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ENERGY ELECTRONS FROM SODIUM

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ABSTRACT

Differential cross sections for the elastic scattering of electrons from sodium have been measured with high angular resolution for incident energies of 54.4, 75, 100 and 150eV and over an angular range of 12° to 140° . The experimental data are compared with calculations based on the First Born approximation, the Glauber approximation and a close coupling impact parameter calculation. Calculations have been carried out for an optical model using the prescription of Vanderpoorten for localizing the absorptive part of the potential. Of the theoretical calculations the optical model is found to best reproduce the general features of the cross section at all energies.

INTRODUCTION

Recently, several calculations on elastic electron scattering from the alkalis (Issa (1976), Vanderpoorten (1976)) have demonstrated the need for accurate high angular resolution experimental data in the intermediate energy range. In particular, the calculation of Vanderpoorten has shown that at least in the case of electron scattering from lithium, the optical model can be used to accurately predict the differential cross sections for elastic scattering of electrons from a target with a high dipole polarizability and in which there is strong coupling between the ground and first excited states.

This paper serves two functions. Firstly we present experimental data for elastic differential cross sections from sodium over a large angular range and secondly we extend the work of Vanderpoorten to electron scattering from sodium.

Previous differential cross section measurements for electron scattering from sodium have concentrated on low incident energies where the close coupling calculations, most notably those of Moores and Norcross (1972), are expected to be valid. To our knowledge the upper energy limit of previous elastic electron-sodium atom experiments has been 20eV (Gehenn & Reichert (1972)). The data presented here are the first in an energy range where intermediate energy approximations can be applied.

Several theoretical calculations have been performed on the electron-sodium system for incident energies above 54.4eV. For example the frozen core Glauber calculation of Walters (1973) and the close coupling impact parameter calculation of Issa (1976) agree for scattering angles less than 20° . Both

of these calculations disagree with the First Born approximation (Walters 1973) at all scattering angles. We have calculated elastic differential cross sections based on two optical models, first the semi-phenomenological model of Furness and McCarthy (1973) and secondly one based on the prescription of Vanderpoorten (1976). The major distinction between these two calculations lies in the description of the imaginary or absorptive part of the optical potential).

We present optical model calculations and experimental data for differential cross sections for elastic electron scattering from sodium for incident energies of 54.4, 75, 100 and 150 eV in the angular region from 12° to 140° .

APPARATUS AND TECHNIQUES

The experimental apparatus was similar to that used in this laboratory for electron scattering experiments on Atomic Hydrogen (Teubner et al. 1974) and the rare gases (Lewis et al. 1974 a, b., Buckman et al. 1977) and is shown schematically in fig. 1. One notable exception has been the incorporation of a larger scattering chamber which provided more extensive shielding from the earth's magnetic field than was available in the previous apparatus. This was accomplished by the rigorous exclusion of magnetic materials from the chamber and its support, by lining the inside of the chamber with high permeability μ -metal shielding and by the use of two pairs of circular helmholtz coils perpendicular and parallel to the scattering plane. The ambient terrestrial magnetic field was thus found to be less than 5×10^{-7} T over a substantial volume enclosing the interaction region.

The atomic beam issued from a joule heated monel oven situated in the

source chamber, the first of three differentially pumped chambers. The oven was of basic design and consisted of a sunken well containing the charge of 2 to 3 grams of sodium which was connected by a long, narrow, heated canal to a stainless steel capillary array at the oven exit. The array was kept at approximately 30°C above the temperature of the well in the back of the oven. The solid volume of the monel block was large compared to that of the well and vapour channel. Although this condition required heating times of many hours, the oven was extremely stable once the operating temperature had been reached. Over a typical data collection period of 4-6 hours, changes in the oven temperature, measured by a thermocouple, were generally less than 1°C .

At the oven exit the sodium beam was 8 mm in diameter with a beam divergence angle of 1.8° . The oven exit was situated 1 cm from the wall of the source chamber and the neutral beam passed through a 5 mm diameter circular aperture in this wall into the second chamber. Here it was modulated at 240 Hz by a rotating toothed wheel. The modulated neutral beam entered the scattering chamber through a 3 mm diameter circular aperture which was aligned on the axis of the capillary array, thus ensuring a well collimated high density beam in the interaction region.

