Elastic scattering of electrons by gadolinium and barium atoms

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Abstract

Total and differential cross-sections for elastic scattering of electrons from gadolinium and barium atoms in a wide energy range were calculated. In the low- and intermediate-energy regions, the phase theory of elastic scattering was used. At low incident energies (<10 eV), an additional polarization potential was introduced. At high incident energies, the Born approximation (keV range) and the Rutherford formula (MeV range) were applied. Our results are in rather good agreement with experimental data of Romanyuk et al. (Pis’ma Zh. Eksp. Teor. Fiz. 32 (1980) 472) for elastic scattering of very-low-energy electrons from barium atoms which confirm its reliability. This agreement is important because these experimental results are in serious disagreement with theoretical calculations of Szmytkowski and Sienkiewicz (Phys. Rev. A 50 (1994) 4007). © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

The problems associated with the penetration of low- and intermediate-energy electrons into matter have attracted much attention in recent years. Simulation of electron passage through matter requires the following interaction processes to be taken into consideration: elastic scattering, excitation and ionization of atoms and Auger-processes. The cross-sections describing the above processes is an essential set of data required in a wide range of applications such as the modeling of radiation effects for both materials and medical research. These cross-sections are needed to follow the history of an incident projectile and secondary radiation for all ranges of energy transferred in individual collisions. Proper understanding of the role of secondary electrons is important because a large number of slow electrons are generated in the process of an electron passing through matter. These secondary electrons interact with other atoms until the electrons are thermalized.

This paper describes the methods for calculating the differential elastic scattering cross-sections of low-, intermediate- and high-energy electrons from gadolinium and barium atoms. Such cross-sections are needed to simulate the angular
scattering of electrons in elastic events, using Monte Carlo methods. As the valence atomic shells of gadolinium and barium atoms are similar, our computations of electron elastic scattering from barium atoms are compared with experimental and theoretical results already available.

2. Computation methods

The accuracy of standard theoretical methods of calculating the elastic scattering cross-sections depends on both the wave function quality and the collision theory used. Applicability of a method depends on the incident electron energy and the target-atom complexity. Our model for computation of the elastic cross-sections is based on the self-consistent Hartree–Fock–Slater (HFS) approach. The statistical approximation of the exchange interaction is used in the HFS method. The Schrödinger equation for radial continuum wave function can be written as follows [1]:

$$\left( \frac{d^2}{dr^2} + \frac{2Z(r)}{r} + V_{ex}(r) - \frac{l(l+1)}{r^2} + \varepsilon_{nl} \right) R_{nl}(r) = 0,$$

where

$$\frac{Z(r)}{r} = \int_0^\infty \frac{1}{r_1} \left( Z_0 - \int_0^{r_1} \rho(x) dx \right) dr_1,$$

$$V_{ex}(r) = -\frac{3}{2} \left( \frac{3}{\pi} \rho(r) \right)^{1/3}, \quad \rho(r) \sum_{nl} R_{nl}^2(r),$$

Here \( r \) is the distance from the nucleus, \( r_1 \) the integration variable, \( \varepsilon_{nl} \) the binding energy of electron in the atom, \( R_{nl}(r) \) the radial wave function of the atomic electron, \( l \) the orbital number, \( Z_0 \) the nucleus charge, \( Z(r) \) the effective charge of the ion field, \( V_{ex}(r) \) the potential of exchange interaction and \( \rho(r) \) is the charge density inside the atom. The integral in brackets in the expression for \( Z(r)/r \) takes into account the inner screening of the nucleus by outer electrons. The wave function is calculated for each pair of the \( n, l \) quantum numbers at the solution of Eq. (1). The eigenvalue \( \varepsilon_{nl} \) is simultaneously determined. Eq. (1) involves the electrostatic and exchange atomic potentials, which are also subject to determination. The potentials are expressed through the wave functions of other atomic electrons. Therefore Eq. (1) is an implicit type and is solved by means of the iterative methods [2]. This equation with additional conditions (Eq. (2)) presents the HFS system.

For high-\( Z \) elements, it is necessary to take into account the relativistic effects, especially for the inner atomic shells. The solution of the Dirac–Hartree–Fock equation [3] with the bicomponent wave function is required. Results of such calculations in the relativistic polarized-orbital approximation were presented by Szymtowski and Sienkiewicz [4]. That approximation is more accurate than the HFS. However, it is possible to take into account the relativistic effects within the perturbation theory using the non-relativistic HFS wave functions. This technique was realized in our model for high-\( Z \) atoms. All the corrections, spin-orbital splitting, contact correction, mass-velocity dependence, were taken into account.

