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DIFFERENTIAL SCATTERING CROSS SECTIONS FOR ELECTRON SCATTERING BY YTTERBIUM ATOM

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Electron scattering by ytterbium atom is studied at energies 10, 20, 40, 60 and 80 eV, by applying a parameter-free complex optical potential. The real part of the complex optical potential includes the static potential $V_{\rm st}(r)$, the polarization potential $V_{\rm pol}(r)$ that consists of the short range correlation and long-range polarization effects and $V_{\rm ex}(r)$ term consisting of electron exchange interaction which is modelled by assuming the electron charge cloud as a free electron gas. The loss of flux into the inelastic channels is included via a phenomenological absorption potential. Our results are compared with the recent experimental measurements.

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1. *Introduction*

The Yb rare-earth atom has electronic ground state configuration [Xe] $4f^{14}6s^2$. The electronic structure of ytterbium makes this atom very interesting for investigation of a number of electron-atom collision processes. This heavy atom ($Z = 70$) provides an important test of relativistic effects in electron-atom scattering. On the other hand, studies of electron impact on Yb are important because of the potential suitability of its vapor as a laser medium. It is also a potential candidate for quantum computing because it has been shown that two non-local Yb atoms can be entangled over a distance of over one meter. This is a substantial advancement in the realization of a quantum computer which would yield super-fast computing which can crack complex problems in physical sciences and other fields.

Recently, differential cross sections (DCS) for electron scattering by ytterbium atoms in the range 2 − 2000 eV have been reported by Kelemen et al. [1] using an optical potential. The DCS for the electron–Yb system have also been measured recently by Predojević et al. [2] by using electron spectroscopy technique in the $10^\circ - 150^\circ$ angular interval at the collision energies of 10, 20, 40, 60 and 80 eV. The evaluation of DCS is a stringent test for any scattering theory employed. Therefore, it is of specific interest to calculate the angular dependence of differential cross sections within intermediate energy range with the aim to compare it with experimental data [2].

The relativistic DCS calculations at 10 eV are compared by Neerja et al. [3] with the Dirac-Fock calculations reported by Yuan [4]. The former calculations showed only one minimum in contrast to two minima predicted by the latter calculation, as observed in the experiment [2]. These calculations used different parameter-free polarization potentials [5, 6]. The exchange interaction between the incident electron and the target atom was taken into account by Neerja et al. [3] with the use of a local modified semi-classical exchange (MSCE) potential [7], while in Yuan work [4], it was taken into account accurately, i.e. in a non-local manner. It is observed that the differences in the manner of taking into account the exchange interaction have resulted in substantially different angular dependences of DCS at 10 eV in Refs. [3] and [4]. Thus, the recent experiment [2] could be used to verify certain theoretical models.

In the present work, a complex optical potential approach is employed in which the real part consists of the static, polarization and exchange potentials, whereas the imaginary part of the optical potential represents the absorption potential that takes into account the loss of flux due to all energetically possible inelastic channels. In order to evaluate the full optical potential, we need target charge density as the basic input. This is in conformity with the density-functional theory. The charge density and the static potential are calculated from the parameterized Hartree-Fock relativistic charge distribution of Salvat et al. [8]. The exchange effects are incorporated by treating the electron cloud as a free gas. The polarization is included via a parameter-free correlation-potential, and the absorption potential is derived according to the procedure devised by Staszewska et al. [9]. The only parameters required are the first ionization potential, which we take as equal to the mean excitation energy and the dipole polarizability of the atom under consideration for the construction of the full optical potential. After generating the full optical potential of the scattering system, we treat it exactly in a partial-wave analysis in terms of a set of first-order coupled differential equations for the real and imaginary parts of the complex phase shift functions under the variable phase approach (VPA) which was applied previously by one of us to calculate the total scattering cross sections for a large number of diatomic and polyatomic molecules [10].