Considerable attention was paid to the possible formation of Na_2 dimers in the sodium beam. Thermodynamic calculations (Janaf 1971) have shown that the dimer concentration in a sodium source depends on the source temperature. We therefore chose to operate the oven at low temperatures, typically 300°C to 350°C , where the dimer concentration was estimated to be between 2.2% and 5.2%. The influence of dimers in the beam was investigated by measuring the angular distribution of elastically scattered electrons as a function of

the beam temperature. No irregularities in the distributions were observed, even at the highest source temperatures of over 400°C.

The electron beam was produced by an electron gun based on a design by Kuyatt (1967) and has been described in considerable detail by Lloyd (1973). The main advantages of this gun were that a well focussed beam could be obtained over an energy range of 20 to 500 eV, with an energy half-width of 300 meV. Final alignment of the electron beam was made with two sets of electrostatic deflection plates mounted in front of the gun. After passing through the interaction region the primary electron beam was trapped in a Faraday cup which consisted of two thin walled concentric cylinders. The beam was focussed by maximizing the current to the central collector. The ratio of the currents to the central and outer collectors varied from 96% at 54.4 eV to 99.5% at 100 eV and above. By scanning the well focussed electron beam across the cup and measuring the collector currents as a function of deflector voltage we estimated that the electron beam was approximately 2.5 mm in diameter at the interaction region. During each run the collector currents were continuously monitored so that corrections for small changes in the incident electron flux could be made.

The energy of the scattered electrons was analysed by a cylindrical mirror spectrometer based on the design parameters of Risley (1972). The energy resolution of this device was 1% which was sufficient to separate the elastically scattered electrons from those which had lost 2.1 eV in exciting the resonance levels. Those electrons which were passed by the energy analyser were detected by a channel electron multiplier.

The electron gun, Faraday cup and electron spectrometer all viewed the same point on the neutral beam axis and the gun-cup system was mounted such that it could rotate either clockwise or anticlockwise about this axis from

12° to 150° relative to the spectrometer. The acceptance angle of the energy analyser was larger than the angle subtended by the interaction region at the entrance to the spectrometer ensuring that the entire interaction region was viewed over the whole angular range. From geometrical considerations the angular resolution of the analyser was estimated to be less than 1.5° .

Pulses from the channeltron were amplified and counted in two gated scalers. The gating of the scalers was controlled by a reference light beam, modulated at the chopping frequency. Thus one scaler recorded electrons elastically scattered from the beam and background and the other those scattered only from the background. The difference in counts between these two scalers after a preset time was thus proportional to the differential cross section for elastic scattering at a particular energy and at a given scattering angle.

The data were placed on an absolute scale by measuring a series of ratios. First the ratio of the elastically scattered signal to the signal arising from the excitation of the 3^2P state in sodium was measured at 54.4 eV and a scattering angle of 15° . The differential cross section for elastic scattering at this angle was then derived from the known value of the inelastic cross section (Kennedy et al. 1977). This cross section, calculated from the distorted wave polarized orbital approximation was in excellent agreement with the measured absolute value of Shuttleworth et al. (1977) and with the close coupling impact parameter calculation of Issa (1976). The absolute value of the differential cross section for elastic scattering at 54.4 eV was therefore determined at every angle. Next the ratios of elastically scattered electrons at each energy to that at 54.4 eV were measured at 15° . Having previously determined (Buckman 1975) that the

transmission of the spectrometer and the efficiency of the detector was independent of the energy over this energy range, these latter ratio measurements placed the complete set of experimental values on an absolute scale. In all ratio measurements, great care was taken to ensure that the electron beam geometries were identical, at all energies. In addition, pulse height spectra were recorded at each energy to ensure that saturation of the detector did not occur.

The major contribution to the error in the absolute value of the cross section at 54.4eV, and therefore at all other energies, arose from the uncertainty in the elastic to inelastic ratio at 15° . Whilst the overall statistical error in the ratio was maintained at less than 0.6%, the possibility of substantially larger systematic errors could not be ignored. Therefore this ratio was determined on thirty separate occasions, the standard deviation of all of these measurements being 15%. Such a relatively large uncertainty reflects the strong forward peaking of the inelastic differential cross section since an uncertainty of only 0.5° in the scattering angle can explain the distribution of the data.

