SOME FEATURES OF LARGE-ANGLE ELASTIC ELECTRON-ATOM SCATTERING AT INTERMEDIATE ENERGIES

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It is shown that the previously observed[1,2] maxima on the energy dependence of the elastic reflection coefficient of intermediate energy electrons incident on solids are related to a singularity in the scattering of intermediate energy electrons by individual atoms. The essence of this singularity is that the integral elastic scattering cross section for intermediate energy electrons scattered through angles between $\pi/2$ and π passes through a maximum at a scattered electron energy which is characteristic for each element. Phase analysis shows that the phenomenon is due to an increase of the contribution of partial cross sections with nonzero orbital angular momenta at a certain characteristic value of the energy. A correlation is established between this effect and the singularities in the angular distribution of electrons scattered through large angles in vapors and gases of certain elements which has been observed earlier in the physics of atomic collisions. Both experiment and theory show that this property of atomic scattering is exhibited by most, if not all, elements in the periodic system.

T HE reflection of intermediate energy electrons from solid surfaces has an interesting property which consists in that the elastic reflection coefficient R is, in general, a nonmonotonic function of the incident electron energy E_p. This phenomenon was first found experimentally for the reflection of electrons from tungsten, and the maximum on the R versus E_p curve was found to occur at approximately 600 eV.[1] It was subsequently established that this phenomenon was not peculiar to tungsten but appeared for most of the elements in the periodic table, and that the characteristic energy at which the maximum appeared was a function of the atomic number Z.[2] In particular, the relation between the characteristic energy E_p^* in electron volts and the atomic number Z is given to a good approximation by the formula

$$E_p^* = \tfrac{1}{8}Z^2 \tag{1}$$

for all Z with the exception of small values. As E_p^* increases, the maximum broadens and the value of R decreases. However, in most cases, the change in R at the maximum is of the order of R itself.

It is now possible to provide an interpretation of this effect which satisfies the experimental data (a preliminary report of this is given in[3]). It may be supposed that this is a purely atomic and quantum-mechanical phenomenon. The solid state aspects have very little effect, especially in the case of polycrystalline targets, and can be shown merely to increase the relatively low atomic scattering cross section through the large angles by a factor of N, where N is the density of atoms of the given element in the target. In addition, it is possible to observe the effect for elements with low vapor pressures. The elastic scattering is therefore noncoherent and multiple, or even single. If the scattering at energies near the characteristic energy E_p^* is multiple then, in addition to the possible collisions with low momen-

tum transfers, it contains one scattering event through angles greater than $\pi/2$. It is important to note that, at the same energies, the total atomic scattering cross section through all angles between 0 and π appears to be a monotonically decreasing function of E_p.

The effect occurs at energies which can be described as intermediate. These are the energies at which, on the one hand, s scattering no longer predominates and, on the other, the Born approximation is not yet valid. In other words, at these energies the atomic back-scattering cross section

$$\sigma_{bs} = 2\pi \int_{\pi/2}^{\pi} \sigma(\theta)\sin\theta\, d\theta, \tag{2}$$

is largely determined by the contribution of partial cross sections corresponding to the first few orbital angular momenta. Since the effect appears to be general right through the periodic table, one would expect that the details of the atomic potential which are different for different atoms are not particularly important in this context. It was therefore hoped that the effect would be describable in terms of a simple model potential. We have, in fact, taken the Mensing potential[4]

$$V(r) = \begin{cases} -Ze^2(1/r - 1/r_0) & \text{for } r \leq r_0 \\ 0 & \text{for } r \geq r_0, \end{cases} \tag{3}$$

which admits of a rigorous solution and the corresponding phase analysis. It can be shown that the atomic back-scattering cross section is given by

$$\sigma_{bs} = \frac{4}{k^2} \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} \frac{(2l+1)(2l'+1)(-1)^{l+l'}}{(l'-l)(l+l'+1)} [\gamma(l,l')$$

$$- \gamma(l',l)] G_+(l) G_-(l');$$

$$\gamma(l,l') = \frac{\Gamma(\tfrac{1}{2}+l/2)\Gamma(1+l'/2)}{\Gamma(\tfrac{1}{2}+l'/2)\Gamma(1+l/2)} \sin\frac{\pi l'}{2}\cos\frac{\pi l}{2},$$

