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Elastic Scattering of Slow Electrons from Alkali Atoms*

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The elastic scattering cross sections for slow electrons incident on sodium and potassium are calculated using a model for the polarization potential which was earlier used for cesium. In all the alkalis studied, the low-energy scattering cross sections show an extreme sensitivity to the exact shape of the polarization potential in the region where r is comparable to the atomic radius of the target atom, indicating the necessity of having an accurate description of the polarization term in the total scattering interaction potential. Results are compared with available experimental data. In its application to the alkali atoms, this model yields results which are in good agreement with current experimental results.

I. INTRODUCTION

In a previous paper[1] a model was proposed to include the polarization potential in the total interaction potential for the scattering of slow electrons by cesium atoms. The method used was similar to that of Robinson[2] except in the form assumed for the polarization term. Of course, the polarization of the target atom plays the same important role in the scattering interaction for the other alkali atoms. In the present paper we extend the use of this model to the scattering of electrons by other alkali atoms, potassium and sodium.

II. METHOD OF SOLUTION

The elastic scattering cross sections for potassium and sodium were obtained in exactly the same manner as that described in I. The model for the effective scattering potential consists of the Hartree or Hartree-Fock potential function for the neutral alkali to which a polarization term of the form

$$V_p(r)=\alpha/2r^4\{1-\exp[-(r/fr_0)^8]\} \qquad (1)$$

is added, where α is the experimental polarizability for the atom in question and the quantity fr_0 is the so-called cutoff parameter. The complete interaction potential which appears in the Schrödinger equation is then

$$V(r)=V_H(r)/r+(\alpha/2r^4)\{1-\exp[-(r/fr_0)^8]\}\,, \qquad (2)$$

where $V_H(r)/r$ is the Hartree or Hartree-Fock potential function. In the present calculations the Hartree potential $V_H(r)$ for potassium was taken from the results of Hartree[3] and of Gibbons and Bartlett.[4] For sodium the Hartree-Fock potential function of Fock and Petrashen[5] was used.

The constant r_0 was again taken as the position of the outermost maximum of the valence electron wave function ($r_0=5.0a_0$ for K, and $r_0=3.5a_0$ for Na) and the parameter f was varied over a small range near $f=1.0$. The polarization potential thus exhibits a shallow peak near the outermost maximum of the valence electron wave function, whose position and magnitude is shifted slightly by varying the quantity f, and goes to zero for $r=0$ and asymptotically to $\alpha/2r^4$ (see Fig. 1 of I). Two different values of the polarizability from the literature[6] were used for each case: $\alpha=36$, 45 Å^3 (248, $326a_0{}^3$) for potassium and $\alpha=24$, 27 Å^3 (161, $182a_0{}^3$) for sodium.

With the experimental polarizability and a choice of the parameter f, the reduced radial equation for the lth partial wave $P_l(r)$

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+2\left(V_H(r)/r+\frac{\alpha}{2r^4}\times\left\{1-\exp\left[-\left(\frac{r}{fr_0}\right)^8\right]\right\}+E\right)\right]P_l(r)=0 \qquad (3)$$

was solved numerically by standard procedures for each value of l from $l=0$ to $l=l_{\max}$, where $l_{\max}$ is determined by the incident energy (values of l through $l=14$ where used at the highest energies considered). The phase shifts were determined as in I and the total cross sections obtained from the expression

$$\sigma=\frac{4\pi}{k^2}\sum_l(2l+1)\sin^2\delta_l\,, \qquad (4)$$

where $k=(2E)^{1/2}$ (atomic units).