The HFS equations are solved with the spatial finite differentiating methods. For this purpose, the initial differential equation (1) is approximated by means of the finite difference Numerov scheme [2]. It gives the possibility to keep the six-order accuracy along the radial steps on a uniform grid. The problem is solved by means of the iterative methods. As 0th approximation for the potential, the solution of Thomas–Fermi equation is used. The self-consistent HFS wave functions and HFS potential are obtained as a result of the system’s solution (1).

The potential of neutral atom at infinity is zero as the nucleus is fully screened by atomic electrons. The atomic electrons move much faster than the incident one. Upon the low-energy incident electron impact, the electronic atom shell is deformed and there is a polarization interaction. In our consideration, the interaction of low-energy incident electron on the atom is taken into account in the approximation of polarization potential. This potential may be presented in the form \( V_p = \beta/(r_0^2 + r^2) \), where \( r_0 \) is the average atom radius, and \( \beta \) is the atomic polarization. Thus, the motion of incident electron is considered in the total potential \( V = V_{HFS} + V_p \) representing the sum
of the HFS and the polarization. The polarization can be rather precisely calculated by means of the formula $\beta = \sum_i f_{0i} / (E_0 - E_i)^2$ [5], where $E_0$ is the energy of the ground atomic state, $E_i$ are the energies of the exited levels, $f_{0i}$ are the oscillator strengths of corresponding transitions. In our computations, these values are determined from the HFS wave functions.

Solving Eq. (1) (without self-consistency) using the potential $V$ gives the total wave functions. To calculate the scattering amplitude, the phase shifts are required. In our model, the evaluation of phase shifts is carried out in the following way. At some rather large distance $r = R$ the phase of total wave function is compared with the phase of wave function calculated under the assumption that the incident electron is moved in the Coulomb field of the nucleus, i.e. in the absence of atomic potential. The difference in these phases will determine the phase shift value. The scattering amplitude is given by the expression [6]

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{n} (2l + 1) \exp(2i\delta_l - 1) P_l(\cos \theta),$$

where $k$ is the wave number, $n$ the number of partial phase shifts which should be taken into account, $\delta_l$ the phase shift corresponding to the orbital quantum number $l$, $P_l(\cos \theta)$ are the Legendre polynomials and $\theta$ is the scattering angle. The number of partial phase shifts can reach about 100 and more. In our model, this number is evaluated in the following manner. Two consequent magnitudes of $f^n(\theta)$ and $f^{n+1}(\theta)$ are calculated by the summation of $n$ and $n + 1$ partial phase shifts, respectively. If the difference between these two scattering amplitudes is less than 0.1%, then the magnitude $f^n(\theta)$ is taken as the scattering amplitude. In a proper way, the number of phase shifts taken into account is increased by one and the above procedure is repeated. For the low-energy electrons the number $n$ is small ($\sim 0.1$). At higher incident electron energy, this number is strongly increased.

The direct computation of scattering amplitudes becomes inconvenient with increasing electron energy. For high-energy electrons, the Born approximation can be used in which the electron interaction with the atomic field is considered to be small and can be taken into account within the perturbation theory. The expression for elastic scattering amplitude in the Born approximation can be written as follows [6]:

$$f(\theta) = \frac{2m}{\hbar^2} \int_0^\infty \frac{\sin Kr}{Kr} V(r)r^2 \, dr,$$

where $K$ is the wave number of the incident electron, $V(r)$ the atomic potential. In our calculations, the HFS potential is used. At high electron energy the role of polarization and exchange effects becomes negligible and they are not taken into consideration.

For very high energies (MeV range), it is possible to take into account the electron interaction with the nucleus only, using the classical Rutherford formula. This formula is applicable at incident electron energies higher than the inner $K$-electron energy.

Eq. (3) can also be used at very high energies (MeV range). However, there is the problem of the accuracy in numerical integration over the fast oscillating function $\sin Kr$. For this reason, at very high electron energies, the Rutherford formula is preferred.

