THE JOURNAL OF CHEMICAL PHYSICS VOLUME 59, NUMBER 1 1 JULY 1973

# Observation of the Compton modified band for the scattering of keV electrons by $H_2$, He, Ne, and Ar*

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(Received 28 March 1972)

Measurements of the energy loss spectrum using keV electrons scattered from $H_2$, He, Ne, and Ar at large scattering angles which define a portion of the Bethe surface are reported. The results are in good agreement with the theory of the Compton effect where the incident x-ray is replaced by a high-energy electron. The angular dependence of the inelastic scattering from $H_2$, He, and Ne with 45 keV incident electrons is found to be in agreement with the first Born approximation including interference and exchange effects assuming weakly bound target electrons. The ratio of the inelastic peak height to the elastic peak height is compared with the results of the binary encounter theory using Hartree-Fock ground state wavefunctions and the results of experiment and theory are found to be in agreement within experimental uncertainties.

## I. INTRODUCTION

Hughes and Mann pointed out in 1938 that the inelastic spectrum of scattered electrons from atoms contained a Compton-like line at large scattering angles.[1] The nonrelativistic theory for electron-electron scattering which gives the basic equation needed in this work was given by Mott[2] in 1930. The relativistic theory for electron–electron scattering given by Möller[3] in 1932 also predicts the existence of an inelastic line associated with energy transfer between two electrons satisfying conservation of energy and momentum. The "Compton modified band" of Hughes and Mann is of course just the nonrelativistic Möller scattering modified by the initial velocity distribution of the target electrons.

Hughes and Mann[1] in their initial work, which seems to be the only work so far reported in the angular and energy loss range to be discussed in this paper, measured the Compton modified band with an energy resolution of about 60 eV at incident electron energies between 1000 and 4000 eV at a scattering angle of 34.2°. As these authors correctly point out, the measurement of Compton profiles by the use of incident electrons rather than x-rays offers two important advantages over the x-ray technique. The first is due to the fact that electrons are more strongly scattered by other electrons than x-rays and hence higher count rates can more easily be obtained. The second point is that the width of the Compton modified band in the electron scattering case is wider relative to the energy loss value at its center than the corresponding x-ray result. A serious disadvantage, not mentioned by these authors, is the effect of exchange scattering[2,3] in the electron case which is not present in x-ray experiments. The first Born theory of scattering suggests that exchange effects are of the order of 25% at a scattering angle of 34° and are thus far from being negligible.[2,3] It would seem that before the advantages of the electron scattering method in the measurement of Compton profiles can be realized the dynamics of the scattering process must be understood in a detailed way.

The purpose of this work is to survey the energy and angular dependence of the Compton modified band in order to test the Born scattering theory. As pointed out by Hughes and Mann the count rates for the inelastic line at large scattering angles and keV incident energies are extremely small. This problem can be overcome to some extent by going to smaller angles and lower energies. However, the Born theory should be better at higher incident energies and the extraction of a Compton profile from scattering data can only be done if the first Born approximation is valid. Another potential advantage of the electron scattering method is that it is relatively easier to obtain higher energy incident electron sources than x-ray sources. This last consideration is not a trivial one when it comes to studying the heavier elements where some target electron binding energies are in the keV range. For these reasons it was decided to investigate the Compton modified bands for the systems $H_2$, He, Ne, and Ar over the energy range 35–45 keV and angular range 25°–45°. This energy range is high enough so that the Born theory should be valid for elements as heavy as Ar. The angular range does not contain the optimum choice of scattering angle for measuring Compton bands but does include one of the more interesting regions for observing large effects on the scattering due to interference and exchange processes.

To obtain Compton profiles from an electron scattering experiment the optimum angular range must be selected by comparing the deviation of the x-ray incoherent scattering factor $S(K)$ with the number of electrons in the target $N$ as a function of momentum transfer with the effects of interference and exchange. The difference $N - S(K)$ decreases with increasing scattering angle while interference and exchange effects increase with increasing scattering angle. The reason for using $S(K)$ as a guide for selecting the scattering angle is that the integral of the Compton modified band over energy loss can be shown[4] to correspond to the term $N$ in the expression for $S(K)$. This means that interference effects between an electron wave scattered by two different target electrons are not included in the binary encounter theory which must be used to show the connection between the Compton profile and the electron energy loss spectrum.[5] For He with incident 40 keV electrons an angle of about 7° should yield a Compton modified band with less than 1% corrections for deviations from electron interference scattering and interference—exchange effects. For a heavier system, such as Ar, the optimum uncertainty for corrections from these two effects is about 10% which is achieved by utilizing a scattering angle of about 25° with 40 keV incident electrons. Any further improvement in the potential measurement accuracy of the Compton profile by electron scattering methods will depend on the development of accurate methods for computing corrections for either one or both of the two major sources of uncertainty discussed above.

