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A simple expression for electronic stopping force of heavy ions in solids

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ABSTRACT

A simple expression for the electronic stopping force of heavy ions in solids is proposed based on an adaption of the Bohr's classical stopping theory. A three-parameter model is constructed by using experimental data for helium, oxygen, argon, krypton and xenon ions in carbon, aluminum, nickel and gold targets at energies from 600 eV/u to 985 MeV/u. Total average agreements between the model and used experimental data are $(-4.5 \pm 47)\%$ and $(-1.6 \pm 7.4)\%$ at energies below and above the Bragg peak, respectively. The good overall agreement makes this model a good candidate for future development in stopping force prediction tools.

1. Introduction

Several unified formulations for the electronic stopping force of heavy ions has been proposed by many authors [1–3] in the hundred-year-history of stopping force theory. Numerous different estimation tools are available for predicting the stopping force, e.g. SRIM-2003 [4], CasP [5] and MSTAR [6,7] to name the few. Most of the prediction tools are semi-empirical. Sigmund and Schinner [8] have developed a model called *binary theory* which is derived from the first principles without any parametrization to experimental data. Also CasP is based on *ab initio* calculations.

The semi-empirical models are based on parametrization of the experimental data on a basis of selected stopping theory. Depending on the ion specie and the energy range in question, estimation tools are based either on the Bohr's classical [9,10], or the Bethe's quantal [11] stopping theories with Bloch's corrections [12] included accordingly. In many cases estimation tools incorporate, in one way or another, the *effective charge* concept [13,14]. The use of effective charge in the calculations of electronic stopping force has been shown to have its restrictions [15].

Neither Bohr's nor Bethe's theory define accurately the electronic stopping force at low energies, which makes their adaption to the experimental data restricted, and increases the complexity of the models at low energies. The typical problem in the semi-empirical schemes is the vast amount of, mostly *non-physical*, parameters which are needed in order to cover different ion–target combinations. Typically the disadvantage in *ab initio* calculations is their complexity, and in some cases their public inavailability, e.g. up-to-date calculations from the binary theory are available only on request from the code developers.

In this work a simple three-parameter model is proposed, which is found to predict stopping force with a reasonable accuracy in wide ranges of energies, projectiles and solid targets. The model is based on the Bohr's classical stopping theory with some modifications made to the original expression, and without using the effective charge concept in the formulation.

2. Methods and calculations

The familiar general relation for the electronic stopping force is given by

$$-\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{m_e v^2} N Z_2 \cdot L, \tag{1}$$

where e and m_e are the electron charge and rest mass, L is the stopping number, v is the projectile velocity, N is the atomic density of the target, and Z_1 and Z_2 are the atomic numbers of the projectile and the target, respectively. The stopping number in the Bohr model can be expressed [17,18] as a function of variable ξ

$$L_{\text{Bohr}} = \frac{1}{2}\ln\{1 + (k\xi)^2\}, \tag{2}$$

where $k = 2e^{-\gamma} \approx 1.1229$, a commonly known coefficient used in the Bohr's theory, with $\gamma \approx 0.577$ being the *Euler's constant*. The variable ξ is defined by

$$\xi = \frac{m_e v^3}{Z_1 \hbar\omega_0 v_0}, \tag{3}$$

where $\hbar\omega_0$ is the mean excitation energy of the target electrons, v_0 is the Bohr velocity. In this work the Bloch relation [19], $\hbar\omega_0 = Z_2 \cdot I_0$, is used with $I_0 = 10$ eV [20]. The Bohr's classical stop-

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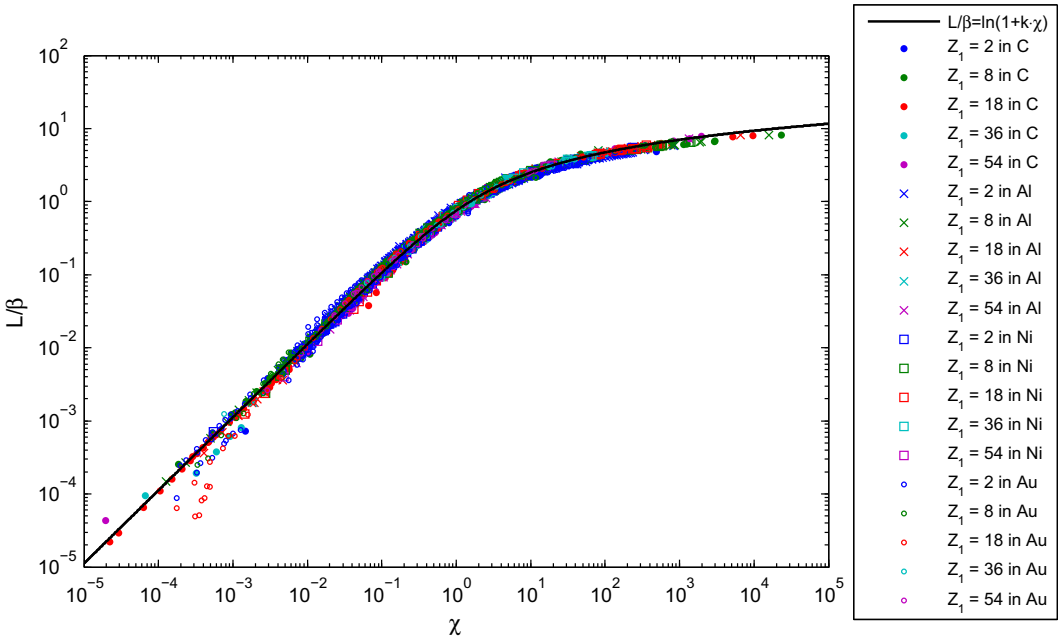

Fig. 1. Experimental stopping numbers derived from Eq. 1 for ion–target combinations given in Table 1 as a function of variable χ. The solid line corresponds to Eq. 5.

ping theory is considered to be valid for heavy ions in velocity range of $2Z_1^{2/3} < \frac{v}{v_0} < 2Z_1$.