THEORY

In the present work we have extended the optical model used by Vanderpoorten (1976) to describe e^{-} -Li scattering to the case of elastic e^{-} -Na scattering. The local optical potential is energy dependent and of the form

$$V(r) = V_s(r) + V_p(r) + V_E(r) + i W(r).$$

The various potentials appearing in this expression were computed using the Hartree-Fock wave functions of Clementi and Roetti (1974). The screening potential, V_s , corresponds to the first-order term in a multiple scattering

expansion of the interaction and is given by $V_s(r) = \langle 0|V|0\rangle$ where $|0\rangle$ is the ground state wave function of the target atom and V is the electron-atom interaction potential.

The polarization potential, V_p , representing the long-range distortion of the target by the incident electron, corresponds to the real part of the second-order potential (Bransden and Coleman (1972)). We have used the local form of this potential obtained by Byron and Joachain (1974) which behaves asymptotically as

$$V_p(r) \underset{r \rightarrow \infty}{\sim} -\frac{\alpha}{2r^4}$$

The value of the static polarizability of sodium, α , was taken to be $\alpha = 165$ a.u. (Teachout and Pack (1971)).

The equivalent exchange potential, V_E , is obtained by localizing the exchange potential appearing in the appropriate continuum Hartree-Fock equations, according to the prescription of Furness and McCarthy (1973).

The resulting potential may be written

$$V_E(r) = \frac{1}{2} \left\{ (E - V_s - V_p) - \left[(E - V_s - V_p)^2 + 2 \sum N_i |R_i|^2 \right]^{1/2} \right\}$$

$$N_i = \begin{cases} (2\ell+1) & 1s, 2s, 2p \text{ orbitals,} \\ (-1)^S & 3s \text{ orbital,} \end{cases}$$

where S is the total spin, E the energy of the incident electron and R_i the radial wavefunction of the i^{th} Hartree-Fock orbital.

The absorption potential, W , which corresponds to the imaginary part of the second-order potential, describes the loss of electrons from the elastic channel. The method for obtaining an equivalent local imaginary potential has been fully described by Vanderpoorten (1975) and Joachain et al. (1977).

RESULTS AND DISCUSSION

Differential cross sections for elastic scattering of electrons from sodium are shown in figure 2 for incident energies of 54.4, 75, 100 and 150eV. The experimental values are given in table 1, with the figures in brackets representing statistical errors only. In addition to statistical errors there is an overall error in the absolute values of 15%.

A striking feature of the measured differential cross sections is their similarity in shape to those for elastic electron scattering from Neon (Williams and Crowe (1975)), particularly at large scattering angles. Such a feature reflects the weak binding energy of the valence electron and indicates that with the exception of the angular region less than $\theta = 30^\circ$, the scattering process is dominated by interactions with the core. The difference between the cross sections at smaller scattering angles can be attributed to the stronger absorption and polarization effects in the sodium atom which are largely a result of this loosely bound valence electron.

At 54.4eV the experimental data are compared with values predicted by the first Born approximation and a frozen core Glauber approximation. Issa (1976) has used the second order potential method of Bransden and Coleman (1972) in a two state model to calculate cross sections at 50eV and all other energies shown. It is clear from the data in figure 2(a) that at lower energies the Born approximation is completely inadequate for describing elastic scattering from sodium at all scattering angles. The frozen core Glauber approximation is in reasonable agreement with the experimental data for scattering angles less than 20° but, not surprisingly, fails for angles

greater than this. Similarly the calculation of Issa at 50eV is in reasonable agreement with experiment for small scattering angles. The semi-classical approximation employed in the calculations by Issa is expected to become valid at larger scattering angles as the incident energy increases (Bransden & Noble (1976)). This feature is in fact observed in the present case and in particular at 150eV (fig. 2(d)) the semi-classical calculation is in excellent agreement with the measured cross sections for scattering angles less than 30° .

The optical model calculations presented in figs. 2(a)-2(d) are in reasonably good agreement with the experimental data over the whole angular range. The largest discrepancy occurs at 54.4eV where there is a considerable difference in the shape of the experimental and theoretical cross sections for scattering angles greater than 40° . At such a low energy the use of an average excitation energy as employed by Vanderpoorten (1976) cannot be expected to be adequate for sodium considering that the orbital energies vary between 4.96eV for 3s electrons and 1101eV for 1s electrons (Joachain et al. (1977)). We have considered the frozen core approximation model for core-excitation states derived by Joachain et al. (1977). A frozen core consisting of $1s^2 2s^2$ electrons gives cross sections which are not noticeably different from those obtained using an absorptive potential including all orbitals. On the other hand a frozen core consisting of $1s^2 2s^2 2p^6$ electrons produces a cross section which is larger than the experimental values at all scattering angles. We have chosen to strictly enforce energy conservation and employ a $1s^2 2s^2$ frozen core at this energy.