III. RESULTS

It was found that the very low-energy cross sections for both sodium and potassium were extremely sensitive to the shape of the polarization potential as determined by varying the parameter f in Eq. (1). This same result was found previously for cesium (see Fig. 2 of I) for approximately the same energy range. In Figs. 1 and 2 we have plotted the results for K and Na which best fit

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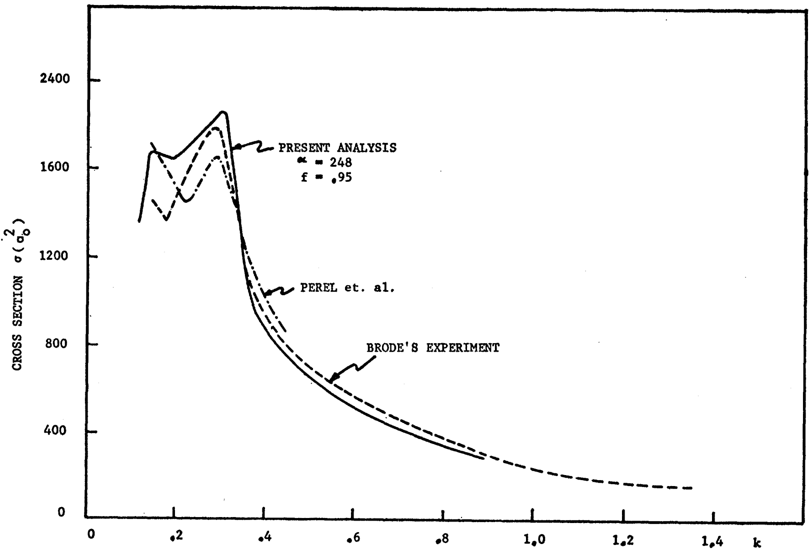

FIG. 1. Total elastic scattering cross sections for potassium yielded by the present model, compared with experimental values of Brode, and Perel *et al.* ($\alpha=248$, $fr_0=4.75$).

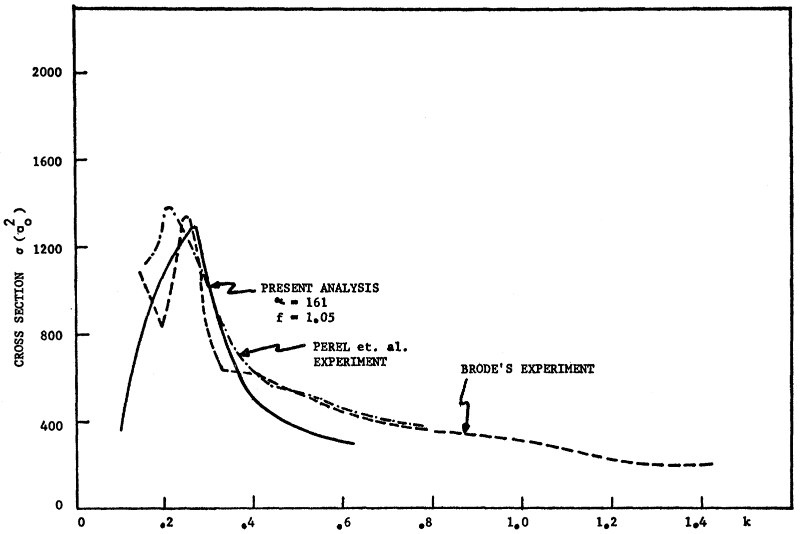

FIG. 2. Total elastic scattering cross sections for sodium from the present model, compared with the result of Brode and of Perel *et al.* ($\alpha=161$, $fr_0=3.675$).

the experimental values of Brode,[7] and of Perel, Englander, and Bederson.[8] These results were obtained with a value of the parameter $f=0.95$ and the experimental polarizability $\alpha=248a_0^3$ for potassium and with $f=1.05$ and $\alpha=161a_0^3$ for sodium. We see that good agreement exists between the present calculations and the available experimental data of Brode and of Perel *et al.*

IV. CONCLUSIONS

From the results obtained here and in I we can conclude that a simple model can be used to describe low-energy electron scattering by the alkali atoms, where the distortion of the target atom by the incident particle makes the major contribution to the scattering cross sections. From the sensitivity of the cross sections to the cutoff parameter of the present model, or more precisely on the position and magnitude of the maximum of the polarization potential, we can appreciate the importance of knowing accurately the contribution to the total scattering interaction due to the distortion of the target atom. The success of the model which we have used is probably due to its having a shape which closely approximates the polarization contribution from the valence electron, particularly in the region near the outermost maximum of the valence electron orbital.

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