Systematic study of channeling stopping-power oscillations for low-velocity heavy ions

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The model used by Briggs and Pathak to calculate the electronic energy loss of low-velocity channeled heavy ions has been explored further to study the velocity dependence of Z_1 oscillations in electronic stopping power. For increasing ion velocities, where the validity of neglecting the target-electron velocities increases, it is found that the magnitude of Z_1 oscillations decreases and by about 2-a.u. velocity the first maxima at $Z_1 = 6$ and the first minima at $Z_1 = 10$ are washed out completely.

I. INTRODUCTION

The Z_1 and Z_2 oscillations in the stopping power of solids for low-velocity channeled heavy ions have been studied in detail both theoretically and experimentally, ever since these were observed first in random situations[1] and later in channeling situations.[2] The theoretical interpretation for these oscillations has been given by several authors. In the beginning all attempts made[3,4] to explain these oscillations were based on modifications of Firsov theory[5] by using a detailed shell-structure model (for the projectile and target atoms) instead of the Thomas-Fermi statistical model. Such attempts were successful in explaining many features of the stopping-power oscillations. However, it was found that (i) the calculated magnitude of oscillations (maxima to minima ratio) was much smaller than that experimentally observed, (ii) the oscillations damp out for higher Z, and more recently it has been found that (iii) the magnitude of stopping is much too sensitive to the choice of wave functions.[6]

An alternative model for low-velocity stopping power for channeled heavy ions was employed by Briggs and Pathak,[7] where one considers the scattering of the target electrons (assumed to form an uniform electron gas) in the potential field of the projectile ion, and, in this process of scattering, the energy is taken away by the target electrons. The energy loss is related to the momentum-transfer cross section for this electron-ion scatttering process, and this cross section has oscillations with respect to Z_1. This approach was found to explain the Z_1 oscillations in the stopping power of channeled heavy ions rather nicely. The major difference between the two approaches discussed above is that the Firsov-theory modification is completely symmetric in Z_1 and Z_2, the projectile and the target atomic number, respectively, and therefore will yield complete symmetry in Z_1 and Z_2 oscillations both for channeling stopping in solids as well as random stopping in solids and gaseous targets. However, the later model[7] used by Briggs and Pathak is *not* symmetric in Z_1 and Z_2. Here, the Z_1 oscillations are embodied in the momentum-transfer cross section, whereas the Z_2 variations come from the corresponding variations in the effective charge density of the assumed uniform electron gas. This point was discussed in connection with Z_2 variation in the channeling stopping power[8] and it was emphasized that in the channeling situation, Z_1 and Z_2 variations do have entirely different origin and symmetry in Z_1 and Z_2 cannot be expected.

The aim of the present paper is to study the systematics of Z_1 and Z_2 variations in the channeling stopping power with increasing velocity of the projectile ion. Experimentally some attempts have been made[9] to study the velocity dependence of Z_1 and Z_2 oscillations in random stopping power. This is because it is known that there are no such oscillations in the high velocity Bethe-Bloch region where the quantal perturbation treatment for stopping power becomes applicable. At these velocities, the above simple model based on elastic scattering of the target electrons from the incident ion is not very useful because the cross sections are now effectively composed of infinite number of partial waves that must be summed. Similarly the Firsov or Lindhard theories for low-velocity heavy-ion stopping (and hence the modifications thereof) are not valid. Therefore a definite knowledge of the velocity where Z_1 and Z_2 oscillations are washed out will be very helpful in establishing more precisely the regions of validity and applicability of two kinds of treatments. Secondly, and perhaps more significantly, such knowledge of systematics of Z_1 and Z_2 oscillations will be of great help in extrapolation, empirical prediction and tabulation of stopping-power data for all projectiles in all targets. For example, lack of such knowledge forced Northcliffe and Schilling to disregard the Z-oscillation effects in their tables.[10]

A short summary of the formulas used is given in the next section and the results are discussed in the last section. Possible experiments have been suggested to test certain new and interesting features in oscillations predicted here.

II. FORMALISM

The mean energy lost by an ion of velocity v to an electron gas of density n is given by[7]

$$-\frac{dE}{dX}=nmv^2Q_d \quad , \tag{1}$$

where m is the electronic mass and Q_d the momentum-transfer cross section, given by

$$Q_d=\frac{4\pi}{k^2}\sum_l (l+1)\sin^2(\eta_l-\eta_{l+1}) \quad . \tag{2}$$

Using atomic units, these two equations [(1) and (2)] can be combined to read

$$-\frac{dE}{dX}=4\pi n\bar{Q}_d=4\pi n\sum_l (l+1)\sin^2(\eta_l-\eta_{l+1}) \quad . \tag{3}$$

Here, η_l is the l th partial-wave phase shift and has been determined by solving the radial part of the Schrödinger equation

$$\frac{d^2G_l}{dr^2}+\left[k^2+U(r)-\frac{l(l+1)}{r^2}\right]G_l=0 \quad . \tag{4}$$

As is well known, for $U(r)$ varying faster than $1/r$, the asymptotic form of the solution G_l of Eq. (4) is

$$G_l(r)\sim\sin(kr-\tfrac{1}{2}l\pi+\eta_l) \quad , \tag{5}$$

and without atomic field [$U(r)=0$], Eq. (4) gives the Bessel function solution whose asymptotic form is

$$G_l(r)\sim j_l(kr)\overset{r\to\infty}{\longrightarrow}\sin(kr-\tfrac{1}{2}l\pi) \quad . \tag{6}$$

The magnitude of the phase shift η_l is then determined by the competition between the attractive potential $U(r)$ and repulsive centrifugal potential $l(l+1)/r^2$ and as such is computed by finding the shift of nodes of the solution (5) with respect to the corresponding node of the Bessel function (6) for large r.

