INELASTIC SCATTERING OF ELECTRONS BY NOBLE GAS ATOMS

M. Ya. AMUS'YA, N. A. CHEREPKOV, and S. I. SHEFTEL'

Physico-technical Institute, U.S.S.R. Academy of Sciences

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The differential cross section for inelastic scattering of electrons (with energies of a few keV) on neon, argon, krypton, and xenon atoms is investigated for the case of small energy losses. The calculation is carried out in Born approximation, and wave functions generated from the Herman-Skillman potential are used for the ejected electron. It is shown that the dipole transition of the atomic electron gives the main contribution; however, the form of the cross section curve depends significantly on the contribution from transitions of other multipole order. The results obtained are compared with experiment. A number of peaks in the differential cross section for scattering on the outer shells of argon, krypton, and xenon are explained. The reasons for the quantitative discrepancy between the calculated and experimental cross sections are analyzed.

1. In the calculation of atomic processes one usually employs the Hartree-Fock approximation, which only takes account of that part of the electron-electron interaction which reduces to a smooth self-consistent field. A further improvement and development of the theory of the atom requires the inclusion of the residual or direct interaction which is neglected in the Hartree-Fock model. Estimates show[1] that the residual interaction plays an important role in a considerable number of processes. A very convenient experiment for a test of the importance of this interaction is one (cf.[2]) in which the differential cross section $\sigma'' \equiv \partial^2\sigma/\partial\epsilon\partial o$ of inelastic scattering of electrons on noble gas atoms is measured as a function of the scattering angle θ of the incident electron and of the energy ϵ transferred to the atom. Such an experiment allows for an unambiguous interpretation, since the increase of the cross section σ'' immediately after the ionization threshold I_i can only result from the removal of an electron from the i th shell. In the region of small energy transfers $\epsilon \ll E$ (E is the energy of the incident electron) one can neglect the interaction of the knocked-out and scattered electrons. If the effect of the residual interaction is small, the process of the ionization of the atom should be well described by the single-particle model, in which the change of state of the remaining electrons is neglected.

The aim of the present paper is to explain the data of the Afrosimov et al.[3] within the framework of a single-particle model. The significant deviation of the results of the calculation from the experimental data in a number of places implies that at the corresponding energies and angles the role of the residual interaction and the many-body effects connected with it are important.

The calculation of the inelastic scattering cross section σ'' was carried out in a region of energies and angles for which experimental data[3] were available (cf. Table I).

Table I

	E, keV	ε, eV	θ, deg		E, keV	ε, eV	θ, deg
Ne	4	20÷200	1; 3; 6	Kr	3	13÷240	1.5; 3; 5
Ar	4	15÷400	1.5; 4; 6	Xe	3	12÷150	1; 4; 6

2. The differential cross section for the scattering of an electron on an atom in first Born approximation is given by the expression[4] [1)]

$$\sigma_{nlm}^{''\varepsilon' l' m} = \frac{8p'}{pq^4}\left|\int e^{-i\mathbf{qr}}\,\psi^*_{\varepsilon' l' m}(r)\,\psi_{nlm}(r)\,d\mathbf{r}\right|^2, \tag{1}$$

where p and p′ are the momenta of the incident electron before and after the scattering, ϵ' is the energy of the knocked-out electron, $\mathbf{q} = \mathbf{p}' - \mathbf{p}$ is the momentum transferred from the incident electron to the atom,

$$\varepsilon = \frac{p^2}{2} - \frac{p'^2}{2} = \varepsilon' + I_{nl}, \tag{2}$$

and $\psi_{nml} = R_{nl}Y_{lm}$ and $\psi_{\epsilon' l' m} = R_{\epsilon' l'}Y_{l' m}$ are the wave functions of the atomic electron in the bound and free states calculated with the help of the Herman-Skillman potential.[5] The radial function of the continuous spectrum is normalized to a δ function in the energy:

$$P_{\varepsilon' l'} \equiv rR_{\varepsilon' l'} \to 2^{1/4}\pi^{-1/2}\varepsilon^{-1/4}\sin\left[\sqrt{2\varepsilon'}\,r + \frac{1}{\sqrt{2\varepsilon'}}\ln(2\sqrt{2\varepsilon'}r) - \frac{\pi l'}{2} + \delta_{l'}\right]. \tag{3}$$

