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Dynamic screening, charge states and energy loss of ions in solids

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The stopping power for light ions in solids is discussed by considering the dynamic screening of the moving ion and its charge states as a function of the ion velocity. Taking into account three different mechanisms for the electron capture and loss, the charge states for H and He moving in Al have been calculated introducing the contributions of the ion charge states and the capture and loss processes. Good agreement with experimental data is found.

1. Introduction

The use of fast ions as probes of the state and dynamic properties of matter dates from the earliest days of modern physics [1]. In the high-speed limit, $v \gg Z_1^{2/3} v_0$ (v_0 is the Bohr velocity and Z_1 the ion atomic number), the ion loses all its electrons and the ion–matter interaction can be described using linear response theory. Fermi [2] was the first to indicate this way to the analysis of the ion energy losses at high speed, and his idea was later developed by Williams [3] and Weizsäcker [4]. Following this, the random phase approximation dielectric function was derived by Lindhard [5], thus enabling a unified description of the single particle and the collective excitations of the electron gas by the incoming ion [6]. In the low velocity limit, $v \ll v_0$, the ion is dressed of its electronic cloud, interacting strongly with the solid; in this limit, the local density approximation (LDA) model has been shown to be very fruitful allowing the calculation of the ion stopping power in metals [7]. For intermediate velocities, $v \approx Z_1^{2/3} v_0$, the ion exchanges electrons with the medium [7,8], and the formal theory of the stopping power should include the different charge states of the ion in its interaction with the solid. This fundamental approach is a difficult task for heavy ions where many electrons participate in the exchange processes. In this communication, we address the problem of calculating the stopping power for the whole range of velocities, including the different loss and capture cross sections associated with the charge exchange processes. In our approach, linear response theory is combined with many-body techniques to calculate the energy loss per unit path length.

2. The model

In our approach for H and He, we assume that there is a well defined bound level for each ion over the whole range of ion velocities [9]. The ion charge states as a function of the ion velocity have been analysed elsewhere [10,11]; here we mention that the equilibrium charge fractions are obtained as the result of the several mechanisms whereby the electrons are either captured or lost by the moving ion. i) In the shell process [12], an electron can make an atomic-like transition from a bound state of an atom in the lattice to a bound state of the moving ion. ii) In the dynamic resonant process [10,12], the moving ion feels a time dependent perturbation due to the lattice potential. This induces transitions between the ion and the metal conduction band. iii) In an Auger process [9,11], electrons are transferred between the ion and the metal assisted by the creation of a third body, a plasmon or an electron–hole pair, in the metal electron gas.

The equilibrium charge fractions of ions with 0, 1 or 2 electrons (Φ^0, Φ^1 and Φ^2) are given in terms of the capture and loss cross sections [9,11], calculated using the mechanisms described above by the following equations:

$$\Phi^0 = \sigma_{\mathrm{LOSS}}(\Phi^1)\,\sigma_{\mathrm{LOSS}}(\Phi^2)\,D^{-1}, \tag{1a}$$

$$\Phi^1 = \sigma_{\mathrm{LOSS}}(\Phi^2)\,\sigma_{\mathrm{CAPT}}(\Phi^0)\,D^{-1}, \tag{1b}$$

$$\Phi^2 = \sigma_{\mathrm{CAPT}}(\Phi^1)\,\sigma_{\mathrm{CAPT}}(\Phi^0)\,D^{-1}, \tag{1c}$$

$$D = \sigma_{\mathrm{LOSS}}(\Phi^1)\,\sigma_{\mathrm{LOSS}}(\Phi^2) + \sigma_{\mathrm{LOSS}}(\Phi^2)\,\sigma_{\mathrm{CAPT}}(\Phi^0) + \sigma_{\mathrm{CAPT}}(\Phi^1)\,\sigma_{\mathrm{CAPT}}(\Phi^0). \tag{1d}$$

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Once the equilibrium charge states are calculated [10,13], we obtain the total stopping power by summing the partial stopping powers for each charge state weighted by the respective charge state fractions, and adding the energy lost per unit path length in capture and loss processes. The stopping powers for each charge state have been calculated in the following way.