## II. EXPERIMENTAL

At large scattering angles a typical energy loss spectrum consists of a sharp elastic line and a Compton modified band. At an incident energy of 35–45 keV the first Born binary encounter theory predicts that a typical energy loss difference between the elastic peak and the Compton line is on the order of 10–25 keV.[5] Therefore, in order to monitor the areas of both peaks in a time which is short compared to possible fluctuations in the experimental conditions, it seemed appropriate to utilize the energy measurement capability of Si surface barrier detectors. The disadvantage of this technique is that the energy resolution of the detector (5 keV FWHM) is rather poor. On the other hand if the energy resolution of the detector is sufficiently broad we can expect the height of an experimentally broadened spectroscopic peak to be nearly porportional to the area of the natural spectroscopic line and approximately independent of its actual line shape. The area of the natural spectroscopic line is of course just proportional to the differential cross section.

Because of these considerations and the extremely small scattering power of atoms in the large angle region it was deemed desireable to employ low energy resolution in the first attempt to study the behavior of the Compton line as a function of both incident energy and scattering angle.

The spectrometer used for the measurement of the large angle electron energy loss spectra consisted of a telefocus gun producing an electron beam of up to 200 $\mu$A beam current in the primary energy range of 35 to 45 keV, which is scattered by a well-collimated gas jet produced by expanding the gas through a hypodermic needle with 0.15 mm inside diameter all contained in a large vacuum chamber in which an ultimate pressure of $6\times10^{-7}$ torr was attained. During an experiment the background vacuum pressure was never allowed to exceed $6\times10^{-5}$ torr. A silicon surface barrier detector, located about 50 cm from the point of scattering, was used for counting and analyzing single scattered electrons. The energy resolution of the detector-amplifier-multichannel pulse height analyzer system was 5 keV FWHM which was sufficient to resolve the two peaks in the spectrum. The energy determination was accurate to within 500 eV. Corrections for scattering from residual gas in the chamber and from the walls, as well as for electron backscattering from the Si detector, were experimentally determined. These corrections introduced an additional uncertainty of about 300 eV in the energetic position of the inelastic peak. The absolute scattering angle was determined to better than 1° and the angular acceptance of the detector apertures was 0.2°. A schematic diagram of the experimental apparatus is shown in Fig. 1.

## III. RESULTS

In Fig. 2 three Compton modified band spectra for He are plotted as a function of scattering angle and energy loss $E$. These results are typical and define an experimentally broadened picture of the high-energy Bethe surface.[6] Note that the spectra have been corrected for background scattering and the low-energy tail of the detector response function. The position of the center of the inelastic peak is defined within about ± 800 eV and the ratio of inelastic peak height to elastic peak height appears to be reproducible to better than ± 5%. Note that the previously reported study by Hughes and Mann,[1] while utilizing superior energy resolution, failed to investigate the angular dependence of the scattering and did not obtain quantitative measurements of the ratio of the intensities of elastic to inelastic scattering.

The present experiments showed that the position of the inelastic peak could be satisfactorily accounted for by free electron momentum and energy considerations[5] over the range of incident energies $E_0$ (35 keV $\leq E_0 \leq$ 45 keV) and scattering angles $\theta$ ($25° \leq \theta \leq 45°$) investigated in this study.

The behavior of the Bethe ridge with incident energy was found to obey the free electron binary encounter relationship