The calculation was carried out for separate shells,

$$\sigma_{nl}^{''\varepsilon'} = \sum_{l'}\sum_{m}\sigma_{nlm}^{''\varepsilon' l' m},$$

as well as for the total value of the differential cross section,

$$\sigma''_{\varepsilon'} = \sum_{nl}\sigma_{nl}^{''\varepsilon'}.$$

The summation over l' was cut off at $l' = l + 3$.[2)]

3. The analysis of the results of the calculation shows that with increasing values of qr_{eff} (r_{eff} is the effective radius of the shell), the cross section σ'' for dipole transitions ($l \to l \pm 1$) decreases rapidly, that for monopole ($l \to l$) and for quadrupole transitions ($l \to l \pm 2$) decreases slowly, whereas the cross section for octupole transitions ($l \to l + 3$) increases in the region of values of qr_{eff} under consideration. With increas-

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1) We use atomic units.

2) The calculations were carried out on the BÉSM-2 computer. The total error of the calculation does not exceed 2%.

ing angle θ the momentum q increases, while r_{eff} increases with shell number n; therefore, although the dipole transition gives the main contribution to the total cross section, the form of the curve for σ'', especially for large angles θ and the outer shells, depends significantly on the transitions of the other multipole orders.

The dependence of σ'' on ϵ' is determined by the behavior of the wave function of the knocked-out electron. For small ϵ' ($\epsilon' < 10$ eV) and $l' > 1$ the first maximum of the wave function lies, owing to the centrifugal barrier, outside the boundary of the atom, and moves even further away from the nucleus with increasing l'. For the above-mentioned energies the effective contribution to the transition matrix elements comes from the peripheral regions of the shells (r_{eff} large), and monopole and quadrupole transitions are important for the calculation of σ''. For larger energies, the first maximum of $P_{\epsilon' l'}$ moves inside the atom, r_{eff} decreases, and the dipole transitions are the most important.

In the cross sections for transitions with several multipole orders there are also additional maxima and minima. These are connected with changes in sign of the matrix elements caused either by oscillations of the radial part of the wave function of the atomic electron $P_{nl}(n - l - 1 \geq 1)$,[7] or by the oscillations of $e^{-i\mathbf{q}\cdot\mathbf{r}}$ for $qr_{eff} > 1$.

4. The cross section for scattering on the outer shells of argon, krypton, and xenon at small scattering angles contains only one maximum corresponding to the dipole transition $np^6 \rightarrow \epsilon'd$. For larger angles ($\theta > 1°$; 1.5°) other maxima appear in the calculated curve. One of these is connected with the knock-out of s electrons of the outer shell (quadrupole transition $ns^2 \rightarrow \epsilon'd$) and occurs directly after the threshold for ionization, while the other is due to the knockout of p electrons (quadrupole transition $np^6 \rightarrow \epsilon'f$). For argon and krypton the maximum of the transition $np^6 \rightarrow \epsilon'f$ (Figs. 1 to 3, double arrow) lies at higher energies than the maximum for the knock-out of s electrons (Figs. 1 to 3, open triangle); for xenon the situation is reversed. Moreover, in the case of xenon peaks appear for $\theta = 6°$ and $\epsilon \approx 37$ and 50 eV which are connected with octupole transitions $5s^2 \rightarrow \epsilon'f$ (Fig. 3, full triangle) and $5p^6 \rightarrow \epsilon'g$ (Fig. 3, triple arrow).