2. *Theory*

All major interactions of electron atom scattering can be represented by a complex, energy dependent, optical potential $V_{\rm opt}(r,k)$ of the form

$$V_{\rm opt}(r,k) = V_{\rm st}(r) + V_{\rm ex}(r,k) + V_{\rm pol}(r,k) + {\rm i}V_{\rm abs}(r,k)\,. \qquad (1)$$

First, we determined the target charge density $\rho(r)$ of the Yb atom. All four potential terms, $V_{\rm st}(r)$, $V_{\rm ex}(r,k)$, $V_{\rm pol}(r,k)$ and $V_{\rm abs}(r,k)$, are functions of $\rho(r)$, thus accurate value of $\rho(r)$ is important in our caculations.

The static potential, $V_{\rm st}(r)$, is calculated from the unperturbed target wave function ψ_0 at the Hartree-Fock level [8]. The potential $V_{\rm pol}(r,k)$ represents approximately the short range correlation and long-range polarization effects [5, 6, 11], while the $V_{\rm ex}(r,k)$ term accounts for electron exchange interaction [12]. The $V_{\rm abs}(r,k)$ term in Eq. (1) is the absorbtion potential [9].

The parameters used in our calculations, taken from the NIST site, are shown in Table 1.

TABLE 1. Parameters used in the present calculations for electron scattering from ytterbium.

Average dipole polarizability (α_d)	141.85 a_0^3
Ionization potential energy	6.2542 eV

After generating the full optical potential of a given electron–atom system, we treat it exactly in a partial-wave analysis by solving the following set of first-order coupled differential equations for the real χ_l and imaginary $\Im m\,\chi_l$ parts of the complex phase shift function under the variable phase approach (VPA) [10],

$$\chi_l'(kr) = -\frac{2}{k}\big[2V_{\rm R}(r)(A^2-B^2) + 2V_{\rm abs}(r)\,AB\big], \tag{2}$$

$$\Im m\,\chi_l'(kr) = -\frac{2}{k}\big[2V_{\rm R}(r)AB - 2V_{\rm abs}(r)\,(A^2-B^2)\big], \tag{3}$$

where

$$A = \cosh \Im m\,\chi_l(kr)\Big[\cos\chi_l(kr)\ j_l(kr) - \sin\chi_l(kr)\ n_l(kr)\Big], \tag{4}$$

$$B = -\sinh \Im m\,\chi_l(kr)\Big[\sin\chi_l(kr)\ j_l(kr) - \cos\chi_l(kr)\ n_l(kr)\Big]. \tag{5}$$

Here $j_l(kr)$ and $n_l(kr)$ are the usual Riccati-Bessel functions [10]. Equations (2) and (3) are integrated up to a sufficiently large r, different for different l and k values. Thus the final S matrix is written as

$$S_l(k) = \exp\big(-2\ \Im m\,\chi_l\big)\exp\big(\mathrm{i}\,2\,\chi_l\big), \tag{6}$$

and the corresponding DCS's are defined as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{4k^2}\sum_{l=0}^{l_{\max}}\Big[\big(2l+1\big)\big[S_l(k)-1\big]P_l(\cos\theta)\Big]^2, \tag{7}$$

where $P_l(\cos\theta)$ is a Legendre polynomial of order l.

3. Results and discussion

In Figures 1 to 5, we display the present DCS for electron scattering from Yb atoms at 10, 20, 40, 60 and 80 eV energies using complex optical potential.