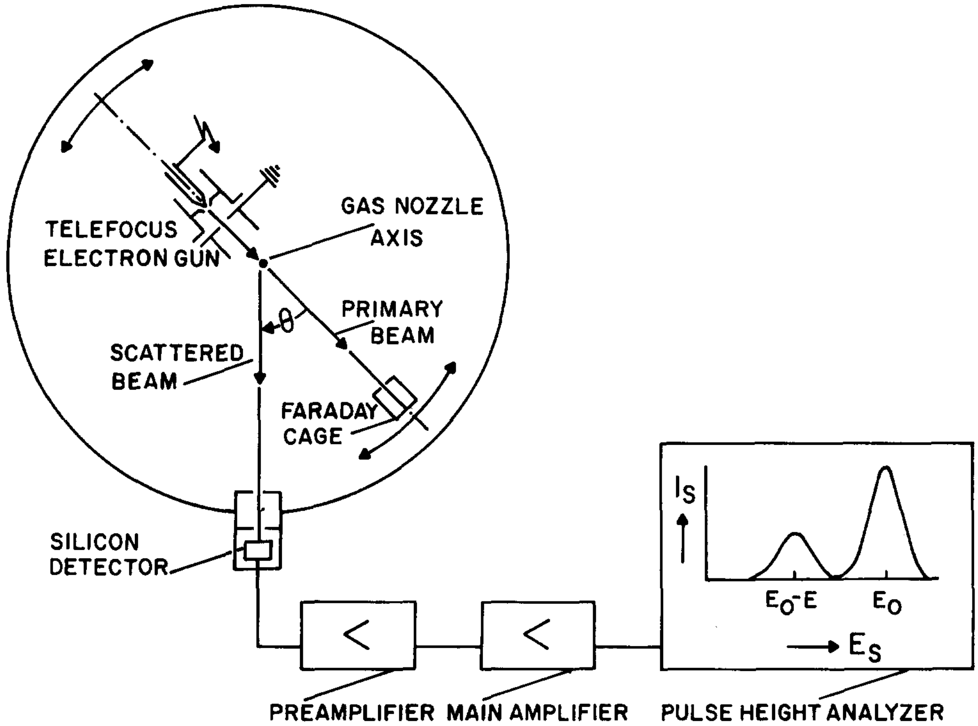

FIG. 1. High-energy large angle scattering electron spectrometer.

$$E = E_0 \sin^2\theta\,[1 + (\beta^2/4)\cos^2\theta + O(\beta^4)]$$

to within the experimental error of ± 0.8 keV. Note that the relativistic correction is less than 0.6 keV in the worst case and was not detectable with the present energy resolution. The variation of the elastic line intensity with incident energy at fixed scattering angle showed a first Born energy dependence of $1/E_0^2$ to within ±4% for He and the results are shown for a scattering angle of 35° in Fig. 3. The data in Fig. 3 have been corrected in the same way as the data in Fig. 2. The variation of the intensity with angle at fixed incident energy could not be easily checked since a slight realignment of the electron and gas beams is required after changing to a new scattering angle.

The single parameter best characterized by these experiments is the ratio, $R$, of the intensity of the inelastic peak at its maximum to the intensity of the elastic peak at its maximum or equivalently the ratio of the two peak areas. The elastic line is assumed to be a narrow Gaussian peak with FWHM of less than 10 eV, as limited by the high voltage source, and with an area proportional to the elastic differential cross section. The inelastic peak can be characterized by a shape which when integrated over energy yields the inelastic differential cross section.

For the systems studied here the elastic cross section is given to an accuracy of better than 1% over the studied range by the relation $d\sigma_{el}/d\Omega = 4Z^2/[K^4(1-\beta^2)]$ in atomic units where $Z$ is the atomic number and $K$ is the elastic momentum transfer $2k\sin(\theta/2)$ with $k$ corrected for relativistic effects ($\hbar k = m_0 c\beta/\sqrt{1-\beta^2}$). Since the independent atom model[7] description was used for $H_2$, $Z^2$ must be replaced by 2. This formula was checked against relativistic partial wave calculations using a Hartree–Fock potential field.[8] Better than 1% agreement between the asymptotic Born result and partial wave calculations were found for He, Ne, Ar,

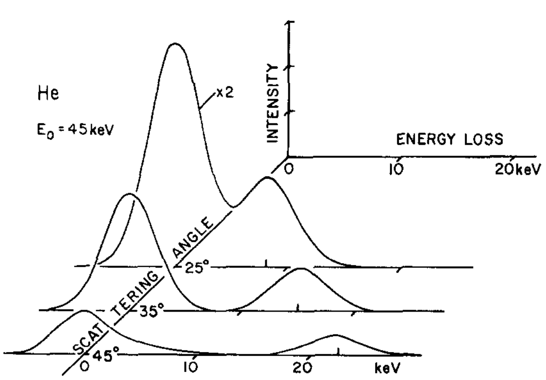

FIG. 2. Experimental electron energy loss spectra at 45 keV primary energy and different scattering angles $\theta$ = 25, 35, and 45° for He. Elastic peak intensities are normalized according to their first Born approximation values.