As the incident energy is increased the agreement between the experimental values and the optical model improves considerably. In particular at 100eV the theoretical curve lies within the experimental errors for all scattering angles less than 90° . The main discrepancy at this energy lies in the position of the minima in the cross section. In fact the optical model consistently

fails to accurately predict the position of the minima at all energies considered with the discrepancy ranging between 3° - 5° . The backward angle behaviour of the optical model cross section at 150eV appears to be somewhat anomalous considering that the agreement with experiment is expected to improve with energy.

The sensitivity of the optical model results to variations in the input potentials was tested both by alterations to the value of the static dipole polarizability α and by considering alternative formulations of the polarization and absorption potentials. At an incident energy of 100eV a 10% change in the value of α did not have a noticeable effect on the differential cross sections. The inclusion of relativistic effects by the method described by McCarthy et al. (1977) was also found to have negligible effect on the computed cross sections. Similarly, the exclusion of exchange did not appear to affect the cross section values significantly. Figure 3 illustrates the relative importance of the various terms in the optical potential. It is interesting to contrast the present case where the absorption potential dominates the polarization potential, except at very large ranges, to the case of electron-rare gas atom scattering where the absorption and polarization potentials are of similar magnitude. Such a situation should provide a stringent test of the imaginary potential.

In addition to calculations using the Vanderpoorten formulation for the imaginary optical potential we have investigated the validity of the Furness-McCarthy potential for the case of alkali targets. This semiphenomenological potential which is considerably easier to calculate than the ab initio form of Vanderpoorten provides an excellent description of the scattering parameters in the case of rare gas atom targets (McCarthy et al. (1977)). However the

cross sections computed using this potential for alkali metal targets differ considerably from the experimental data at all incident energies considered here.

CONCLUSIONS

Of the various theoretical calculations in the literature it appears that the optical model best reproduces the general features of the observed differential cross sections. It is clear that in the elastic scattering of electrons from sodium, the very strong coupling between the ground and first excited state in the atom implies that the absorptive part of the optical potential plays an extremely important role in the description of the scattering process. The description of the absorptive potential in the model of Furness & McCarthy (1973) is clearly an oversimplification which, although it can readily be applied with great success to elastic scattering from the inert gases fails rather badly in the case of the alkalis.

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TABLE I: Elastic Differential Cross Sections (in $a_0^2\text{sr}^{-1}$) for electrons scattered by sodium atoms. The numbers in brackets represent the percentage statistical error in the cross section. There is an additional systematic error in each point of 15%. Where no figure appears the error is less than 1%.

Angle (deg)	Energy (eV)			
	54.4	75	100	150
12	14.92	13.58	14.14	12.08
15	9.51	8.48	8.01	7.21
20	4.03	3.87	3.78	3.32
25	1.92	1.82	1.95	1.83
30	0.899	1.02	1.13	1.11
35	-	0.672	-	-
40	0.413	0.471	0.474	0.37
50	0.258	0.279	0.224	0.168
60	0.198	0.181	0.129	0.0838 (2.4)
70	0.134 (1.1)	0.115	0.076 (1.2)	0.0466 (2.4)
80	0.0888 (1.1)	0.0629	0.0412 (1.6)	0.0274 (2.8)
90	0.0465 (2)	0.0272 (1.4)	0.0159 (2)	0.0154 (4.8)
95	-	0.0123 (4.1)	0.00928 (3.9)	0.0122 (7.9)
97.5	-	-	-	0.011 (11)
100	0.0234 (3.4)	0.00429 (8.1)	0.0058 (5)	0.0117 (8.6)
105	0.00894 (6.2)	0.00208 (11.5)	0.00839 (3.9)	0.0144 (6)
108	0.00230 (12)	-	-	-
110	0.00181 (12)	0.006 (8)	0.0145 (2.3)	0.0184 (5.8)
112	0.00223 (11)	-	-	-
115	0.0124 (5.8)	0.016 (3.5)	-	-
120	0.0395 (3.2)	0.0387 (1.9)	0.0439 (1.5)	0.0348 (5)
130	0.140 (1.2)	0.0867	0.103 (1.1)	0.0591 (2)
140	0.283	0.179	0.187	0.0895 (1.8)