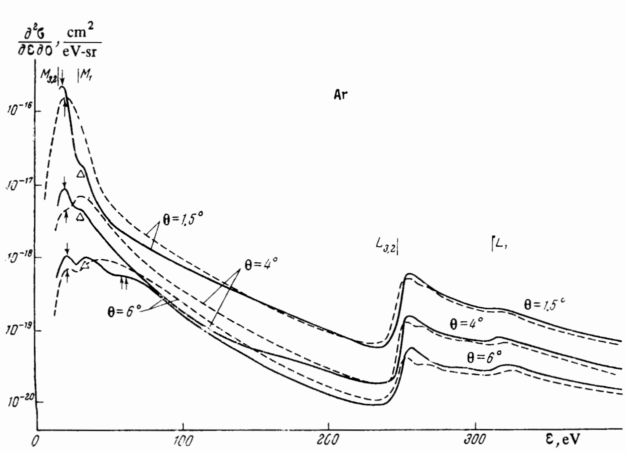

FIG. 1. Cross section for inelastic scattering of electrons on argon. Solid curve: calculation, dashed curve: experiment. Single arrows mark the maxima corresponding to the transition $3p^6 \rightarrow \epsilon'd$, double arrows correspond to the transition $3p^6 \rightarrow \epsilon'f$, and Δ to $3s^2 \rightarrow \epsilon'd$.

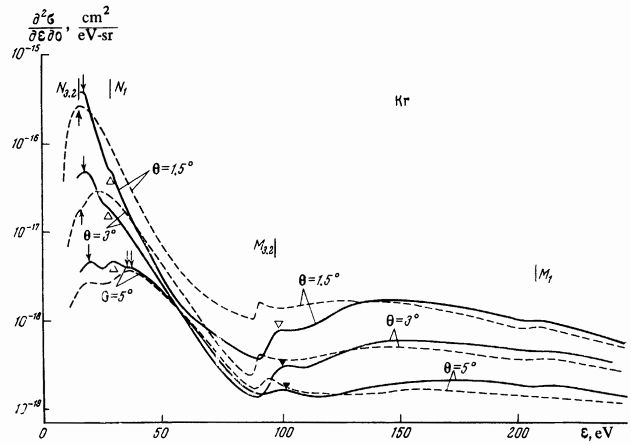

FIG. 2[3] Cross section for inelastic scattering of electrons on krypton. Single arrows mark the maxima corresponding to the transition $4p^6 \rightarrow \epsilon'd$, double arrows correspond to the transition $4p^6 \rightarrow \epsilon'f$, Δ to $4s^2 \rightarrow \epsilon'd$, ∇ to $3d^{10} \rightarrow \epsilon'p$, and $\blacktriangledown$ to $3d^{10} \rightarrow \epsilon'd$.

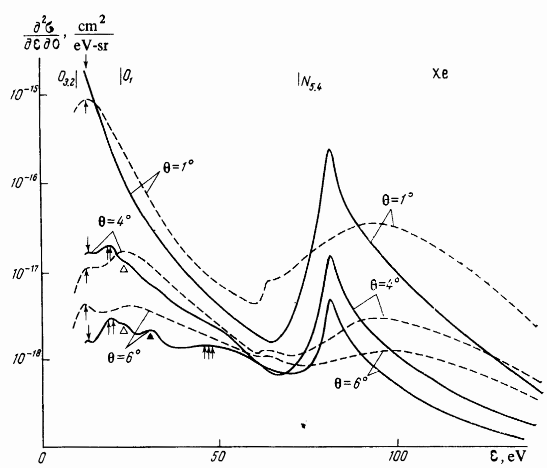

FIG. 3. Cross section for inelastic scattering of electrons on xenon. Single arrows mark the maxima corresponding to the transition $5p^6 \rightarrow \epsilon'd$, double arrows correspond to the transition $5p^6 \rightarrow \epsilon'f$, triple arrows to $5p^6 \rightarrow \epsilon'g$, Δ to $5s^2 \rightarrow \epsilon'd$, and $\blacktriangle$ to $5s^2 \rightarrow \epsilon'f$.

In the experiment, only one maximum in addition to the dipole maximum is visible, since the transitions $np^6 \rightarrow \epsilon'f$ and $ns^2 \rightarrow \epsilon'd$ are practically indistinguishable. With increasing angle θ the relative contribution of the additional maxima increases, in the calculation as well as in experiment, as compared to that of the dipole transition, and they move toward the region of large energy transfers ϵ. Thus the calculated cross section σ'' for the outer shells is in qualitative agreement with experiment. However, the quantitative discrepancies are large. The calculated value of the cross section in the region of the first maximum due to the dipole transition $np^6 \rightarrow \epsilon'd$ is larger than the experimental value by a factor of 1.5 to 2.