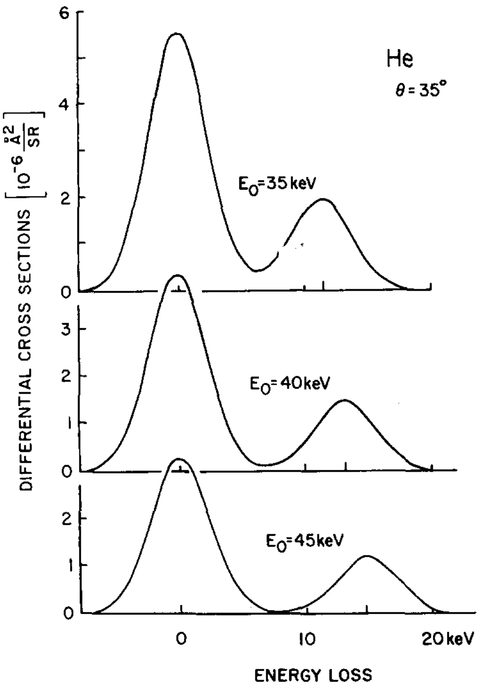

FIG. 3. Experimental electron energy spectra at 35° scattering angle and different primary energies $E_0 = 35$, 40, and 45 keV for He. The elastic peak at 35 keV is normalized to the theoretical first Born approximation differential cross section. Relative experimental elastic peak intensities agree within 4% with first Born approximation.

and $H_2$ in the range of $K$ and $E_0$ of these experiments. Inelastic multichannel coupling effects[9] such as polarization and absorption should be unimportant at the incident energies and scattering angles considered in this work.

For the inelastic scattering the differential cross section can be given by either

$$d\sigma_{\text{inel}}/d\Omega = [4N/K^4(1-\beta^2)]\,[(1+2\beta^2\,|\,\epsilon_0|\,)/3m_0c^2N]\,\delta_1 \tag{1}$$

or

$$\frac{d\sigma_{\text{inel}}}{d\Omega} = \frac{\cos\theta}{\cos^4(\theta/2)}\ \frac{4N}{K^4(1-\beta^2)}\ 1+\left[\frac{2\beta^2\,|\epsilon_0|}{3m_0c^2N}\right]\delta_2, \tag{2}$$

where $N$ is the number of electrons in the atom and $|\,\epsilon_0|$ is the total electronic energy of the ground state of the atom and $\delta$ is a correction for exchange and interference effects. The quantity $\delta$ is given in the first Born approximation as

$$\delta_{1,2} = 1 - K^2\int[d\mathbf{p}\,\rho(\mathbf{p})/|\,\mathbf{k}_s-\mathbf{p}|^2] + K^4\int[d\mathbf{p}\,\rho(\mathbf{p})/|\,\mathbf{k}_s-\mathbf{p}|^4]\ , \tag{3}$$

with

$$\delta_1 \simeq 1 - 4\sin^2(\theta/2) + 16\sin^4(\theta/2), \tag{3'}$$

and

$$\delta_2 \simeq 1 - \tan^2\theta + \tan^4\theta, \tag{3''}$$

where $\rho(\mathrm{p})$ is the one electron momentum distribution function of the target and $k_s^2$ is the energy of the scattered electron. The relativistic term involving $|\,\epsilon_0|$ was derived from an expression given in Ref. 3 with the neglect of all nondiagonal terms in the scattering operator and is not important in this work. Equations (1) and (2) are derived by the approximate use of closure over all excited electronic states of the first Born expression for the differential inelastic cross section. Assuming that all target electrons have infinite binding energies yields Eqs. (1) and (3′) while Eqs. (2) and (3″) come from the assumption that all target electrons are free.

Because of the difficulties with background scattering and in some cases insufficient energy resolution it was not possible to collect data for Ar at each of the three scattering angles used in this study. It might be mentioned that the absolute value of the Born differential cross sections studied here are of the order of $10^{-22} - 10^{-23}\,\text{cm}^2$ whereas the elastic cross section in the forward direction is on the order of $10^{-16} - 10^{-17}\,\text{cm}^2$. This means that the scattered intensities for the present study are at least 5 orders of magnitude smaller than those encountered in the forward direction where most experiments in this energy range have been carried out.

The experimental results for the peak ratio $R$ for $H_2$, He, Ne, and Ar are presented in Table I as a function of scattering angle. Note that angular data for the three angles could be obtained only at 45 keV for the reasons discussed earlier. The simplest way to relate $R$ to theory, is to assume that the instrumental broadening is large compared to natural linewidths so that the height of the experimentally broadened peak is proportional to the peak area and the ratio $R$ is given by

$$R \simeq (N/Z^2)\,\delta_1 \tag{4a}$$

or

$$R \simeq (N/Z^2)\,[\cos\theta/\cos^4(\tfrac{1}{2}\theta)]\,\delta_2. \tag{4b}$$

While the experimental results agree better with the predictions of Eq. (4b) than (4a) it is clear that a systematic difference still remains.

