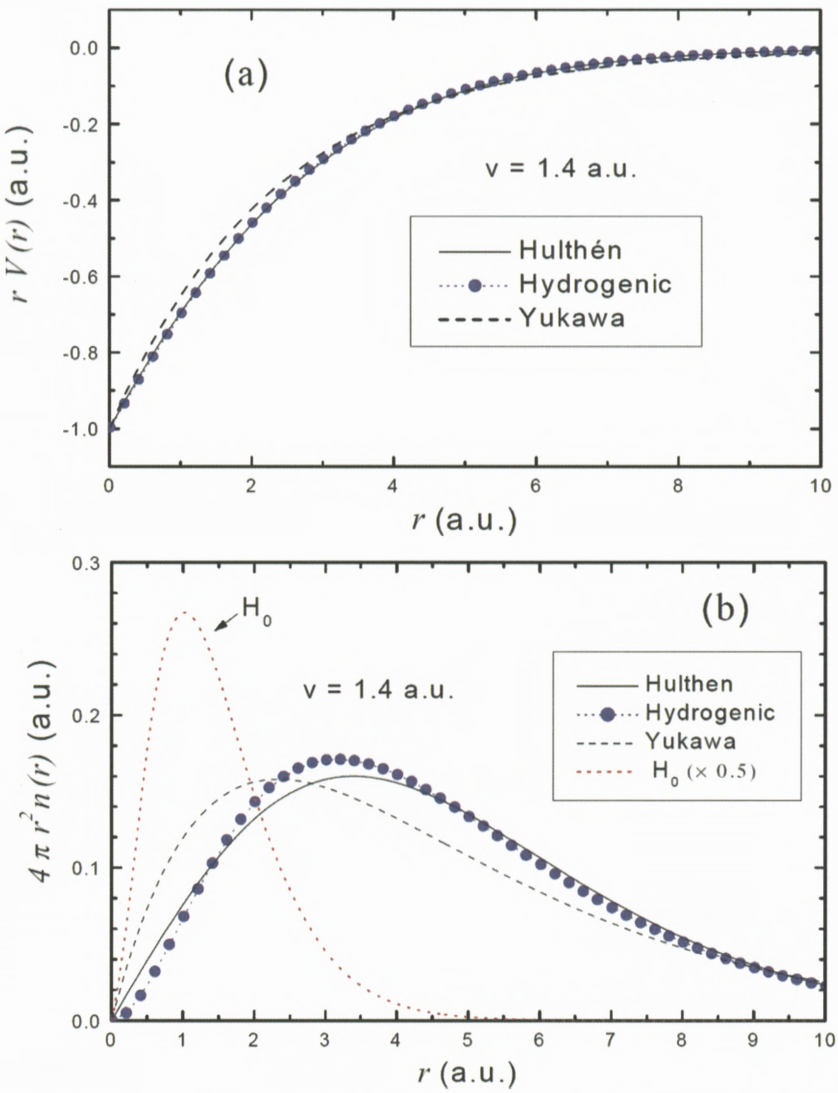

Figure 7. Values of the potentials (part a), and corresponding screening densities (part b) for the three potential models (Hydrogenic, Hulthén and Yukawa), with screening constants α adjusted by the extended Friedel sum rule method as discussed in the text.

For further illustration, Figure 7 shows the values of the potentials (part a), and the corresponding screening densities (part b) for the three adjusted potentials indicated before (with the α-values determined by the extended Friedel sum rule). Also included in this figure is the normal electron density for the free hydrogen atom (reduced by a factor 0.5). One observes a remarkably close agreement between the three potentials (as a result of the adjustment made by the extended Friedel sum rule); second, the screening cloud is much more spread than the normal density of the hydrogen atom; this is a dynamical effect on the screening charge. Of course the present results yield only a spherically averaged view of the screening phenomenon but they are still useful for illustrative purposes.

Similar calculations for slow ions ($v < v_F$) show that the screening densities become similar to the normal hydrogen density (although in these calculations they represent the density of free electrons undergoing scattering). Under these conditions, the corresponding phase shifts and stopping coefficients obtained with the different models are also expected to be quite similar (see Lifschitz and Arista, 1998, for specific calculations).

The conclusion drawn from these calculations is that slow protons in metals behave as free particles dressed by a screening cloud of conduction electrons; this conclusion is backed by full size band structure calculations as indicated earlier (Vargas et al., 1986; Vargas and Christensen, 1987). At higher velocities ($v > v_F$) bound states appear, and at the same time the coupling between the projectile and the target weakens, so that a good approximation may be to consider a base of states composed by the separate projectile and free-electron-gas wavefunctions (in the sense of the zero-order approximation of time-dependent perturbation theory), and then calculate the transition probabilities corresponding to capture and loss processes (Cross, 1977; Lakits et al., 1990; Alducin et al., 2003).