FIGURE CAPTIONS

- Figure 1. Schematic diagram of the experimental apparatus.
- Figure 2. Elastic differential cross sections for electrons scattered by sodium atoms at incident energies of (a) 54.4eV (b) 75eV (c) 100eV (d) 150eV. - - - - Optical model calculation, -.-.- First Born approximation (Walters 1973), — Second order potential calculation (Issa 1976).
- Figure 3. Absolute value (in atomic units) of the terms contributing to the optical potential. V_{st} - static potential, V_{pol} - polarization potential, W - absorption potential (including all orbitals). The incident energy is 100eV.

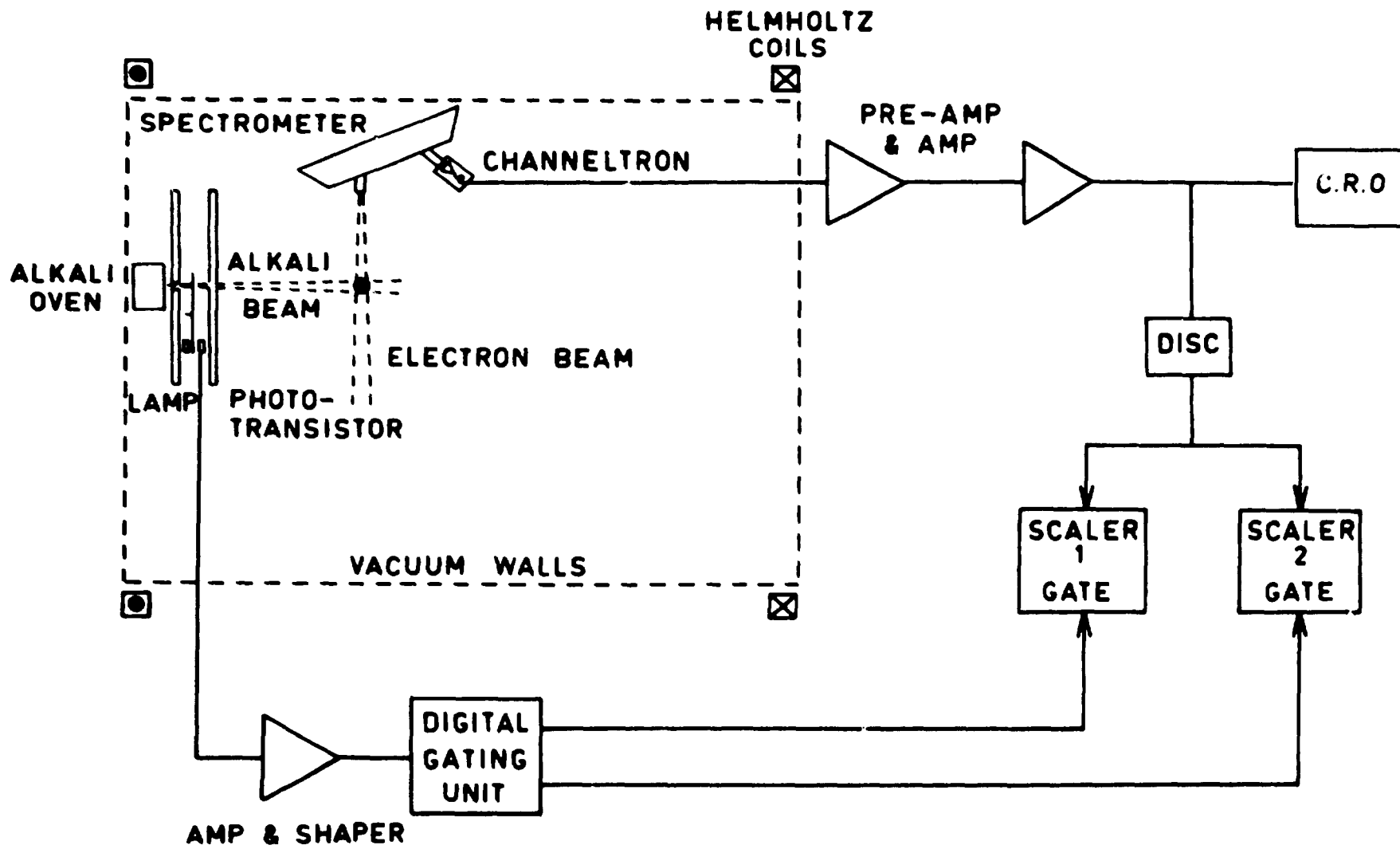


Fig. 1.

