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Systematic study of channeling stopping-power oscillations for low-velocity heavy iona. II

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Recent study of velocity dependence of channeling stopping-power oscillations with respect to projectile atomic number Z_1 has been extended to heavier ions. It is found that the shifting of positions of maxima and minima accompanied by the gradual merger of consecutive peaks reflecting the energy dependence of phase shifts and bound states continues. The need for an experimental test of these predictions has been emphasized.

Apart from some finer details like target-electron velocity averaging, inclusion of the effects, of the Pauli exclusion principle, and actual variation of charge states of different projectiles in solids, the theory for Z_1 oscillations in the electronic stopping power as proposed by Briggs and Pathak,¹ using a model of target electron scattering in the potential field of projectile ions has successfully explained all essential features observed in channeling experiments.² The Z_2 variations in channeling stopping power have also been explained in this model.³ Recently, however, it has been realized that a knowledge about velocity and material dependence^{4, 5} of stopping-power oscillations will be most helpful for a better understanding of the physics behind the basic phenomena. We have recently studied theoretically' the velocity dependence of Z_1 oscillations using the Briggs-Pathak model and found that first maxima around $Z_1 = 6$ and first minima around $Z_1 = 10$ are almost completely washed out by 2 a.u. velocity. Moreover, the decrease in the oscillation amplitude is accompanied by a gradual shift in the position of maxima and minima towards the higher- Z_1 side by about 2 to 3 units. It was suggested that an experimental test of these predictions should be undertaken. Specifically, it is worth mentioning that no channeling experiment to measure systematically the stopping powers for different projectile ions has ever been undertaken for projectile velocities higher than 1.5×10^8 cm/sec, to check the phase and magnitude of oscillations. For random situations, the only work in this direction seems to be that of Ward et $al.$, 6 showing that the maxima and minima at $Z_1 = 6$ and 10 are washed out by about 2 a.u. velocity of projectiles, but even here, nothing is known about extrema at higher- Z_1 values.

The aim of this paper is to extend our previous work⁵ (referred to as I) to higher- Z_1 values and to show that shifts in the positions of maxima and minima with increasing projectile velocities is a real effect and should be observable. An experiment to test it

would be of great value for a better understanding of Z oscillations in stopping power.

The procedure and the model used have been discussed in I. The basic formula for the mean energy lost by an ion of velocity v to an electron gas of density n is written in atomic units as

$$
-\frac{dE}{dX} = 4\pi n \overline{Q}_d
$$

= $4\pi n \sum_{l} (l+1) \sin^2(\eta_l - \eta_{l+1})$ (1)

where the *l*th wave phase shift η_l in the targetelectron wave function is obtained by solving the radial part of Schrödinger equation

$$
\frac{d^2G_l}{dr^2} + \left(k^2 + U(r) - \frac{l(l+1)}{r^2}\right)G_l(r) = 0
$$
 (2)

and comparing the asymptotic form of $G₁$, i.e.,

$$
G_l(r) \sim \sin(kr - \frac{1}{2}l\pi + \eta_l)
$$

with the corresponding solution without potential, namely,

$$
G_l(r) \sim j_l(kr) \sim \sin(kr - \frac{1}{2}l\pi) \quad . \tag{3}
$$

The interaction potential used in these calculations is Moliere-type Thomas-Fermi potential

$$
U(r) = \frac{1}{r} \sum_{i=1}^{3} a_i \exp(-b_i r) \quad . \tag{4}
$$

The results for momentum transfer cross section \overline{Q}_d are plotted in Fig. 1 for $Z_1 = 2$ to 80 [and the stopping power is obtained through the formula (1)] for $k = 0.75$ to 2 a.u. in steps of 0.25. First we discuss the case of $k = 0.75$, the one dealt with earlier¹ in detail because of availability of experimental results at this velocity, for Z_1 values up to 54. It was seen that the peaks around $Z_1 = 21$ and 38 are connected with the filling of $3d$ and $4d$ shells. Now we find another maximum in the momentum-transfer cross section in

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FIG. 1. Variation of momentum-transfer cross section \overline{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. (1).

the region where the $4f$ shell is being filled, consistent with the interpretation given earlier.¹ We notice, however, the effect of changing k from 0.75 to 2 a.u. First, the shifting of extrema predicted for lower Z_1 continues. The minimum around $Z_1 = 27$ shifts continuously as k increases from 0.75 to 2 a.u. More interesting is the effect occurring near the minimum at $Z_1 = 45 - 46$ and maximum near $Z_1 = 37$ and $60-61$. As k increases, a gradual shifting and distortion of shape takes place simultaneously and by $k = 2$ a.u., the minimum around $Z_1 = 45-46$ has vanished altogether and a prominent peak representing a merger of the two peaks at 37 and 60, appears at $Z_1 = 50$. The way this happens (which we noticed by having a closer look at curves for $k = 1, 1.25$, and 1.5) is similar to merger of peaks at $Z_1 = 6$ and 20 which formed a broader single maximum before $Z_1 = 32 - 34$.

Physically, this is clearly related to the energy ef- fect on the bound states and corresponding phase shifts. As energy [i.e., k in Eq. (2)] increases, the step-function rise of the phase shift for a given partial wave is transformed into a gradual rise⁷ and various partial cross sections in momentum transfer tend to interfere with each other resulting in a broadening of the extrema and an eventual merger. This is what is happening to the third and fourth peaks which now

merge to give a single peak at $Z_1 = 50$ in the region of earlier minima, and is essentially a combination of partial cross sections corresponding to $l = 2$ and 3, i.e., ^df and fg partial cross sections.

Since the velocity up to which the electronic stopping increases with the projectile velocity depends upon Z_1 and is given approximately by $v_0Z_1^{2/3}$ where v_0 is Bohr velocity, the vanishing of stopping-power oscillations for higher Z_1 will take place at velocities much higher compared to the lower- Z_1 case. This is presumably the reason for survival of oscillations (with changed phase as explained above) for higher Z_1 even for 2 a.u. whereas the first maximum and first minimum are washed out almost completely by this velocity.

In conclusion, it should be emphasized that an experimental verification of the above predictions for shifting of oscillations and change in phase will be extremely helpful in the further development of channeling stopping-power theories in the low- and medium-velocity region.

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- ¹J. S. Briggs and A. P. Pathak, J. Phys. C $\frac{7}{1}$, 1929 (1974); A. P. Pathak, J. Phys. F 4, 1883 (1974).
- 2L. Eriksson, J. A. Davies, and P. Jespersgaard, Phys. Rev. 161, 219 (1967); J. Bottiger and F. Bason, Radiat. Eff. 2, 105 (1969).
- $3A. P.$ Pathak, J. Phys. C $7.$ 3239 (1974); J. L. Whitton, Can. J. Phys. 52, 12 (1974).
- 4D. Ward, H. R. Andrews, I. V. Mitchell, W. N. Lennard, and R. B. Walker, Can. J. Phys. 57, 645 (1979).
- 5A. P. Pathak, Phys. Rev. B 22, 96 (1980).
- 6D. Ward, J. S. Forster, H. R. Andrews, I. V. Mitchell, G. C. Ball, W. G. Davies, and G. J. Costs, AECL Report No. 5313 (unpublished).
- 7S. T. Manson, Phys. Rev. 182, 97 (1969).