2.1. Experimental Evidences: Positrons, Positive Muons and Pions

According to the previous analysis, no bound states of protons in metals would be expected for velocities smaller than about one atomic unit. In principle, it might be expected that the energy loss of slow protons would yield information to confirm this. However, the theoretical evaluation of stopping powers at low energies is not currently as accurate as it is at high energies (in the perturbative regime) and so it seems that for the moment it cannot provide a final test of this point (for instance, the best available calculations using density functional theory for protons and helium ions do not show a very satisfactory agreement with experiments (Martínez-Tamayo et al., 1996).

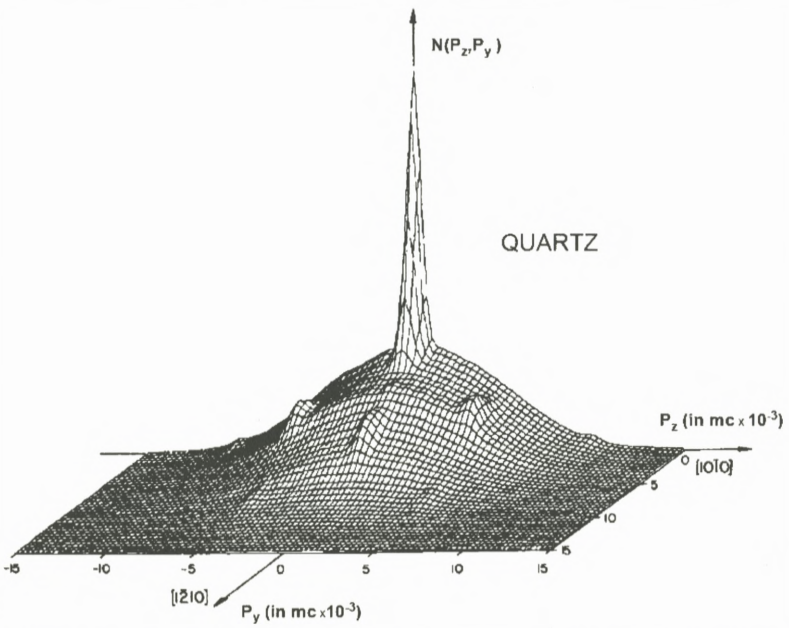

Figure 8. Angular-correlation distribution of gamma rays corresponding to positronium annihilation in crystalline quartz (experiment by Berko et al., 1977).

But there are other experimental methods that are more sensitive to the electronic environment around an impurity ion and could provide more conclusive information on the charge state problem. In particular, such is the case of experiments done with positrons and positive muons or pions.

Experiments on positron annihilation in solids reveal a sharp distinction between metals and semiconductors or insulators (West, 1973, 1974; Brandt and Dupasquier, 1983). Figures 8 and 9 show two typical spectra (Berko et al., 1977) of angular correlations between the two gamma rays (emerging in opposite directions) produced by the annihilation of individual positrons in solids. In these experiments the positrons, coming from an external source, are completely slowed down and approach thermal equilibrium with the lattice before annihilating (Brandt and Arista, 1982). Figure 8 corresponds to an insulator (a quartz crystal) while Figure 9 is for a metal (Al, with $r_s = 2.07$). The prominent and narrow peak observed in Figure 8 is explained by the mechanism of electron capture (positronium formation) prior to annihilation; here the angular width corresponds to the momentum distribution of the positronium wavefunction (the small periodic crispations are produced by the effects of the lattice on this wavefunction). By contrast, the wider shape in Figure 9 corresponds to the spectrum of positron an-

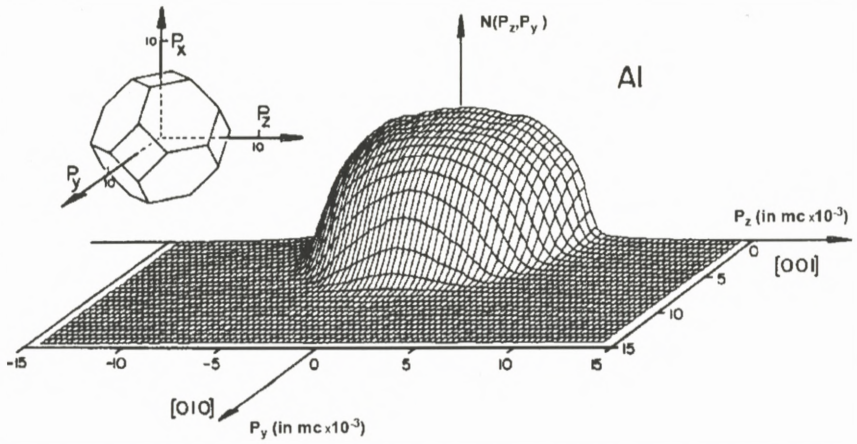

Figure 9. Angular-correlation distribution of gamma rays corresponding to the annihilation of free positrons in aluminum (experiment by Berko et al., 1977).

nihilation in metals; this result is representative of similar spectra found for other metals (Donaghy and Stewart, 1967a, 1967b; Stewart et al., 1962; West, 1973, 1974). In this case the width of the angular distribution is directly related to the radius of the Fermi sphere, indicating that the positron does not capture an electron but annihilates as a free particle with the conduction electrons of the metal. The usual explanation given to this different behavior is that positrons cannot bind electrons in metals due to the strong screening produced by free electrons (West, 1973, 1974; Brandt and Dupasquier, 1983).

