

Theoretical stopping power of copper for protons using the shellwise local plasma approximation

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(Dated: April 8, 2009)

We present a theoretical study on the energy loss by protons in solid copper. The *ab initio* shellwise local plasma approximation (SLPA) is employed for the inner-shells, and the Mermin dielectric function for the valence electrons. The partial contribution of each sub-shell of target electrons is calculated separately, including the screening among the electrons of the same binding energy. Present results are obtained using the SLPA and the known Hartree-Fock wave functions for copper. The theoretical curves are compared with the experimental data available and with the semi-empirical SRIM08 values, showing very good agreement in a large energy region (5 keV-30 MeV).

PACS numbers:

I. INTRODUCTION

The stopping power of ions in solids is a necessary ingredient of many areas of basic science and material technology [1, 2]. There are numerous detailed models to describe the response of outer electrons as a free electron gas (FEG) [3, 4, 5]. In many cases the stopping due to the FEG is enough for energies reaching up to the maximum of the stopping. But for targets with the full *d* or even *f* subshells, the bound electron contribution plays an important role even at intermediate energies. The description of bound electrons from first principles is a heavy task, especially for multielectronic atoms (see, for example the binary collisional formalism in Refs. [6, 7]).

In this work we describe the bound electron contribution to the stopping power by employing a many electron model, the shellwise local plasma approximation (SLPA). This is based on the local plasma approximation (LPA) [8, 9, 10] to deal with bound electrons as an inhomogeneous free electron gas. We apply this model within the dielectric formalism [11, 12, 13] but assuming independent shell approximation [14]. This means that in the SLPA the electrons of the same binding energy respond to the ion passage as a whole (collectively), screening the interaction with the impinging ion. This binding energy (or ionization gap) is included explicitly by employing Levine and Louie dielectric function [15].

The SLPA allows us to calculate the different moments of the energy loss by the ion when at least one of the bound electrons is ionized. This is an *ab initio* calculation – no parameter is included – whose only inputs are the atomic densities of the different subshells and the corresponding binding energies. Once the electronic wave functions are available, the SLPA applies to the different

targets with the same degree of complexity. This model has been applied successfully to describe experimental stopping cross sections of elements with $Z \leq 54$ (using the Hartree-Fock wave functions and binding energies) [16], and also for very heavy elements like Au, Pb, and Bi for which numerical solutions of the Dirac equation were needed [17].

In what follows we present our theoretical results for the stopping of protons in Cu ($Z=29$, [Ar] $3d^{10}4s^1$). The aim of this contribution is to use Cu as a testing case for the SLPA because it is a well known element (experimentally [18, 19] and theoretically [20, 21, 22]), and because we can employ the known Hartree-Fock wave functions [23, 24] to obtain the subshell densities to include in the SLPA.

We organize this work in two steps. First, we describe briefly the theoretical calculation, and then we present results for stopping cross sections of Cu for protons and compare our *ab initio* theoretical values with the experimental data available [18] and with the semi-empirical SRIM08 results [19].

II. THEORETICAL CALCULATIONS

The SLPA introduces two important differences to the known LPA. One of them is the shell-to-shell calculation. Mathematically it implies a separate dielectric function for each subshell of bound electrons, and the total response as the addition of these independent contributions. Physically, the electrons are screened only by those of the same binding energy and not by the rest.

The second one is the explicit inclusion of the binding energy by using the Levine-Louie dielectric response [15] instead of Lindhard one [25]. This dielectric function takes into account the ionization gap so that the contribution is null if the ionization threshold is deeper than the energy transferred [14]. The Levine-Louie dielectric

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response maintains the characteristics of Lindhard [25] (linear response, electron-electron correlation), and satisfies the f -sum rule (particle number conservation). More detail about the SLPA can be found in Refs. [14, 16].

For a bare ion of charge Z_P and velocity v , the stopping cross section due to the ionization of the nl subshell of target electrons, is expressed as

$$S_q^{nl} = \frac{2Z_P^2}{\pi v^2} \int_0^\infty \frac{dk}{k} \int_0^{kv} \omega \operatorname{Im} \left[\frac{-1}{\epsilon_{nl}(k, \omega)} \right] d\omega, \quad (1)$$

The dielectric function $\epsilon_{nl}(k, \omega)$ is calculated as a mean value of a local response [13]

$$\operatorname{Im} \left[\frac{-1}{\epsilon_{nl}(k, \omega)} \right] = 4\pi \int_0^{R_{WS}} \operatorname{Im} \left[\frac{-1}{\epsilon^{LL}(k, \omega, \delta_{nl}(r), E_{nl})} \right] r^2 dr, \quad (2)$$

where $\delta_{nl}(r)$ and E_{nl} are the local density of electrons $\delta_{nl}(r)$ and ionization gap, respectively, obtained from the atomic Hartree-Fock tabulated by Bunge *et al.* [23]. The spatial integration is performed over the atomic dimensions within the solid Cu (i.e., R_{WS} is the atomic Wigner-Seitz radius, related to the atomic density $\delta_{at} = [\frac{4}{3}\pi R_{WS}^3]^{-1}$).