A new variable is introduced where the variable ξ is scaled with reciprocal of the velocity-independent screening parameter $s \cong 1.2\frac{Z_1^{1/3}}{Z_2^{1/2}}$ from [21] as follows

$$\chi = a \cdot s^{-1} \cdot \xi, \tag{4}$$

where a is a fixed fitting parameter. It has been found that experimental stopping numbers follow relation

$$L = \beta \cdot \ln(1 + k \cdot \chi), \tag{5}$$

where β is a moving fitting parameter corresponding to each ion–target combination, see more below. The relation between experimental stopping numbers derived from Eq. 1 and χ is illustrated in Fig. 1.

The considered ion–target combinations are given in Table 1. All experimental stopping force data used in this work has been taken from Paul's database [16]. These ions–target combinations were chosen, on one hand, because a relatively large amount of experimental data are available for them, and on the other hand, these represent combinations from *light ions in light target* to *heavy ions in a heavy target*. This way the validity of the model is tested properly.

In the first step, data fit is done by using Eq. 5, which gives parameters a and β. In Fig. 2 these parameters are plotted as a function of ratio $\frac{Z_1}{Z_1}$. It is observed that parameter a is relatively constant for all values of $\frac{Z_1}{Z_2}$. There is a weak downward trend in a as a function of $\frac{Z_1}{Z_2}$. However, it is found not to improve the model if this trend is taken into account by increasing one extra parameter for determining a.

Hence, in the next step a constant parameter $a = 0.2853$ is used in fitting parameter β. Now, β is observed to be relatively well behaved as a function of $\frac{Z_1}{Z_2}$, which is also illustrated in Fig. 2. For further modeling a function

$$\beta = b_1 \cdot \sqrt{1 + b_2 \ln\left(\frac{Z_1}{Z_2}\right)}, \tag{6}$$

Table 1
The ions and targets used in this work with corresponding energy ranges and number of data points. The data is taken Paul's database [16]. The average differences and their standard deviations at energies below (*lo*) and above (*hi*) the Bragg peak are given for each ion–target combination. The difference is defined by $\Delta = \frac{\frac{dE}{dx}_{\text{exp.}} - \frac{dE}{dx}_{\text{this work}}}{\frac{dE}{dx}_{\text{exp.}}}$.

Ion–target	$E_{\min}$ (keV/u)	$E_{\max}$ (MeV/u)	Data points	$(\Delta \pm \sigma)_{lo}$ (%)	$(\Delta \pm \sigma)_{hi}$ (%)
He–C	1.4	7.00	315	−0.5 ± 11.8	1.6 ± 5.9
O–C	1.3	690.00	189	1.2 ± 9.5	−3.3 ± 7.3
Ar–C	0.6	985.00	97	−11.9 ± 15.3	−6.1 ± 7.2
Kr–C	2.4	42.31	38	−28.5 ± 28.2	−2.3 ± 2.2
Xe–C	1.5	780.00	50	−13.8 ± 12.8	−1.6 ± 2.1
He–Al	3.7	13.01	482	14.5 ± 4.7	−0.7 ± 8.5
O–Al	1.3	690.00	172	7.5 ± 5.6	−2.0 ± 5.7
Ar–Al	5.6	985.00	52	−12.2 ± 11.0	−3.7 ± 4.8
Kr–Al	28.6	42.78	34	−9.1 ± 4.2	0.9 ± 2.2
Xe–Al	100.0	780.00	31	−13.1 ± 6.0	3.0 ± 3.5
He–Ni	1.3	7.20	262	−11.1 ± 8.1	−9.3 ± 3.5
O–Ni	12.5	92.14	169	2.8 ± 8.3	0.1 ± 4.7
Ar–Ni	16.8	75.73	39	−10.7 ± 15.5	−0.4 ± 4.6
Kr–Ni	511.0	42.50	44	3.5 ± 4.3	0.8 ± 3.4
Xe–Ni	100.0	26.31	37	−7.4 ± 7.5	−0.5 ± 3.2
He–Au	0.8	13.01	768	1.3 ± 23.0	−1.6 ± 7.8
O–Au	4.3	89.31	272	5.8 ± 13.9	0.7 ± 7.7
Ar–Au	5.8	83.55	83	−65.0 ± 161.2	1.7 ± 3.2
Kr–Au	28.6	43.01	35	9.5 ± 10.2	−0.5 ± 4.1
Xe–Au	100.0	26.32	34	3.8 ± 9.5	1.8 ± 1.6