It could be argued that these results do not apply directly to protons due to the significant mass difference (in fact, the relevant parameter is the reduced mass of the system which is only affected by a factor 1/2). Hence we may turn to consider additional evidences arising from experiments on spin rotation and relaxation of positive muons and pions stopped in different materials (Patterson, 1988; Morenzoni, 1992; Morenzoni et al., 2002; Major et al., 1992). The evidence arising from these experiments is fully consistent with the previous picture of positrons: in the case of metals the muons/pions decay (by positron/muon emission) as free particles, whereas in the case of insulators, semiconductors, or organic materials, they capture an electron, forming a stable bound state, before decaying. Also, the charge distribution around muons in interstitial positions in Ni and other metals, measured by the intensity of the hyperfine field, demonstrated a strong screening of muons by conduction electrons, but not a bound state (Vargas and Christensen, 1987). The explanation of the different behavior

between metals and non-metals is, as in the case of positrons, based on the strong screening effect that avoids the formation of bound states in metals.

2.2. Discussion

As illustrated, there is a consistent explanation of the behavior of positrons and positive pions and muons in the different types of solids, irrespective of the different masses between these particles. Thus, one would expect a similar behavior in the case of slow protons. The closest comparison is of course between protons and positive muons/pions.

The theoretical analysis provides physical arguments to expect that no bound states would be formed for velocities below the Fermi velocity in metals. There is no consensus on this point in the ion-beam community, but it should be noted that it is in agreement with all the experimental evidence coming from positron, muon and pion experiments.

According to this view, the physical picture of the behavior of protons in solids would be the following.

(a) Metals: one may distinguish two ranges:

  (i) for $v < v_F$: bound states are not formed (except perhaps for high-r_s materials) and the protons propagate through the lattice as strongly screened ions;
  (ii) for $v > v_F$: bound states appear and a collisional equilibrium between H^0 and H^+, determined by capture and loss processes, is established. The neutral and negative fractions observed when slow (1–20 keV) hydrogen beams emerge from metals may be explained by electron capture processes taking place at the exit surface (Bhattacharya et al., 1980; Verbeek et al., 1980).

(b) Insulators, semiconductors and organic materials: here an equilibrium between H^0 and H^+ is expected at all energies (with a predominant fraction of H^0 at low energies).

While for the moment a complete theoretical proof of this picture cannot be given (a full size theoretical model would require self-consistent many-body calculations including non-linear screening plus dynamical and lattice-potential effects), we may note that it is consistent with all the existing experimental evidences cited before.

3. Heavy Ions

The question of the charge states of heavy ions in solids is one of the main problems in trying to achieve a definitive theoretical framework for the evaluation of ion stopping and ranges. As in the case of light ions, one common difficulty is the fact that measurements of the charge states of ions emerging from solid targets provide only indirect information on the internal charge state distributions. Yet, alternative methods to measure the equilibrium charge state of ions in solids (Della-Negra et al., 1987) may yield useful information in this respect.

There are extensive experimental studies that provide detailed information on the charge state distributions (Shima et al., 1986, 1992), as well as convenient empirical fittings to the data (Nikolaev and Dmitriev, 1968; Schiwietz and Grande, 2001). But the question of charge states of ions moving within a solid was for many years an open issue. In particular we may note the old controversy between two models that has remained open through the years: the Bohr–Lindhard (BL) (1954) and the Betz–Grodzins (BG) models (Betz, 1972).

The BL model considers that the fast sequence of collisions experienced by the ion within a solid produces an enhancement in the excitation and ionization probabilities, leading to an increased equilibrium charge. The effect of the passage through the surface, in the case of swift ions, is not considered to be very relevant, due to the high velocity condition, and so the mean exit charge $\bar{q}_{\rm exit}$ is expected to be close to the mean charge $\bar{q}$ inside the solid. Instead, the BG model considers that the effect of repeated collisions within the solid produces ions with several excited electrons in outer shells, but those electrons remain mostly attached to the ion until it emerges into vacuum; after this, the ion would decay by emitting electrons *via* Auger processes. According to this model, the mean charge states $\bar{q}$ of the ion inside the solid should be significantly smaller than the exit values $\bar{q}_{\rm exit}$. A detailed discussion of this problem within the context of non-linear calculations of the energy loss has been given recently (Lifschitz and Arista, 2004); the results of this study show a disagreement with the BG model and provide a plausible explanation to the old controversy.

It may be noted that the BG model was initially inspired in the apparent lack of gas-solid differences in the energy loss values, which was associated to similar values of charge states. However, small gas-solid differences in the stopping were found later on by Geissel et al. (1982), whereas, on the other hand, the Auger electrons predicted by the BG model were not found.