3. Results

The model presented above was used to calculate the total and differential cross-sections for the elastic scattering of low- and intermediate-energy electrons with gadolinium and barium atoms. To test the reliability of our model we have compared the results obtained with the experimental and theoretical data available. Results of such comparison for elastic scattering of electrons from barium atoms are presented in Fig. 1. Our results are in rather good agreement with the experimental data obtained by Romanyuk et al. [7,8]. However, an essential qualitative disagreement with the theoretical results of Szymkowsi and Sienkiewicz [4] is observed, even though the last ones were obtained using the relativistic polarized-orbital approximation [3]. This disagreement is somewhat surprising because the method they
used is more accurate than our approach. In Szmytkowski and Sienkiewicz's work [4], it was assumed that the maximum at energy 2 eV is due to the appearance of near-threshold resonance in $d$ partial waves. One can see from our results that there is the peak in this energy region but its magnitude is smaller and is in the limits of the computation accuracy. In the very-low-energy region, the theoretical results of the work in [4] are in serious discrepancy with the experimental data. It should be pointed out here that the experimental results might be in error. However, from simple physical consideration it is clear that with the electron energy decreasing, the time it stays in the atomic field is larger and therefore the cross-section should be greater. Our computation results confirm the behavior of experimental cross-sections in the very-low-energy range. It is rather difficult to point out the origin of calculation errors in theoretical results of Szmytkowski and Sienkiewicz [4] (the maximum at 2 eV and the cross-section falling off in the very-low-energy region). It might be associated with the simplifications used in the relativistic polarized-orbital model and incorrect determination of the partial phase shifts and its number.

Total elastic scattering cross-sections for gadolinium and oxygen atoms computed using our model, as a function of energy, are shown in Fig. 2. An inflection in these curves in the keV range is due to the transition from the phase theory to the Born approximation. It may be seen that the elastic cross-section is a decreasing function with increasing electron energy.

Our computations of differential cross-sections for barium are shown in Fig. 3 along with experimental (Wang et al. [9] and Jensen et al. [10]) data, and theoretical results of Szmytkowski and Sienkiewicz [4]. Calculations were made for barium atoms at incident electron energies of 20, 60 and 100 eV, respectively. Satisfactory agreement between the calculated and reference data is seen. The elastic scattering cross-sections are a non-monotonic function of the angle. They have usually the peak at zero angle and several local minima and maxima. The accuracy of the cross-sections (especially at a minimum) strongly depends on the computation error of the partial phases and the atomic potential including the polarization. The difference in cross-section minima depends on the approach used, it might be a few orders of magnitude.

Fig. 4 illustrates the dependence of differential elastic scattering cross-sections calculated using our model on the scattering angle for gadolinium atom. Fig. 4(a) shows our calculated values of

![Fig. 1. Comparison of total cross-sections for electron scattering from barium atoms. Present work (---), Szmytkowski et al. [4] (--), and (-----), Romanyuk et al. [7] experiment (▲).](image1)

![Fig. 2. Total elastic scattering cross-sections of electrons from gadolinium and oxygen atoms.](image2)
di/C128erential cross-sections for the very-low-energy range of incident electrons. The scattering probability at angles where the cross-sections have their peaks is comparable with that at zero angle. With the energy increase the scattering at zero angle is more probable (see Fig. 4(b)). In Fig. 4(c), the result obtained using the Born approximation is also presented. At high incident electron energy the differential cross-sections obtained using the phase theory are strongly oscillating functions. The Born approximation gives those as a monotonically decreasing function of the scattering.
angle. Therefore, it is possible to choose some energy values for which the accuracy of the Born approximation and the phase theory are comparable and to use the Born approximation for electrons of higher energy. The value of the chosen energy depends essentially on the atomic number of the target.

4. Conclusions

We have calculated electron elastic scattering from gadolinium and barium atoms in a wide energy range. For low- and intermediate-energy ranges, the phase theory of elastic scattering is used. At low incident energies (<10 eV), the additional polarization potential is introduced. At high incident energies, the Born approximation (keV range) and the Rutherford formula (MeV range) are applicable. The most important result is confirmation of the experimental total cross-sections by Romanyuk et al. [7,8] in the very-low-energy region. The methods presented for computation of the elastic scattering cross-sections have some systematic error in each energy range. This error depends also on the complexity of the target atom. In our treatment, the calculations were performed with the HFS approximation taking into account the polarization effects. The exchange and spin interactions between incident and atomic electrons were not taken into account. Therefore, according to our assessments, the systematic error in the differential cross-sections might be a factor of 2–3. Despite this error, the quantitative agreement with experimental data is rather satisfactory. For scattering of intermediate-energy electrons (several hundreds of eV), the role of the polarization, exchange and spin effects is significantly decreased. However, the accumulation of computation errors is increased. The scattering cross-section is the sum of alternating series. The terms of this series contain the partial scattering phases, which are calculated with some error. For this reason at high energies the differential cross-section will have a set of non-physical oscillations. For scattering of high-energy electrons (tens or hundreds of keV) the Born approximation is sufficiently accurate and can be used. In the MeV-energy range the elastic scattering cross-sections are determined with a good accuracy using Rutherford formula. To improve the computation accuracy of elastic cross-sections, serious modification of our model is required. This presents large difficulties, especially in the low-energy region.

References