$$G_{\pm}^{-1}(l) = 1 \pm i\frac{A_l N_{l+\frac{1}{2}}(kr_0) - (k/k_0)N_{l+\frac{3}{2}}(kr_0)}{A_l J_{l+\frac{1}{2}}(kr_0) - (k/k_0)J_{l+\frac{3}{2}}(kr_0)},$$

$$A_l = 1 - \frac{1+l-\Sigma}{1+l}\frac{F(2+l-\Sigma, 2l+3, 2k_0 r_0)}{F(1+l-\Sigma, 2l+2, 2k_0 r_0)}.$$

In these expressions k = $(2mE_p)^{1/2}\hbar^{-1}$, Γ is the gamma function, F is the confluent hypergeometric function, and N and J are the Neumann and Bessel functions, respectively. The quantity Σ in the arguments of the confluent hypergeometric functions and in the factors in front of these functions is defined as follows:

$$\Sigma = \frac{me^2 Z}{\hbar^2}\left(\frac{2me^2 Z}{\hbar^2 r_0} - k^2\right)^{-1/2}, \tag{5}$$

where r_0 is the atomic boundary of the Mensing potential. The quantity k_0 is defined by

$$-k_0^2 = k^2 - 2me^2 Z / \hbar^2 r_0.$$

It is found that k_0 is a real quantity at the energies at which the maximum of the cross section σ_{obs} is observed.

Figure 1 shows the $\sigma_{bs} = \sigma_{bs}(E_p)$ curves calculated from Eq. (4) for chromium (Z = 24), copper (Z = 29), and molybdenum (Z = 42). The atomic radius was assumed to be equal to one half of the minimum distance between the atoms in the lattice of the corresponding crystal. In the case of chromium, $r_0 = 1.27 \times 10^{-8}$ cm, for copper $r_0 = 1.28 \times 10^{-8}$ cm, and for molybdenum $r_0 = 1.39 \times 10^{-8}$ cm. These three elements were selected for the following reasons. It is clear that the Mensing potential is a poor approximation to reality for r approaching r_0. On the other hand, for elements that are too light, E_p^* is such that even simple estimates show that the main contribution to large-angle scattering is due to the "outer" region of the atomic potential. We note, by the way, that for light elements, experiment shows a deviation from Eq. (1). There was, therefore, very little point in considering elements with low Z. In this plan, chromium is a suitable and, at the same time, relatively light, element. Copper was chosen because both it and nickel give an experimental $\sigma_{bs} = \sigma_{bs}(E_p)$ curve with the characteristic double-hump maximum. In copper this structure is better defined than in nickel. Finally, molybdenum is a suitable and, at the same time, relatively heavy element for which the double series in l and l' in Eq. (4) converges at a still acceptable rate. For heavier elements the series in Eq. (4) converges slowly. This complicates the study of Eq. (4) and reduces the accuracy of the numerical results necessary for the plotting of the curves.

In all three cases, the theoretical curve has a clearly defined maximum roughly in the region in which this is found experimentally. The agreement between the theoretical and experimental values of E_p^* is very good for Cr and less good for Mo. However, it is important that, in the latter case, the theory still indicates the presence of a maximum. The agreement between theory and experiment insofar as the position of the maximum is concerned can probably be improved by a better choice of r_0 but this, in our view, is not of particular interest owing to the fact that a model potential has been assumed [Eq. (3)]. It is striking that, in the case of copper, the theory gives the double-hump curve which is, in fact, observed experimentally. For the value of r_0 adopted for copper, the theoretical and experimental curves are found to be shifted relative to one another by about 25 eV. The experimental curves to the right of the maximum usually lie somewhat higher than the theoretical curves and this seems to us to be connected
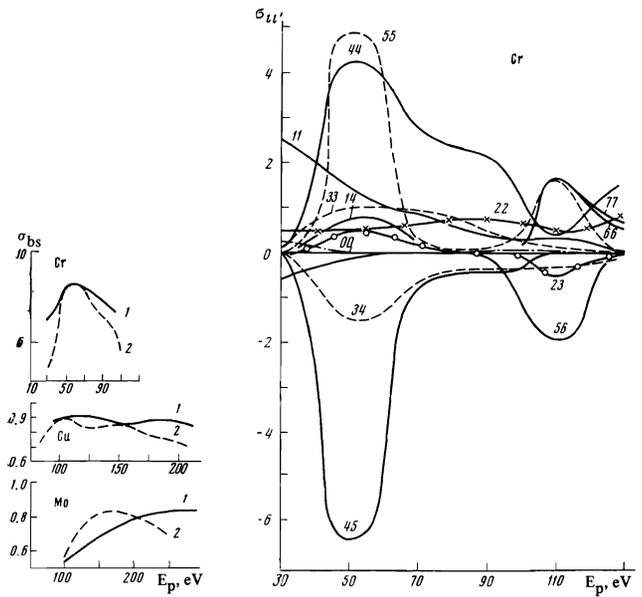
FIG. 1   FIG. 2