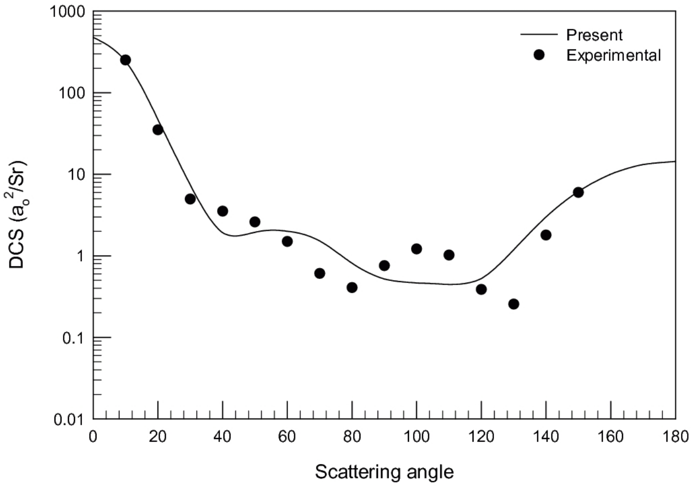

Fig. 1. Differential cross sections for electron scattering from Yb *atoms at energy 10* eV.

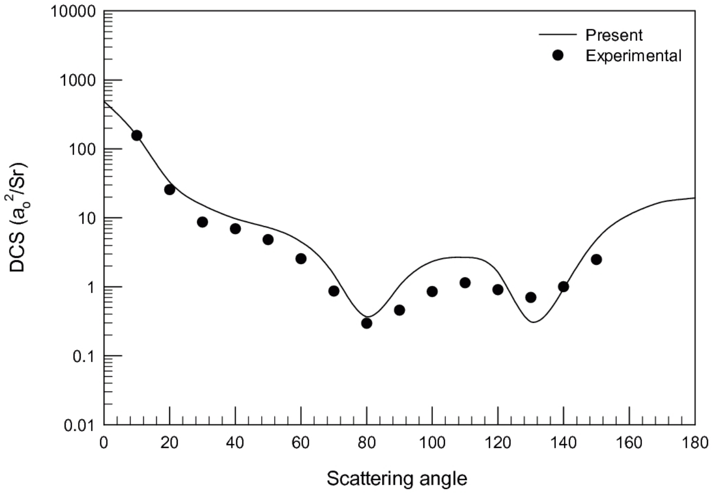

Fig. 2. Differential cross sections for electron scattering from Yb *atoms at energy 20* eV.

In particular, the structure of dips and humps (both in magnitude and width) changes when the absorption effects are switched on. A similar feature was also no-

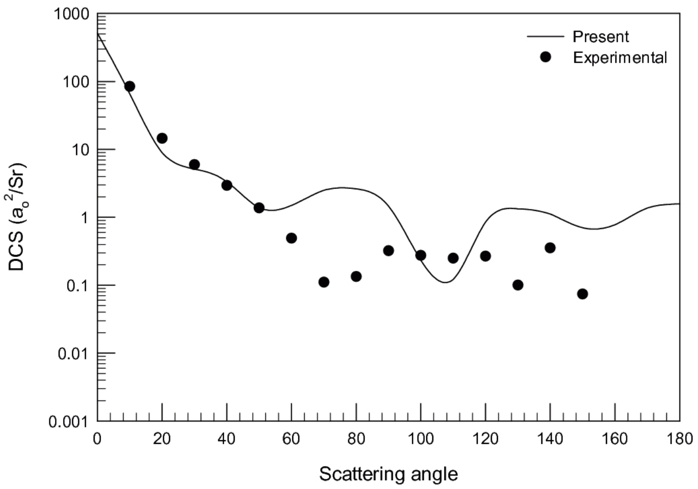

Fig. 3. Differential cross sections for electron scattering from Yb *atoms at energy 40* eV.