The study of the charge states of ions moving in solids is thus a fundamental aspect in the field of ion-solid interactions. An important problem in this respect is the wide discrepancy among the values assumed in different places. An example

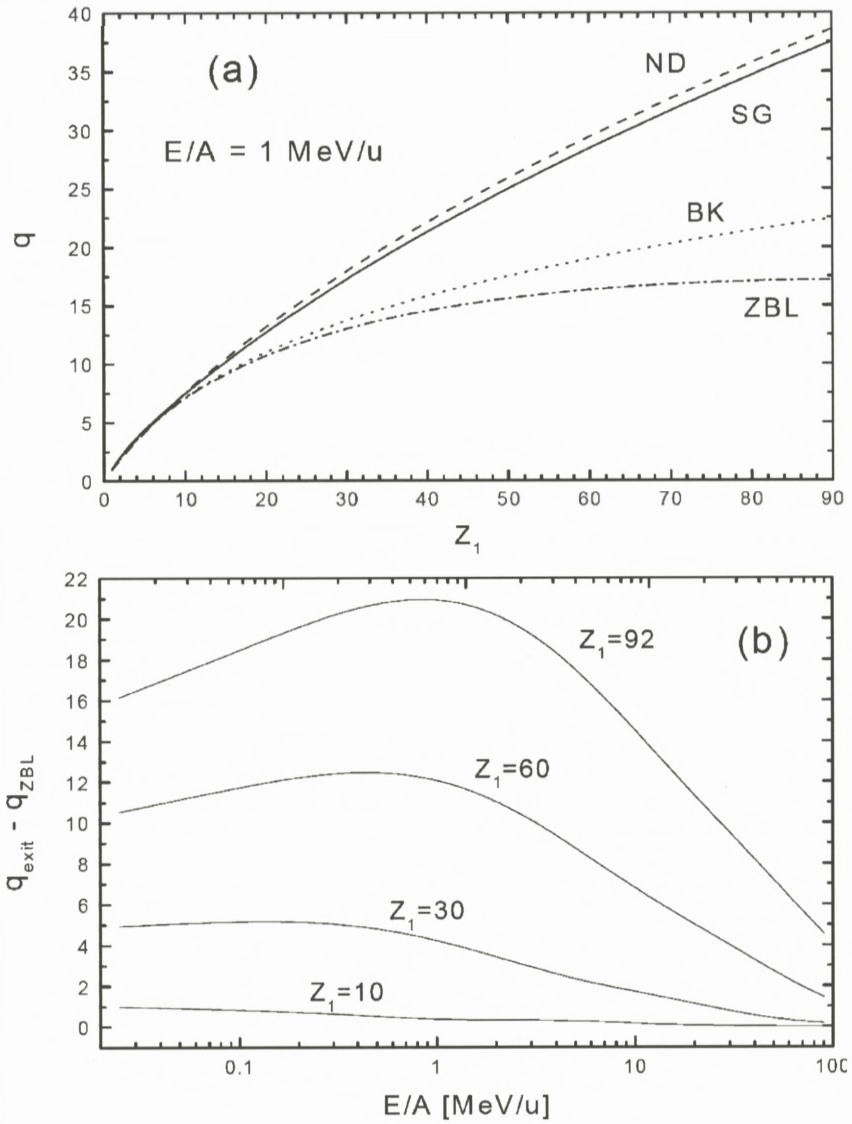

Figure 10. (a) Different approaches to the mean charge of ions in solids. Curves ND and SG: fitting values to the mean charge of ions emerging from solid foils according to Nikolaev and Dmitriev (ND) and Schiwietz and Grande (SG) respectively; BK: ion charge values calculated by Brandt (1975) and used in the Brandt–Kitagawa model; ZBL: recommended values by Ziegler et al. (ZBL) (1985) obtained by fitting stopping power values with the BK model. (b) Difference between the mean exit charge q_{exit} (represented by the empirical SG values), and the average ionization values by Ziegler et al. q_{ZBL}, for various atomic numbers, as a function of ion energy.

of the most frequent assumptions is shown in Figure 10. Part (a) of this figure shows the fitting expressions to the mean charge of ions emerging from a solid foil obtained by Nikolaev–Dmitriev (ND) and Schiwietz–Grande (SG), the q-values of the Brandt–Kitagawa (BK) model (Brandt, 1975; Brandt and Kitagawa, 1982), and the expression for the "ionization" values given by Ziegler et al. (ZBL) (Ziegler et al., 1985). The BK model calculates the mean ion charge using a previous model by Brandt (1975) based on the velocity-stripping criterion by Bohr and assuming a Thomas–Fermi model for the electron velocities in the atom. The ZBL formula is the result of a large number of fittings based on the BK model for heavy ions scaled to equal-velocity proton values. As observed in the figure, large discrepancies arise for heavy ions. Part (b) of this figure shows the difference between the mean charge values measured at the exit of solid foils and the charge values recommended in the ZBL approach. As observed, very large differences arise for heavy ions on a wide range of energies below and over 1 MeV/u. Hence, this range of energies is of central interest for the present analysis.

The purpose of the following is to try different stopping models, together with different q-values, in order to analyze some basic differences dealing with linear *versus* non-linear approaches, and finally, to discuss the origin of these discrepancies.