For the H^- or He^0 state we have calculated the stopping power using the LDA method as explained in the refs. [7,11]. This is well justified because those charge states only appear at low velocities, when the LDA approach is appropriate. For the other charge states, the stopping power is calculated using linear response theory: this is also well justified because these other charge states only appear at high velocities.

The energy lost in capture and loss processes has to be calculated using the different microscopic processes contributing to the electronic charge exchange. In the case of an Auger process, for example, one has to take into account the third body excitation, electron–hole pair or plasmon, created in the electron gas, having an energy ω, and, at the same time, the electron or hole energies created in the metal due to the loss or capture processes, respectively. This yields the following energies: $[\omega + E_{\text{electron}}]$ in a loss process, whereby an electron is transferred to the metal, and $[\omega + E_{\text{hole}}]$ in a capture process, when an electron is transferred to the ion. In the resonant and shell processes only the electron and hole energies have to be considered, since no third-body excitation has to be created in the metal.

This argument yields the following energy losses per unit path [14]. In the Auger capture and loss processes we obtain:

$$\frac{\mathrm{d}E^{\mathrm{C,L}}_{\mathrm{Auger}}}{\mathrm{d}x} = \frac{2D_s}{v} \sum_{|\boldsymbol{k}+\boldsymbol{v}| \gtrless k_F} \int \mathrm{d}\omega \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^2} (\boldsymbol{q} \mp \boldsymbol{k})\boldsymbol{v} \frac{4\pi}{q^2} \times \mathrm{Im}\left\{ -\frac{1}{\epsilon(\boldsymbol{q}, \omega)} \right\} |M_{k,0}(\boldsymbol{q})|^2 \times \delta^{\mathrm{C,L}}(\omega - \boldsymbol{q}\boldsymbol{v} \mp E_{k,0}), \quad (2a)$$

for the resonant capture and loss processes we obtain:

$$\frac{\mathrm{d}E^{\mathrm{C,L}}_{\mathrm{Resonant}}}{\mathrm{d}x} = \frac{2\pi D_s}{v} \sum_{G} \sum_{|\boldsymbol{k}+\boldsymbol{v}| \gtrless k_F} |V(G)|^2 (\boldsymbol{G} \mp \boldsymbol{k})\boldsymbol{v} \times |M_{k,0}(\boldsymbol{G})|^2 \delta(\boldsymbol{G}\boldsymbol{v} \pm E_{k,0}), \quad (2b)$$

and for the capture shell process we obtain:

$$\frac{\mathrm{d}E^{\mathrm{C}}_{\mathrm{Shell}}}{\mathrm{d}x} = n_{\mathrm{at}} \sum_{n} \left(E_n - E_b + \tfrac{1}{2}v^2 \right) \sigma_{n,0}. \quad (2c)$$

In these equations, $\boldsymbol{G}$ is a reciprocal vector, $V(G)$ is the Fourier transform of the effective crystal potential acting on the incoming electron, $E_{k,0} = E_b + k^2/2$ and $M_{k,0}(\boldsymbol{q}) = \langle s | e^{i\boldsymbol{q}\boldsymbol{r}} | \boldsymbol{k} \rangle$. E_b and $|s\rangle$ are the binding energy and wavefunction of the bound electron [11]. $|\boldsymbol{k}\rangle$ is a plane wave orthogonal to $|s\rangle$ and $\epsilon(q, \omega)$ is the solid dielectric response function. E_n is the energy of the electron bound to the nth shell of the Al atom, and $\sigma_{n,0}$ is the cross sections for the $n \to 0$ transition. In reaching eqs. (2) we have also used the energy conservation laws: $\omega = \boldsymbol{q}\boldsymbol{v} \pm E_{k,0}$ and $E_{k,0} = \boldsymbol{G}\boldsymbol{v}$ for the Auger and resonant processes respectively, and the balance between all the capture and loss processes.

3. Results

The results for the stopping power of H and He moving with velocity v in Al are shown in figs. 1 and 2 as the thick solid line (labeled TOTAL). The stopping power for the bare ions calculated in linear response theory, using the Lindhard dielectric function is shown in the same figure for comparison. The different contributions to the TOTAL curve have been separated showing the charge states and the capture and loss contributions as a function of the ion speed.