The dielectric response, given by Eq. (2), considers only the electrons in the nl subshell. In this way the contribution of each shell of target electrons is obtained separately. An orbital version of the LPA was introduced many years ago by Meltzer *et al.* [26] within the logarithmic high energy limit of the stopping number. Instead, in the SLPA we calculate a dielectric response of each shell, and it is valid even in the intermediate energy range.

The independent shell description in the SLPA considers explicitly the energy threshold E_{nl} of each shell (ionization of inner shells). The Levine and Louie model [15] defines the dielectric function as

$$\operatorname{Im} [\epsilon^{LL}(q, \omega, k_{nl}^F)] = \begin{cases} \operatorname{Im}[\epsilon^L(q, \omega_g, k_{nl}^F)] & \omega > |\epsilon_{nl}| \\ 0 & \omega < |\epsilon_{nl}| \end{cases} \quad (3)$$

with $\omega_g = \sqrt{\omega^2 + \epsilon_{nl}^2}$ and $\epsilon^L(q, \omega, k_{nl}^F)$ being the usual Lindhard dielectric function [25]. This modified SLPA has already been applied successfully in recent calculations of stopping power [16, 27], energy loss straggling [28] in solids, and also in multiple ionization cross sections of rare gases [14].

III. RESULTS

In order to compare with the experimental data available we calculate total stopping cross sections. These values are obtained as the addition of the bound electron and the FEG contributions. The former calculated with the SLPA formalism as described before. The latter by employing the dielectric formalism with the Mermin dielectric function [29].

The characteristic plasmon frequency and width of the Cu FEG are $\omega_p = 0.703$ a.u. and $\gamma = 0.950$ a.u. respectively. This implies a mean value of electrons in the FEG $Ne = 3.14$, and a Seitz radius $r_S = 1.82$ a.u.. These values were obtained from the optical data of energy loss function [30] by considering only the first important peak. The number of electrons in the FEG is similar to the experimental value recommended by Isaacson [31]. To keep the total number of electrons, we considered Cu as [Ar] $3d^{7.86}$ and 3.14 electrons as FEG.

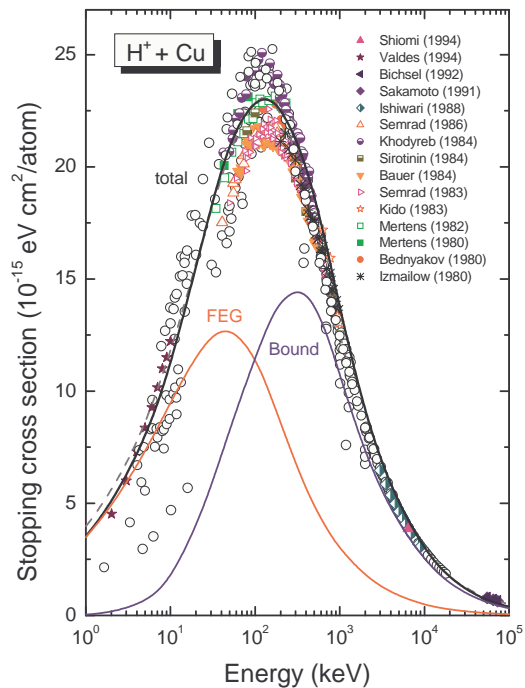


FIG. 1: Stopping cross sections of Cu for protons. Curves: Solid-lines, present theoretical results for the contributions by bound electrons (SLPA) and the FEG, and total stopping as the addition of the previous two; dash-line, SRIM08 results [19]. Symbols: black hollow-circles, sets of experimental data compiled by H. Paul [18] corresponding to (1935-1979); different symbols signed within the figure, experimental data in Refs. [32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46].

In Fig. 1 we plot our total stopping cross sections of Cu for protons, and compare them with the experimental data available [18], and with SRIM08 results [19]. The contribution from the FEG and the bound electrons are displayed separately. About the experimental data, we indicate separately only the data since 1980, while previous one is plotted together with a single type of symbol. The agreement with the experimental data and with the SRIM08 curve is good. This is a perturbative formalism,

which is not expected to describe the data for ion energies below 30 keV. However, we have obtained a very good agreement even with the measurements by Valdes *et al.* [32] in the low energy region. The FEG results obtained with the Mermin dielectric function, even perturbative, are rather good for protons in Cu at such low energies. Figure 1 shows that the stopping maximum is correctly described in energy and value. For energies above that of the stopping maximum, the description is good, but shows an overestimation around 2 MeV. This behavior of the SLPA has already been noted in previous works [17, 47] and it is under study.

IV. CONCLUDING REMARKS

In this work we test the *ab initio* SLPA for the stopping of Cu for protons. This is a perturbative model

which works within the dielectric formalism by considering the response of bound electrons as that of a free electron gas of inhomogeneous density. The SLPA introduces the independent shell approximation to the usual formalism. The theoretical results are compared with the experimental data available and with the semi empirical SRIM08 values, showing good agreement in a large energy region (5 keV-30 MeV).

Acknowledgments

This work was partially supported by the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), the Universidad de Buenos Aires, and the Agencia Nacional de Promoción Científica y Tecnológica de Argentina.

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