First, I will briefly recall the calculation of the stopping power for dressed ions according to the dielectric function formulation (Lindhard, 1954; Ferrell and Ritchie, 1977; Brandt and Kitagawa, 1982). The energy loss in this case is given in terms of the dielectric function $\varepsilon(k, \omega)$ by the expression

$$\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{2e^2}{\pi v^2} \int_0^\infty \frac{\mathrm{d}k}{k} |f(k)|^2 \int_0^{kv} \omega \, \mathrm{d}\omega \, \mathrm{Im} \frac{-1}{\varepsilon(k, \omega)}, \tag{2}$$

where $f(k)$ is the ion form factor, which is calculated from the Fourier transform of the ion-charge density $\rho_{\mathrm{ion}}(\vec{r})$, by

$$f(k) = \int d^3r \, \mathrm{e}^{i\vec{k}\cdot\vec{r}} \rho_{\mathrm{ion}}(\vec{r}) \, . \tag{3}$$

In particular, in the BK model $f(k)$ may be expressed analytically, for any ion charge q and atomic number Z_1, by

$$f_{\mathrm{BK}}(k) = Z_1 \frac{q/Z_1 + k^2\Lambda^2}{1 + k^2\Lambda^2} \, , \tag{4}$$

where Λ is the screening radius of the ion (which depends also on q and Z_1). In the simplest case of bare nuclei, $f(k) = Z_1$.

The use of a dielectric description, as well as the use of a free electron gas picture, is more adequate to deal with the excitation of conduction electrons in

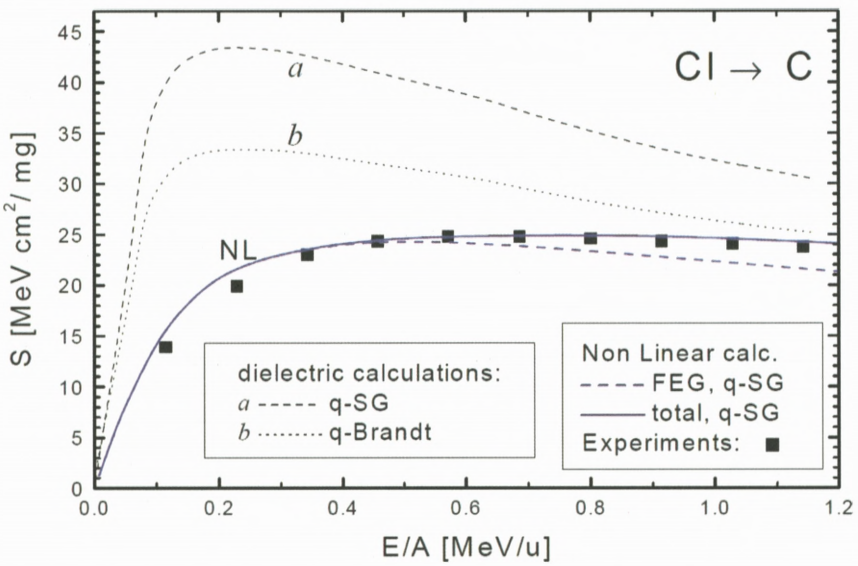

Figure 11. Calculations of stopping cross sections for Cl ions in carbon using linear and non-linear models. Curves *a* and *b*: dielectric calculations corresponding to the following assumptions on the ion charge: (a) empirical values by Schiwietz–Grande (SG), (b) Brandt statistical-ion model (Brandt, 1975). The two blue curves denoted NL are the results of the non-linear calculations using the SG values of ion charges, considering only the electron gas contribution (dashed line) and including K-shell ionization (continuous line). The solid symbols are experimental values (Boot and Grant, 1965; Paul, 2006).

metals or valence electrons in semiconductors. A more comprehensive scheme may be built using a description in terms of Mermin functions derived from optical data and including also inner shells (Abril et al., 1998). The present calculations will be restricted to a carbon target where the dominant energy loss is produced by the excitation of valence electrons, and the contribution of the K-shell may be included as a separate correction.

The calculations were made using the dielectric function obtained by (Lindhard, 1954) for the free electron gas. To integrate Equation (2) according to this formulation one must separate the contributions of plasmon (given by a line integral) and single particle excitations. The numerical method was described in a previous publication (Arista, 1978).

Results of these calculations are shown in Figures 11 and 12, for Cl and Ni ions in carbon foils ($r_s = 1.6$). The figures show the results of the linear (dielectric) formulation and of the non-linear quantal calculations considering different ion charge values. The curves denoted *a* and *b* are dielectric calcu-