For H the intermediate regime [14] appears for $0.8 < v < 1.2$; in this case all the three charge states appear to be relevant and their fractions are in the range 20–40%. For $v \approx 1.2$ a.u. the contributions from H^- and H^+ are comparable, each being about 30% of the total, while that of H^0 is about 10%. The inelastic processes of

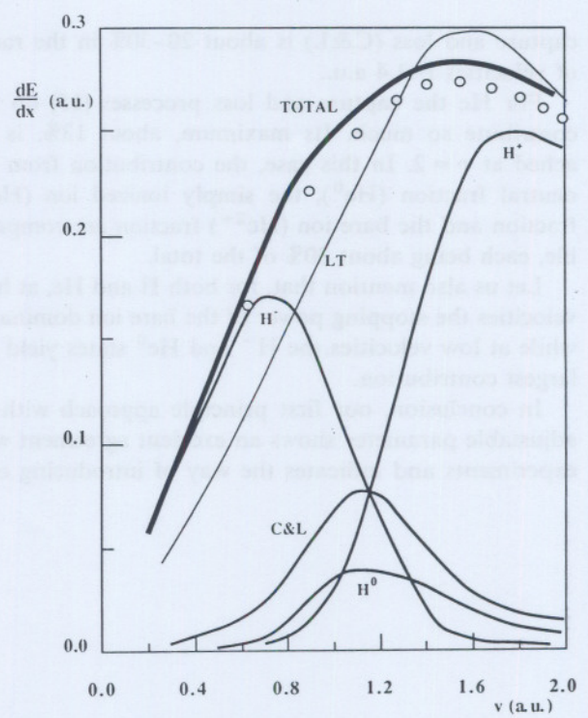

Fig. 1. Stopping power in atomic units of Al for H as a function of the ion speed. TOTAL: our results; LT: linear theory; H^+, H^0, H^-: charge fractions contributions; C&L: capture and loss contributions.

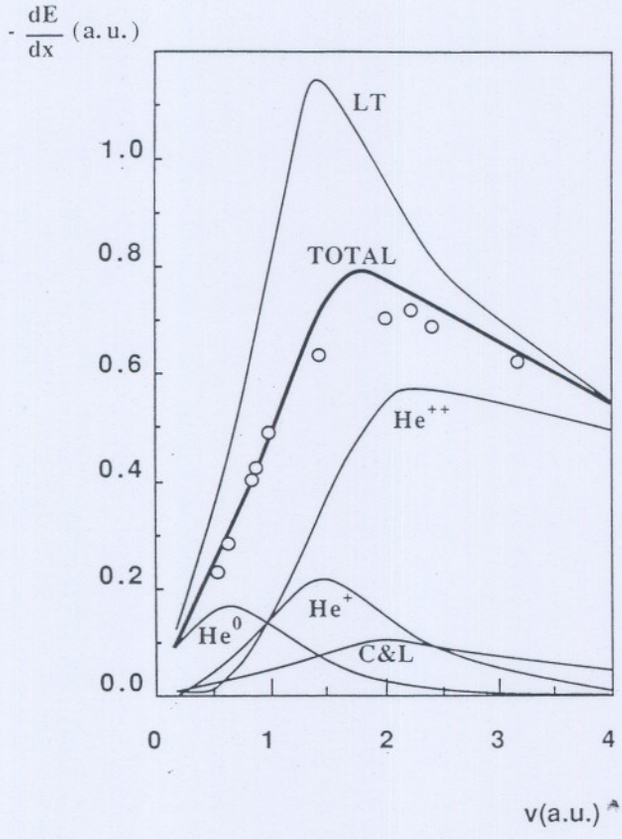

Fig. 2. As fig. 1 for He.

capture and loss (C&L) is about 20–30% in the range of velocities 1–1.4 a.u..

For He the capture and loss processes [15] do not contribute so much. Its maximum, about 13%, is reached at $v = 2$. In this case, the contribution from the neutral fraction (He^0), the simply ionized ion (He^+) fraction and the bare ion (He^{2+}) fraction are comparable, each being about 30% of the total.

Let us also mention that, for both H and He, at high velocities the stopping power of the bare ion dominates, while at low velocities the H^- and He^0 states yield the largest contribution.

In conclusion, our first principle approach with no adjustable parameter shows an excelent agreement with experiments and indicates the way of introducing capture and loss processes in the stopping power calculation. These processes are shown to yield important contributions to the total stopping power.

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