In order to resolve this remaining difference between theory and experiment a somewhat more sophisticated theory was used. It was assumed that the shape of the peaks in the inelastic energy loss spectrum for the exchange and interference

TABLE I. Ratios of inelastic to elastic differential cross sections for $H_2$, He, Ne, and Ar at an incident electron energy of 45 keV as a function of scattering angle.

| Element | Angle | $R$ Experiment | Eq. (4a) $(N/Z^2)\delta_1$ | Eq. (4b) $(N/Z^2)[\cos\theta/\cos^4(\theta/2)]\delta_2$ | HF Compton profile times $\delta_2$ folded with the instrument response function |
|---|---|---|---|---|---|
| $H_2$ | 25° | 0.66 ± 0.10 | 0.85 | 0.83 | 0.76 |
| | 35° | 0.57 ± 0.06 | 0.77 | 0.75 | 0.62 |
| | 45° | 0.90 ± 0.18 | 0.76 | 0.97 | 0.70 |
| He | 25° | 0.40 ± 0.04 | 0.42 | 0.41 | 0.40 |
| | 35° | 0.36 ± 0.04 | 0.38 | 0.37 | 0.35 |
| | 45° | 0.40 ± 0.08 | 0.38 | 0.49 | 0.45 |
| Ne | 25° | 0.073 ± 0.004 | 0.085 | 0.083 | 0.071 |
| | 35° | 0.058 ± 0.003 | 0.077 | 0.075 | 0.059 |
| | 45° | 0.072 ± 0.007 | 0.076 | 0.097 | 0.072 |
| Ar[a] | 25° | ··· | 0.047 | 0.046 | 0.037 |
| | 35° | 0.022 ± 0.006 | 0.043 | 0.041 | 0.031 |
| | 45° | ··· | 0.042 | 0.054 | 0.037 |

[a] Values obtained at 40 keV.

terms were identical to the shape of the direct peak. This is of course a very tenuous assumption since no theoretical investigations into this matter have yet been made and at 45° all three contributions are of equal magnitude in Eq. (4b). The approach to be used here then is to make the assumption and then compare the results with experiment. Assuming that the inelastic peak shape is given accurately by the binary encounter theory[5] the peak height was computed by using the theoretical Compton modified band shape, calculated with a Hartree-Fock wavefunction folded with the experimental peak shape which was taken as the shape of the elastic band in the forward scattering direction where all peaks for inelastic processes are close to the elastic peak and hence not resolved by the detector. There is a small uncertainty in determining the experimental peak shape caused by the presence of the low energy tail but this was taken into consideration in assigning the experimental uncertainties. Note that an independent atom model description was used in the case of $H_2$.

It was found that the experimentally broadened theory was in agreement with all cases studied with the exception of $H_2$ where the wavefunction used was quite poor and Ar where the magnitude of the effect is quite small. Hence within the accuracy of the present experiment it does not appear that there are major qualitative differences in the shapes of the interference and exchange contributions to the scattering and the shape of the direct scattering term.

In summary, the work reported here has shown that:

(a) The angular dependence and energy dependence of the position of the Compton modified band are in agreement with the predictions of binary encounter theory for the targets, angular, and incident energy regions studied.

(b) The first Born theory of exchange and interference scattering assuming weakly bound target electrons was found to agree with experiment for $H_2$, He, and Ne.

(c) The effect of the finite breadth of the velocity distribution of the target electrons was observed in all cases. The results agree with the predictions of Hartree-Fock theory but are not sensitive to minor changes in the wavefunction.

(d) The shape of the exchange and interference contributions to the Compton modified band must be qualitatively similar to the shape of the contribution to the direct band. Note that if the exchange and interference peaks had the same shape but were very dissimilar to the shape of the direct peak that the scattering at 45° would be identical to the direct contribution. At other angles this would not be the case however.

Work is currently underway to improve the energy resolution by employing an electrostatic velocity analyzer with a resolving power of better than 10 eV.

The authors wish to thank Dr. L. Vriens for helpful suggestions during the course of this work.

[*] Contribution No. 2185 from the Chemical Laboratories of Indiana University. The authors wish to acknowledge support from the AFOSR Grant No. AFSOR-70-1900.

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