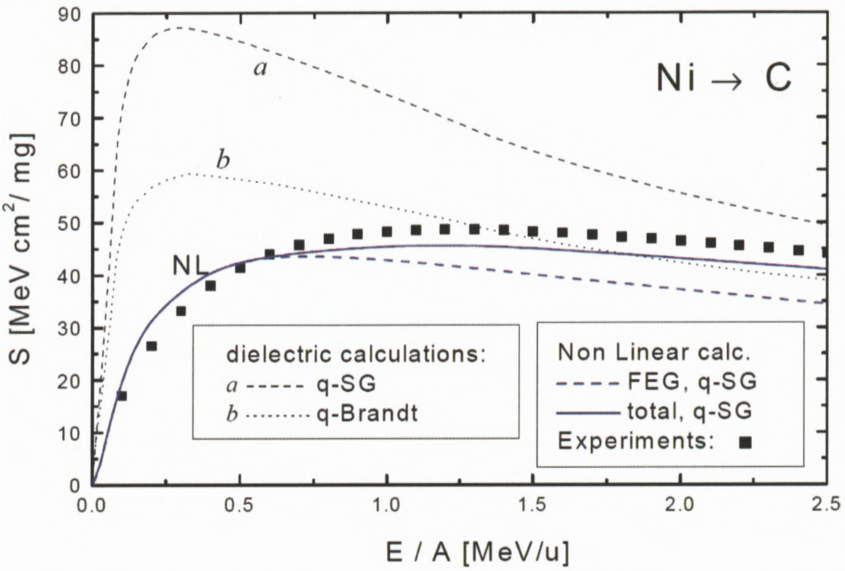

Figure 12. Same as in Figure 11 for Ni ions in carbon; the solid symbols are empirical values according to the fitting by Konac et al. (1998).

lations corresponding to the following assumptions on the equilibrium charge states $\bar{q}$ of the ions: (a) empirical values by Schiwietz and Grande (2001) (derived from experiments with emerging ion beams), (b) Brandt statistical-ion model (Brandt, 1975; Brandt and Kitagawa, 1982). The curves denoted NL are the results of non-linear calculations based on the extended Friedel sum rule according to the method described in Arista (2002) and using the Schiwietz–Grande values of ion charges (Schiwietz and Grande, 2001). This method is fully non-perturbative and based on numerical integrations of the Schrödinger equation for the scattering of electrons by the field of the moving ion. A correction due to K-shell ionization has been included in the non-linear calculations following Arista (2002) and Arista and Lifschitz (2004) yielding the result indicated by the solid blue line. The solid symbols are experimental values from Boot and Grant (1965) and Paul (2006).

As it may be observed, the calculations based on the linear formulation overestimate the values of the stopping power. The reason for this behavior is simple: the basic assumption of the dielectric approach is the linear response of the medium, which produces a quadratic dependence of the stopping power on the ion form factor $f(q)$, Equation (2), and is the same reason why the stopping of bare ions in the Bethe model increases with Z_1^2. In the case of

heavy ions this produces a significant overestimation of the energy transfer to the medium. A more realistic description, such as the non-linear method for heavy ions (Arista, 2002; Arista and Lifschitz, 2004), takes into account the effect of "saturation" in the energy transfer. In the ZBL method, the values of $\bar{q}$ are fitted to the experiments by a calculation procedure that is based on the BK model; in this way it compensates the intrinsic overestimation of the linear approach by using a reduced value of $\bar{q}$. Instead, the non-linear calculation shows a good agreement with the experiments when the SG values of $\bar{q}$ are used. Conversely, if the non-linear calculations were made using the ZBL values for $\bar{q}$ the results would be too low (Arista and Lifschitz, 2004).

It may be noted that other non-perturbative methods (Grande and Schiwietz, 1993, 2002; Maynard et al., 2000, 2002; Sigmund and Schinner, 2000, 2002) may be used to obtain appropriate stopping power values in this energy range, although the present aim is not to perform a fine test of stopping evaluation methods but to illustrate the relevance of charge state assumptions on these calculations.

Another illustrative comparison is made in Figure 13 which shows the calculated values of the stopping cross sections for a fixed ion velocity ($v = 10$ a.u.) as a function of the atomic number Z_1 (which may be thought of as representing the interaction strength). Calculations using the two referred methods are included. The letter L here refers to linear calculations (using the described approach, Equations (2–4)) for two different ion charge values: the empirical SG values ($\bar{q}_{\mathrm{SG}}$) (Schiwietz and Grande, 2001) and the Brandt model ($\bar{q}_{\mathrm{Brandt}}$). The NL curves correspond to the non-linear calculations according to the method of Arista (2002) and Arista and Lifschitz (2004)); curve (a) corresponds to the stopping power of a free electron gas (FEG) for the case $\bar{q} = \bar{q}_{\mathrm{SG}}$, while curve (b) includes the contribution due to K-shell ionization. The additional curve (c) is the result of stopping calculations with the non-linear method using the heavy-ion charge model by Brandt ($\bar{q}_{\mathrm{Brandt}}$). The data symbols are the fittings to experimental values according to Konac et al. (1998) and Hubert et al. (1990). A good agreement between the non-linear calculations (curve (b)) and the empirical values is observed for atomic numbers below 50, but for higher Z_1 an increasing discrepancy is observed. This behavior was also observed in previous calculations and probably indicates a deficiency in the ion-potential model (a modified Molière potential) for the heaviest ions (Arista, 2002). We note also a fair agreement between the non-linear curve (a) and the linear calculation using $\bar{q} = \bar{q}_{\mathrm{Brandt}}$. However, a significant disagreement (which grows with Z_1) is observed between the non-linear calculations corresponding to $\bar{q}_{\mathrm{SG}}$ and $\bar{q}_{\mathrm{Brandt}}$ (curves (a) and (c)). This is a consequence of the important differences in the ion charge values already noted in