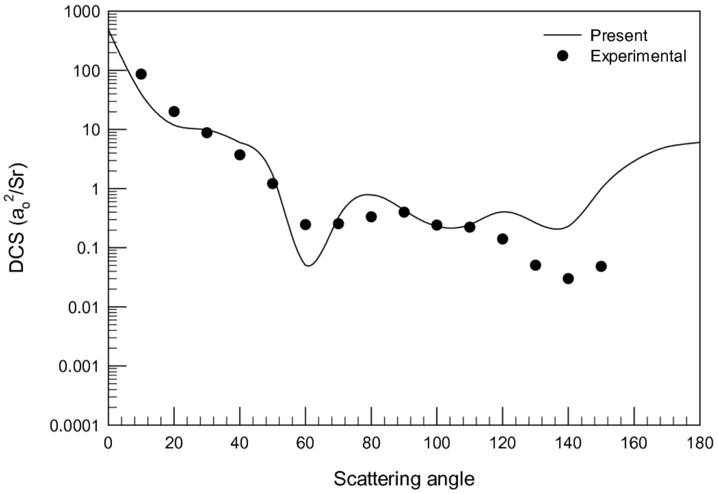

Fig. 4. Differential cross sections for electron scattering from Yb *atoms at energy 60* eV.

ticed by Jain, Etemadi and Karim [13] in one of their non-relativistic calculations on electron scattering from argon and krypton atoms at high energies. Dorn et al. [14] observed a similar feature in their experiment on elastic scattering of spin-polarized electron xenon atoms. They also confirmed it by their Dirac-Fock calculations including polarization and absorption potentials. This reduction is appreciable here also, particularly at 60 and 80 eV energies.

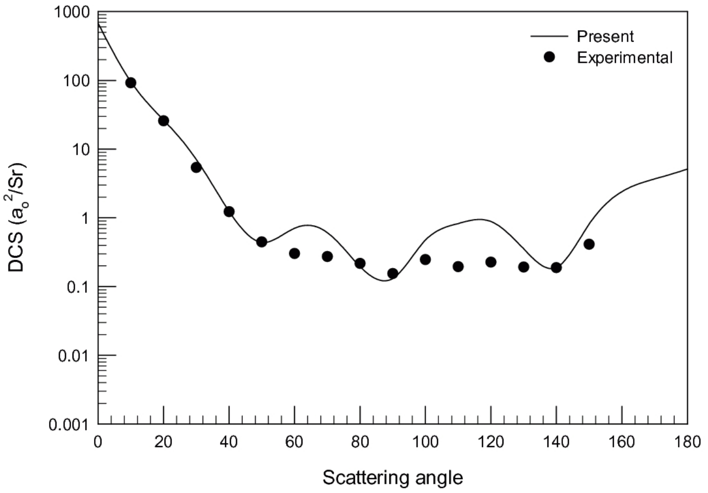

Fig. 5. Differential cross sections for electron scattering from Yb *atoms at energy 80* eV*.*

In comparison of our calculations with the experimental results of Predojević et al. [2], it is observed that qualitatively the salient features are reproduced well for incident energies of 20 and 60 eV. For other energies the agreement with the experimental data is also good.

4. *Conclusions*

We calculated the DCS of electron scattering by Yb atom for projectile energies 10, 20, 40, 60 and 80 eV by employing a parameter-free complex optical potential, which consists of all major interactions of the electron–Yb atom. The present work shows good agreement with the experimental work of Predojević et al.

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DIFERENCIJALNI UDARNI PRESJECI ZA RASPRŠENJE ELEKTRONA ATOMIMA ITERBIJA

Proučavamo raspršenje elektrona na enegijama 10, 20, 40, 60 i 80 eV primjenom bezparametarskog kompleksnog optičkog potencijala. Realni dio optičkog potencijala uključuje statički potencijal $V_{\rm st}(r)$, polarizacijski potencijal $V_{\rm pol}(r)$ koji se sastoji od kratko-dosežnih korelacija i dugo-dosežnih polarizacijskih efekata i član $V_{\rm ex}(r)$ koji se sastoji od elektronskog međudjelovanja izmjene, a izražen je pretpostavivši oblak elektronskog naboja kao slobodan elektronski plin. Gubitak toka u neelastične kanale uključuje se preko fenomenološkog apsorpcijskog potencijala. Postignuti ishodi uspoređuju se s nedavnim eksperimentalnim podacima.