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Elastic electron scattering by silver atom

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ABSTRACT

The experimental and theoretical studies of elastic electron scattering by silver atom have been carried out. The experimental investigation was based on crossed beam technique with effusive atomic beam being perpendicularly crossed by electron beam. The measurements were performed at electron-impact energies (E_0) of 10, 20, 40, 60, 80 and 100 eV and for a range of scattering angles (θ) from 10° up to 150°. The absolute differential cross sections (DCSs) have been obtained from the elastic-to-inelastic (the unresolved silver resonant lines $4d^{10}5p\ ^2P_{1/2,\ 3/2}$) intensity ratio at $\theta = 10°$ at each E_0. Calculations have been performed using the parameter-free complex optical potential (OP) with the inclusion of spin-orbit interaction for the same E_0. Comparison between present experiment and theory has been made.

1. Introduction

The low and intermediate energy electron scattering from metal atoms has been studied extensively recently. Detailed knowledge on the differential cross sections (DCSs) is essential for explaining and understanding the basic interaction in the electron atom scattering processes, particularly, at certain electron energy and scattering angle. In our previous paper [1], we gave a short review of our experimental work on electron interactions with metal atoms (Ca, Yb and Pb) in the intermediate electron energy range from 10 to 60 eV.

In our previous paper [2], we reported on the results of both experimental and theoretical investigations of elastic electron-indium scattering. We have reported differential, integral (Q_I), momentum transfer (Q_M) and viscosity (Q_V) cross sections and have determined the positions of critical minima. Comparisons were made for the energies from 10 to 100 eV and as shown, theoretical calculations carried out using a model phenomenological complex potential with the inclusion of spin-orbit interaction can be applied to elastic electron scattering by In atom, i.e. to predict the behaviour of both the angular and the energy dependences of DCSs within a wide energy range as well as the positions of critical minima.

We consider here the data on the elastic electron scattering by silver atoms. Silver has the highest thermal and electrical conductivity of any metal and is of widespread importance in many applications. It has the electron configuration of krypton plus ten electrons in 4*d* and one in 5*s* orbitals – ([Kr] $4d^{10}5s$) – with the $^2S_{1/2}$ ground-state level. Unfortunately, very limited information is available on the elastic electron-silver cross sections especially in the energy range considered here. Fink and Ingram [3] investigated the influence of the spin in the elastic low-energy scattering from gaseous atoms. They solved the Dirac equation using relativistic Hartree–Fock–Slater scattering potential but their calculations excluded the exchange of the incident electron with the atomic electrons and charge-cloud polarization. Werner [4] utilized the CPC code of Yates [5] and also solved the Dirac equation using empirical potential from the paper of Bonham and Strand [6]. In this approach, the polarization and the exchange potentials also were not taken into account. Jablonski et al. [7] analyzed elastic DCSs for six elements including silver at the energies from 100 to 10,000 eV. DCSs were calculated from a relativistic Dirac partial wave analysis using the Thomas–Fermi–Dirac (TFD) and Dirac–Hartree–Fock (DHF) potentials.

To the best of our knowledge, there are no experimental results on elastic electron-silver scattering. The reason for the lack of experimental investigations on this topic could be the high working temperature (approximately 1300 K), which is necessary to vaporize the silver sample and to produce well collimated effusive atomic beam.

In the present paper, the results of both experimental and theoretical studies of elastic electron scattering by Ag atoms are presented. The angular distribution of elastically scattered electrons was measured in the intermediate energy range up to 100 eV at scattering angles from 10° to 150°. Corresponding theoretical

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results were obtained using the parameter-free complex optical potential (OP) with the inclusion of spin-orbit interaction well-tested by us earlier [2,8–12]. The real part of this potential consists of static, local exchange, polarization and spin-orbit potentials while the imaginary part of OP takes into account the absorption effects. The atomic characteristics are calculated in the local approach of the density functional theory (DFT). We have obtained the results using two different approaches, i.e. calculations with and without absorption.

2. Experimental techniques and procedures

The experimental set-up used by us to measure the angular distributions of electrons elastically scattered from silver atoms is identical to that described elsewhere [1,2,13]. Therefore, we shall not describe them in detail and only a brief summary will be given.

The measurements were carried out using the perpendicularly crossed electron and atom beams. Electrons from hairpin thermoelectron source pass the systems of cylindrical electrostatic lenses made of gold plated oxygen-free high conductivity copper and hemispherical electrostatic energy selector made of molybdenum (electron monochromator). A monoenergetic beam of electrons (full width at half maximum, FWHM, being near 120 meV) from the monochromator was perpendicularly crossed by the silver atomic beam. The primary electron current was of the order of 10–50 nA, depending on the impact energy. Elastically scattered electrons were analyzed and detected as a function of scattering angle at fixed electron-impact energy by a hemispherical electron energy analyzer and channeltron as a single-electron detector. The analyzer is of the same type as the monochromator and it can rotate around the atomic beam axis from -30° to 150° with respect to the incident electron beam.

The experiment was carried out in a vacuum chamber, which was shielded by a double μ-metal shield, so (providing) magnetic field was below 2×10^{-7} T. Two oil diffusion pumps with liquid nitrogen traps provided differential pumping of the vacuum chamber and electron optical system. The background pressure was about 10^{-5} Pa.