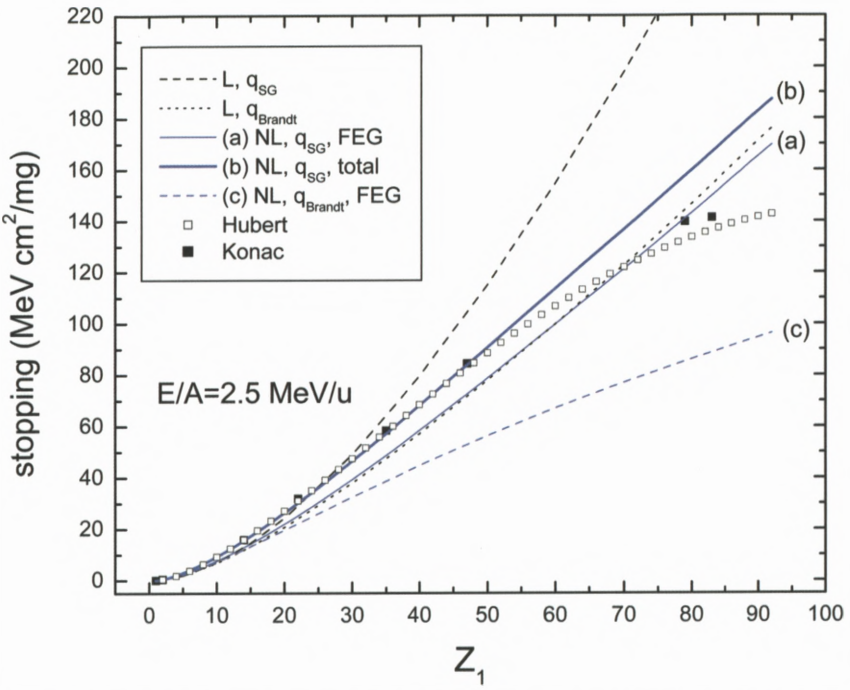

Figure 13. Calculated and empirical values of stopping cross sections for a fixed ion velocity ($v = 10$ a.u.) as a function of the atomic number Z_1. Letter L denotes linear calculations (dielectric approach) for two different ion charge values: the empirical values by Schiwietz and Grande ($\bar{q}_{SG}$), and the values of the Brandt model ($\bar{q}_{Brandt}$). The solid lines are the non-linear (NL) calculations described in the text: curve (a) corresponds to the stopping power of a free electron gas (FEG) for the case $\bar{q} = \bar{q}_{SG}$, curve (b) includes the contribution to the energy loss due to K-shell ionization, and curve (c) is the result of non-linear calculations using the ion charge model proposed by Brandt ($\bar{q} = \bar{q}_{Brandt}$). The data symbols are the fittings to experimental values using the approaches by Konac et al. (1998) and Hubert et al. (1990).

Figures 10a and 10b. A similar disagreement was found in previous calculations when the ZBL values for $\bar{q}$ were used (Arista and Lifschitz, 2004).

The fact that the NL results in these figures are in reasonably good agreement with the experiments suggests that the approximation of the ion charge inside the solid by the value of the corresponding emerging ion charge is fairly good (although a difference of a few units of charge, but much smaller than the differences shown in Figure 10b, may not be excluded). In this way the results of the non-linear approach show a disagreement with the Betz, Brandt and ZBL models of ion charge, being instead compatible with the BL model (Lifschitz and Arista, 2004).

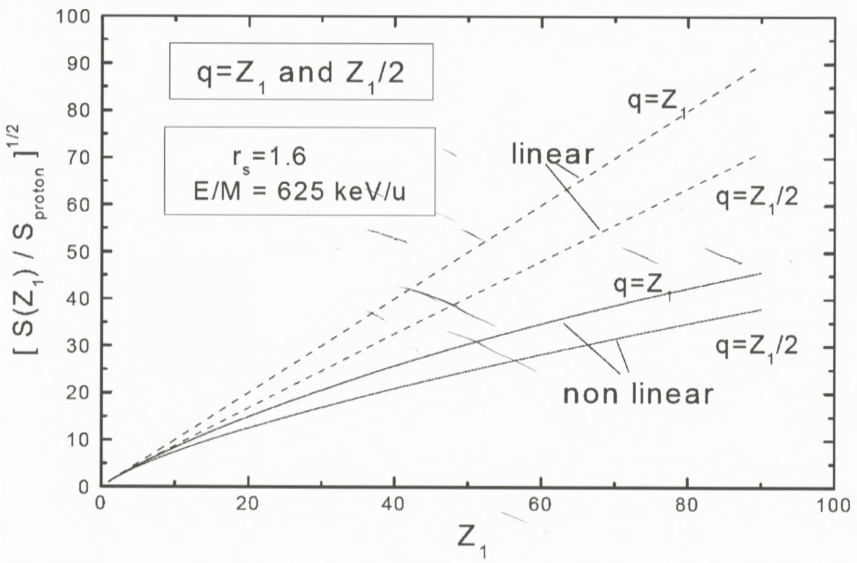

Figure 14. Illustrative calculations of stopping power ratios, shown as $[S(Z_1)/S_{\text{proton}}]^{1/2}$, where $S(Z_1)$ and S_{proton} are the stopping powers of ions and protons at the same velocity, $v = 5$ a.u. The present calculations correspond to fully charged ($q = Z_1$) and half-charged ($q = Z_1/2$) ions, using the linear (dashed lines) and non-linear (continuous lines) methods described in the text.