The atomic field $U(r)$ in which the target electrons are scattered is taken to be statistical Thomas-Fermi potential. For use in the numerical calculations, this was fitted to a sum of screened Coulomb form (i.e., Moliere type)

$$U(r)=\frac{1}{r}\sum_{i=1}^{3}a_i\exp(-b_ir) \quad . \tag{7}$$

The reason to choose this simple potential is based on our experience which has shown that the potential in Eq. (7) demonstrates quite clearly[7,8,11] the occurrence of stopping-power oscillations. Recourse to a potential which is calculated with the shell structure explicitly taken into account (for example the Hartree-Fock potential) only gives rise to isolated peaks[7] which are not observed experimentally because they correspond either to large radii outer shells (for example $3s$ in Na) or to Ramsaur-Townsend effect, both of which cannot be expected to be observed in a stopping-power experiment in solid targets. The Z_1 oscillations in stopping power are essentially contained in the momentum-transfer cross section $\bar{Q}_d$. The target electron velocity has been neglected in all of the above equations because the main purpose here was to establish an upper limit of projectile velocity beyond which the Z oscillations in stopping power should not be expected. In any case, this assumption of neglecting target electron velocity becomes more and more valid as the projectile velocity increases beyond 1 a.u.

III. RESULTS AND DISCUSSION

Using the above equations, we have calculated the various partial-wave phase shifts and evaluated the momentum-transfer cross section $\bar{Q}_d$ for $k=0.75$ to 2.0 a.u. in steps of 0.25. The results are displayed in Fig. 1 for $Z_1=2$ to 24. The stopping power in the uniform-electron-gas model is obtained simply by using the formula (1) with appropriate effective electron gas density. We notice from Fig. 1 that as k increases, the magnitude of the oscillations (i.e., maxima to minima ratio) decreases systematically and by $k=2.0$ a.u., the first maxima around $Z_1=6$ and first minima around $Z_1=10$ are completely washed out. This decrease in the oscillation amplitude is also accompanied by a gradual shift in the positions of first maxima and first minima towards the higher-Z_1 side by about 2 to 3 units.

We remember[7,11] that the origin of the Z_1 oscilla-

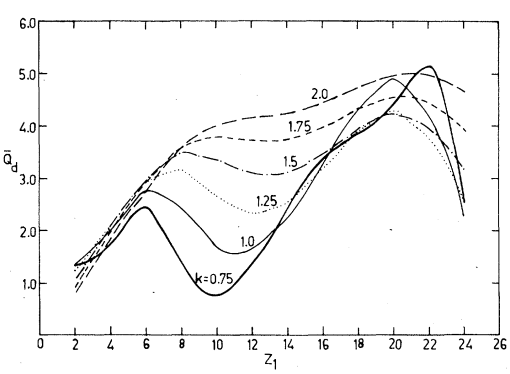

FIG. 1. The variation of the momentum-transfer cross section $\bar{Q}_d$ with the projectile atomic number Z_1 for various values of projectile velocity given in atomic units, by $k=0.75$, 1.0, 1.25, 1.5, 1.75, and 2.0. The stopping power is obtained through Eq. (3).

tions is contained in the way the various shells are filled in the Periodic Table. The first peak around $Z_1 = 6$ comes from $l = 1$ partial cross section in the expression for $\bar{Q}_d$ since the p-wave phase shift goes through a change by π corresponding to the filling[12] of the $2p$ shell while the d-wave phase shift is zero. Similarly, the second peak comes from $l = 2$ partial cross section corresponding to the filling of the $3d$ shell. Now as the energy (and hence k) increases, the near step-function increase (actually at $k = 0$, the phase shift increase is literally a step function[13]) by π in the appropriate phase shift η at given Z, tends to be smeared out and by $k = 2$ a.u. it becomes nearly monotonic increase. Therefore, by the time the $l = 1$ partial cross section in $\bar{Q}_d$ has a chance to drop corresponding to η_1, going through π, the next partial cross section (for $l = 2$) has started contributing, and as a result we get monotonic increase in the total $\bar{Q}_d$ with Z_1, thus washing out first maxima and first minima almost completely. These results are in agreement with the experimental results of Ward *et al.*[9] for random stopping oscillations, where the Z_1 oscillations are found to vanish at about $k = 2$ a.u. velocity. However, more experiments on channeled stopping-power oscillations for a wider range of velocities will be useful. At the same time more calculations for higher Z_1 values and for higher velocities are required and are being attempted.

It may be mentioned that the Z_2 variations in the channeling stopping power have different origin and interpretations. These are due to the corresponding variations in the effective electron density encountered in the channels.[8] Therefore these are expected to show up until the onset of the high-velocity Bethe-Bloch region where the long-distance plasma excitations start contributing to the process of energy loss. In fact, Ward *et al.*[9] do indeed find that Z_2 variations persist up to 8 a.u. velocity. In this respect it seems worth emphasizing that a detailed experimental study similar to that of Ward *et al.*[9] for random situations like gaseous targets regarding velocity dependence of Z_2 oscillations will be of great value for investigations concerning the origin and interpretation of Z_2 oscillations. Specifically, because the Z_1 and Z_2 oscillations in the random materials and gaseous targets are found to be very similar[1,14]; as also expected from modified Firsov theory,[4] as against those in channeling situations,[8,15] a detailed comparison of velocity dependences of Z_1 and Z_2 oscillations for gaseous targets will be extremely useful in clarifying and establishing the basic similarities and differences in the two situations.

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