The additional minima and maxima connected with the change of sign of the matrix elements (cf. the end of Sec. 3) do not show up in the total cross section. They are covered up by transitions of other multipole orders.

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[3]Note added in proof. For $M_{3,2}$ and M_1 in the figure read $M_{5,4}$ and $M_{3,2}$, correspondingly.

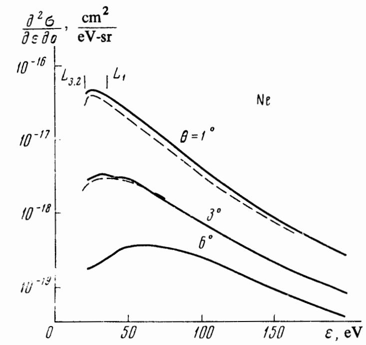

FIG. 4. Dependence of the calculated and experimental cross sections for the scattering of electrons σ'' by neon atoms on ϵ for various angles θ. Solid curve: calculation, dashed curve: experiment.

The effective radii $N_{5,4}$ of the subshells of argon and $M_{5,4}$ of the subshells of krypton are appreciably smaller than the radius of the outer shells; for the angles under consideration the dipole transition $nd^{10} \rightarrow \epsilon'f$ is therefore predominant. Only directly at the ionization threshold of krypton, the small peak at $\theta = 1.5°$ corresponds to the dipole transition $nd^{10} \rightarrow \epsilon'p$ (Fig. 2, upside-down open triangle), while that at $\theta \geq 3°$ corresponds to a monopole transition (Fig. 2, upside-down full triangle). The disagreement between calculation and experiment is not very big for krypton, but reaches a factor of 5 to 9 for xenon (Fig. 3).

The main contribution to the cross section for scattering on the L shells of argon and neon comes from the dipole transition $2p^6 \rightarrow \epsilon'd$ (Figs. 1 and 4). Therefore, both in the calculation and in experiment, a single maximum appears which is somewhat removed from the threshold. The contribution from the ionization of the L_1 subshell of argon shows up as a slight rise. The agreement with experiment is completely satisfactory. We note only that the calculated values in the region of the ionization threshold are 1.2 to 1.5 times larger than the experimental ones.

5. Thus the results of the calculation agree qualitatively with experiment. The quantitative discrepancies are connected with the use of the Born approximation and with the neglect of many-particle correlations. The criterion for the applicability of the Born approximation is the smallness of the parameter $\alpha = Z_{eff}/p \ll 1$. Estimates of the spatial regions giving the most important contributions to the integration permitted us to determine the effective charge Z_{eff} seen by the incident electron, and to obtain a table of values of the parameter α. It is seen from Table II that the Born approximation works well for $\theta \leq 4°$ for electron scattering on neon and argon and for $\theta \leq 3°$ for scattering on krypton and xenon. For larger scattering angles one should expect

Table II. Dependence of the parameter α on the scattering angle of the incident electron θ

	θ, deg					
	1	1,5	3	4	5	6
Ne	0.13		0.23			0.30
Ar		0.21		0.34		0.40
Kr		0.24	0.35		0.45	
Xe	0.21			0.47		0.59

significant discrepancies owing to the inaccuracy of this approximation.

Hence, for small angles θ, the difference between the calculated and experimental values can only be explained by many-body effects. The largest discrepancies were found for scattering on the $N_{5,4}$ subshell of xenon and on the outer shells of argon, krypton, and xenon, i.e., where many-body effects are most significant.

More detailed information on the many-electron correlations can be obtained by separating the contributions from the various subshells. This requires an experiment in which the scattered (fast) and knocked-out (slow) electrons are measured simultaneously. The determination of the energies of these electrons allows one to confirm that the knock-out of an atomic electron is not accompanied by an excitation of the atom.

In conclusion the authors regard it their duty to thank L. A. Sliv and G. F. Drukarev for useful comments on this work, and I. M. Band and M. B. Trzhaskovskiĭ for help with the calculations.

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