3.1. Saturation Effects in the Energy Loss

As already mentioned, a very basic difference between linear and non-linear approaches for swift heavy ions is the possibility – in the non-linear approach – of accounting for the saturation effect in the energy loss (Arista, 2002; Arista and Lifschitz, 2004). This effect arises from a more complete description that includes the effects of higher-order terms in the interaction.

To illustrate this effect I include in Figure 14 various simplified calculations assuming frozen ion charges: full charge ($q = Z_1$) and half charge ($q = Z_1/2$), according to the linear (dashed lines) and non-linear (continuous lines) models. Here the results are plotted in the form of "effective charge ratios": $[S(Z_1)/S_{\text{proton}}]^{1/2}$, where $S(Z_1)/S_{\text{proton}}$ is the ratio of the corresponding ion and proton stoppings for the same velocity. Clearly the linear calculation for $q = Z_1$ yields a straight line ($S \propto Z_1^2$ behavior). The non-linear results show a more moderate increase with ion charge in both cases. It should be noted that in most of this range the interaction parameter $\eta = Z_1 e^2/\hbar v$ is larger than 1, and therefore in the case of bare ions the behavior of the non-linear calculations may be well explained by a simple estimation based on the Bloch approximation. Thus, in the case of bare

ions the effect of saturation in the energy loss is already contained in the Bloch formula. The main new feature of the non-linear approach is that in contains both Bloch and Barkas corrections for dressed ions.

4. Summary

The question of charge states of light and heavy ions in solids remains being one of the most challenging problems in the field of ion-solid interactions. Two main difficulties combine to make this question a very tough one both from experimental and theoretical sides. The main experimental problem lies in the impossibility of obtaining precise values of the charge states of the ions inside the solid, at least from the conventional type of experiments using ion beams, so that one has to rely on indirect or external evidences. In the case of protons there are some alternative sources of information using subatomic particles, which consistently produce a rather well defined picture separating the cases of metallic and non-metallic materials. In the case of metals, the evidences support Brandt's conjecture in a more restricted sense: slow protons, as well as other positive point particles, would not bind electrons due to the strong screening conditions imposed by the metallic environment and so the protons remain as free but strongly screened ions. However, when the proton velocity increases the screening weakens and hydrogenic bound states appear. On the other hand, in the case of non-metallic materials, the screening is lower, and so it allows the existence of both free protons as well as neutral hydrogen atoms at all velocities, with corresponding charge state fractions determined by capture and loss processes.

Heavy ions are in principle still more complicated systems due to the much larger number of possible charge states and corresponding capture and loss processes that may take place (Echenique et al., 1990). A complete theoretical analysis of charge equilibrium and charge state fractions is a highly complicated issue since the cross section values for the elementary processes are not precisely known, having to deal in most cases with only rough estimations. The experimental side of this question is much more evolved; in particular, there are extensive sets of measurements of charge state distributions and mean values (q_{exit}) for ions emerging from solid foils (Shima et al., 1986, 1992). An important question that arises from these studies is the striking difference that may be found in some cases between these experimental values and those of the ion charges used in some phenomenological approaches and computer codes. The origin of this problem has been clarified by the recent calculations based on non-perturbative approaches (Arista, 2002; Arista and Lifschitz, 2004; Lifschitz and Arista, 2004). A very important difference between linear (or perturbative) and non-linear

(non-perturbative) methods is the absence of saturation effects (Bloch type of corrections) in the former case, which tends to enhance the stopping power values calculated with the linear/perturbative approach. This deficiency has been compensated in a heuristic way in the past by using comparatively lower values of ionization charges (like in the ZBL approach). It should be stressed that these values do not physically represent the real charge of ions travelling through a solid, and it follows that the use of these values in a different context may lead to erroneous results.

It should be noted that the question of slow heavy ions has not been included in this analysis. The most appropriate methods currently available for electronic energy loss calculations appear to be those based on density functional theory (for metallic targets) or alternative quantum methods. There are also a few recent calculations that describe changes in the electronic energy loss of slow ions due to inner-shell vacancies (Juaristi and Arnau, 1996; Juaristi et al., 1999).

The areas of ion charge states in solids and related energy loss processes still offer many open questions to be clarified from the theoretical point of view. Among these, an accurate theoretical treatment of capture and loss processes is one of the most challenging issues. A quantitative description of these processes may be the key to access the problem of charge state distributions and charge equilibrium in solids. The use of non-perturbative methods and the inclusion of dynamical effects should be considered as essential requirements for future studies on this line.

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