FIG. 1. Back-scattering cross section (relative units) of Cr, Cu, and Mo atoms: 1—experimental, 2—theory.

FIG. 2. Dependence of the partial cross section $\sigma_{ll'}$ (in relative units) on the energy of electrons undergoing elastic backward scattering by Cr. The two numbers marked against each curve represent the orbital angular momenta l and l' respectively.

with the fact that inelastic scattering has been neglected in the theory.

In order to be able to understand the nature of the nonmonotonic behavior orbtained in this way, it is useful to consider the dependence of the partial cross sections on the energy of the scattered electrons. Figure 2 shows that theoretical dependence of the partial cross section $\sigma_{ll'}$ as functions of E_p in the case of chromium (we are, of course, concerned with the partial cross section for back scattering; the subscripts bs are omitted both here and henceforth). Chromium is convenient because of the relatively rapid convergence of the series in Eq. (4), so that to obtain a quantitative picture it is sufficient to restrict one's attention to partial cross sections with l and l' not greater than 7. Partial cross sections with l and l' equal to 8 are found to be negligible. It is clear from Fig. 2 that σ_{00} is small throughout the energy range in which we are interested. The maximum begins to appear as a result of the increase in σ_{33}, σ_{14}, and σ_{23}. Appreciable contributions are provided by σ_{22} and even σ_{11}. The very large values of σ_{44} and σ_{55} on the left slope of the σ_{bs} maximum are largely compensated by the large interference terms σ_{34} and σ_{45}. Nevertheless, on the same slope of σ_{bs} the cross sections σ_{44} and σ_{55} provide an appreciable although not decisive contribution to σ_{bs}. The top of the σ_{bs} maximum corresponds to an energy E_p for which σ_{55} and the interference cross section σ_{45} fall rapidly and cease to compensate the contribution of σ_{44}. Further decrease in σ_{44} leads to a reduction in the back-scattering cross section σ_{bs}.

A qualitatively similar situation occurs in the case of copper and molybdenum with the one difference that, for example, in the case of copper, there is a resonance

increase in the partial cross sections σ_{88} and σ_{99}, and in the interference cross section σ_{89}. We thus see that the nonmonotonic behavior of the $\sigma_{bs} = \sigma_{bs}(E_p)$ curve appears as a result of the rapid increase in the individual partial cross sections, which has a resonance character. To the left of the maximum on the σ_{bs} curve these partial cross sections are quite large for $l = l'$, but their contribution to σ_{bs} is suppressed as a result of the strong interference between the corresponding waves. For a subsequent small increase in energy (for large Z—this is, in fact, a relatively large increase) the interference ceases to suppress large-angle scattering and the $\sigma_{bs} = \sigma_{bs}(E_p)$ curve shows the maximum. This, in turn, means that when $E_p = E_p^*$ one can expect a rapid change in the angular dependence of the differential cross section.

Existing published data confirm this conclusion. Such a sudden change in the angular dependence of electron scattering in xenon, argon, krypton, and mercury was observed by Arnot[5] (some other interesting data are also given in[6,7]). The nature of the resonance increase in certain partial back-scattering cross sections for $E_p \to E_p^*$ requires further investigation. It appears to us, however, that this increase is connected with the presence of virtual levels with nonzero orbital angular momentum. The overall character of the above effect suggests that it may be useful in applications, since the formula given by Eq. (1) can, in principle, be used to identify elements in, for example, the surface layers of a target.

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