Well collimated effusive atomic beam was produced by heating silver sample in an atomic oven. The oven was heated to about 1300 K by two separate resistive bifilar heaters, one for the top of the stainless steel crucible and nozzle and one for the body of the crucible. They provided a variable temperature difference between the top and bottom and enabled the top of the system to be maintained at approximately 100 K higher temperature than the bottom in order to prevent clogging and minimize dimer production. The working temperature was controlled by two thermocouples (top and bottom). The new design (reduced thicknesses of oven walls, additional shielding and water-cooling) allows one to reach higher temperatures, reduces heat transfer and radiation losses from the oven and avoids overheating of surrounding components. A liquid-nitrogen cold trap was placed above the oven and interaction region in order to prevent chamber contamination.

Typical overall energy resolution FWHM was 120 meV, while the angular resolution of the spectrometer was estimated to be 1.5°. Before each measurement, the angular distribution of scattered electrons was measured from -10° to $+10^\circ$ and the real zero scattering angle was determined according to the symmetry of inelastic scattering at negative and positive scattering angles around the instrumental zero.

The angular dependence of elastically scattered electron intensities at E_0 = 10, 20, 40, 60, 80 and 100 eV were corrected to effective path length correction factors [14] determined for the current experimental conditions to get relative DCSs. The absolute DCS values were obtained from the measurements of intensity ratios of elastic and $4d^{10}5p\ ^2P_{1/2,\,3/2}$ signals at scattering angle of 10° at each impact energy.

3. Theory

In the present study, the calculations of the scattering cross sections were carried out within the framework of the optical potential method, both with and without taking into account of the absorption effects. We used the complex potential (SEPASo approach [8]) as the OP with absorption

$$V^{\pm}_{opt}(r,E) = V^{\pm}_{R}(r,E) + iV_a(r,E) \tag{1}$$

Calculation without absorption, when only a real part of potential (1) is used as the OP

$$V^{\pm}_{opt}(r,E) \equiv V^{\pm}_{R}(r,E) = V_s(r) + V_e(r,E) + V_p(r) + V^{\pm}_{so}(r) \tag{2}$$

similarly [8] will be called the SEPSo approach.

The terms of V_s, V_e, V_p, V_{so} and V_a in Eqs. (1) and (2) are the static, exchange, polarization, spin–orbit and absorption potentials. Notation "±" corresponds to the values of the total electron angular momentum $j = \ell \pm 1/2$, ℓ being the electron orbital momentum. Here the atomic units (a.u.) are used: $\hbar = e = m_e = 1$, $E = k^2/2$ is the energy and k is the momentum of the incident electron.

The calculations in the SEPSo and SEPASo approaches allow one to obtain the real and complex partial phase shifts $\delta^{\pm}_{\ell}(E)$. To calculate the absolute $\delta^{\pm}_{\ell}(E)$ values, similarly to [8–11], we used the well-known variable phase method. Having the phase shifts, one can calculate the scattering amplitudes and differential elastic cross sections. For this purpose we used the expressions (2)–(4) from [10]. It is natural, that in case of SEPASo-calculation, these expressions include complex phase shifts $\delta^{\pm}_{\ell}(E)$.

The total electron density $\rho(r)$ of silver atom was calculated within the framework of the local scalar-relativistic DFT approximation with the exclusion of electron self-action energy (see, e.g. [9] and references therein). As a result of the least-square approximation of the initial tabulated data for $\rho(r)$, the best approximation was obtained with the use of the analytical expression (A1) (see Appendix A). The static potential V_s is calculated by the analytical expression (A2) and, as well as in [15], is related to expression for $\rho(r)$.

The local exchange potential in the free electron gas approximation was taken as the potential $V_e(r,E)$ (see [9] and references therein). The ionization potential for silver atom necessary for V_e calculations is $I = 7.5763$ eV [16].

Similarly to [10], we used here as the polarisation potential $V_p(r)$ consisting of two parts. At small $r \leqslant r_c$ distances this potential is equal to the correlation-polarization potential $V^{SR}_p(r)$ in a form of Eq. (9) from [17]. At large $r > r_c$ distances, the potential has a well-known asymptotic form $V^{LR}_p(r) = -\alpha_d/2r^4$. The static dipole polarizability of silver atom $\alpha_d = 52.59a_0^3$ was found within the framework of the relativistic time-dependent DFT approach (see [9]). Note that the experimental value $\alpha_d = 42.51a_0^3$ was obtained with the 50% accuracy [18]. The two parts of the polarisation potential, $V^{SR}_p(r)$ and $V^{LR}_p(r)$, have their first intersection at $r_c = 6.408a_0$ point. Spin–orbit interaction of the incident electron with the target atom was taken into account using the potential $V^{\pm}_{so}(r) \sim dV_s/dr$ [19] (see also Eq. (5) in [8]).

As an imaginary part of OP (1) we used the modified f2 version of the absorption potential $V_a(r,E)$ from [20], Eq. (1). The physical modification suggested here consists of two items. First, similarly to [21], we included the polarization potential V_p in the expression for the local speed of the scattering electron $v_{loc} = [2(E - V_{sep})]^{1/2}$, where $V_{sep} = V_s + V_e + V_p$. Second, we included the V_p in the expression for the f2 version parameters $\alpha(r,E)$ and $\beta(r,E)$: $\alpha = k_F^2 + \Delta - 2V_{sep}$ and $\beta = \alpha$ (compare with Eq. (21a) in [20]). The