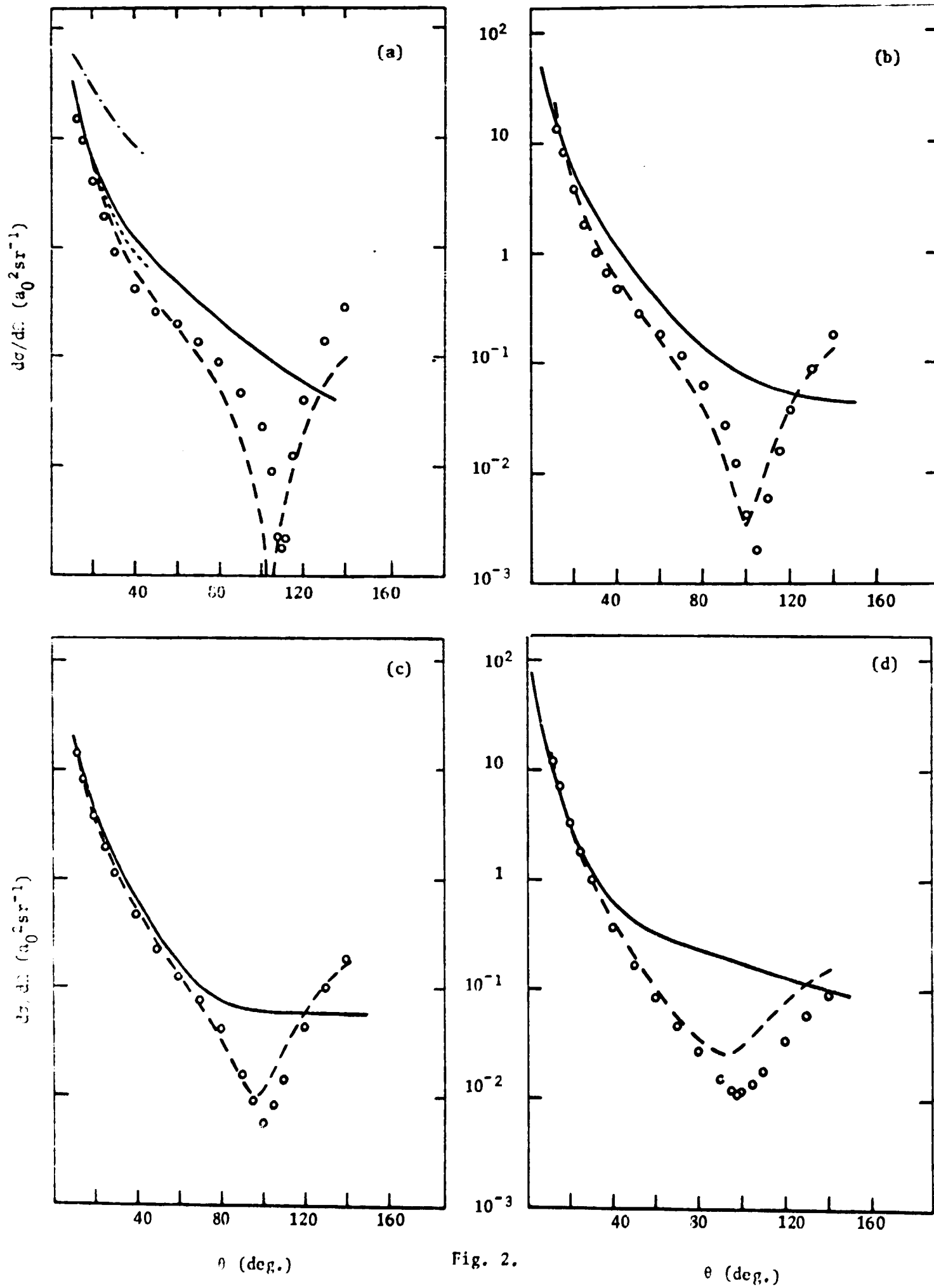


Fig. 2.

Fig. 3

