Study of Rayleigh Scattering Cross-Sectionsfor 40 keV Photons at Large Angle

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ABSTRACT

In the present measurements, theoretical Rayleigh scattering cross-sections have been measured. Differential cross-sections for the Rayleigh scattering for the 40 keV photons have been evaluated at an angle of 141 for all the elements in the atomic region 1 Z 99. The two basic theoretical approaches to calculate the Rayleigh scattering amplitude and scattering cross-sections are form factor (FF) approximation and state of art S-matrix approach. The modified form factor (MF), modified form factor incorporating the anomalous scattering factor (MFASF) and S-matrix cross-sections for all the elements have been interpolated from the values available assuming the same energy dependence as that for the MFASF values.

Keywords: Rayleigh, cross-section, X-rays, MF, MFASF, S-matrix

Introduction

A photon interacts with an atom through different processes involving interaction with atomic electron through photoelectric effect, scattering, i.e., elastic and inelastic scattering from electrons, and pair production around the nuclear field. In the photoelectric effect the energy of the incident photon should be either greater than or equal to the binding energy of an electron and it gets completely absorbed resulting in the emission of photoelectron with energy equal to the energy of incident photon minus the binding energy of the electron. In the elastic scattering process, the energy of the scatter photon remains same as that of the incident photon. In this process only

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the momentum is transferred, i.e., direction of the scatter photon changes [1,2]. The elastic scattering from the bound electrons,at lower photon energies, gives the dominant contribution to the photon-atom scattering amplitude, which is known as Rayleigh scattering. The scattering of photons from a virtual electron-positron pair created in the field of nucleus is called Delbruck scattering. In the inelastic process, the energy as well as momentum of the scatter photon changes. Inelastic scattering is of two types, i.e., Compton scattering and Raman scattering. Compton scattering is the inelastic scattering resulting in ionization of the atom and Raman scattering involves excitation of the interacting electron to higher energy unoccupied bound state. In case the incident photon energy is slightly less than binding energy of interacting electron, it proceeds by creation of a virtual hole in the respective shell/subshell with the corresponding electron excited to an unoccupied state. Simultaneously, an electron from a higher-shell fills this hole followed by emission of a photon whose energy corresponds to the difference between final and initial holes. It can also result in a radiationless transition. The term resonant Raman scattering (RRS) has been usually employed whether the excited electron is in bound state or occupies a continuum state.When the energy of incident photon exceeds $2m_oc^2$> 1.02 MeV, it interacts with the Coulomb field of a nucleus and the incident photon disappears with the creation of an electron-hole pair. This process of interaction of photon with atom is known as pair production. Basic photon-atom interaction processes in the x-ray energy region are shown in figure 1. The term cross-section is used as a measure of probability of the occurrence of a particular interaction process.

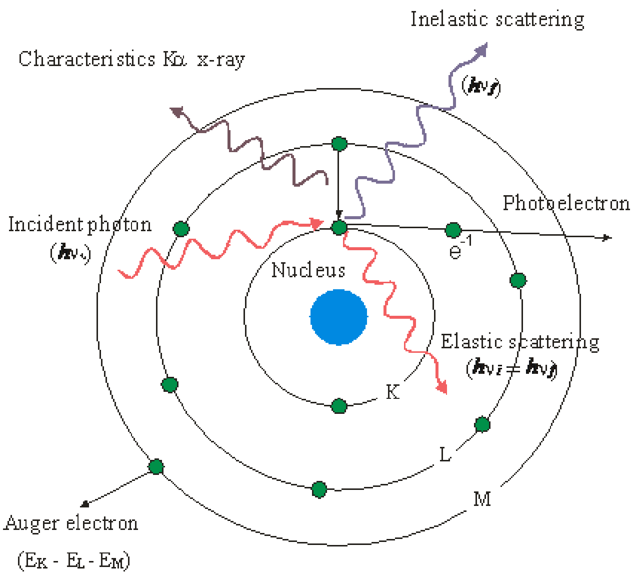

Figure 1: Basic photon-atom interaction processes in the x-ray energy region.

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The elastic scattering of photons from atom involves no transfer of energy and there exist a phase relationship between the incident and scattered photons. An isolated atom itself is a composite system of nucleus and bound electrons. The scattering of photons from bound electrons is known as Rayleigh scattering. In the x-ray energy region (< 100 keV), the scattering the scattering from the nucleus is very small and Rayleigh scattering is the only domiating elastic scattering process. In case of rayleigh scattering , the scattering contribution from the bound electrons in a given atom has definte phase relationship to each other. Therefore Rayleigh scattering is also known as coherent scattering. The internal state of the atom is same after the scattering process, only some momentum has to be transfered during the scattering process. For momoatomic gases, incdent photon of energy 10 keV transfer large momentum and scattering is no more coherent. But in case of solid, the recoil momentum is transferred to the whole crystal andscattering from the different atoms in crystal will be coherent. The two basic theoretical approaches to calculate the Rayleigh scattering amplitude and scattering cross-sections are form factor (FF) approximation and state of art S-matrix approach.

Form-factor formalism

The Thomson differential scattering cross-section for scattering of unpolarized photons by a classical free electron is given by

$$\frac{d\ {}_{T}}{d\Omega} = \frac{1}{2} r_o^2 \left(1 + \cos^2\theta\right) \quad (1)$$

Here θ is the scattering angle and r_o is the classical radius of the free electron.

The atomic form factor for a spherical symmetric atom containing one electron is given by

$$f(q) = 4 \int_0^\infty \rho(r) \frac{\sin(qr)}{qr} r^2 dr \quad (2)$$

where ρ(r) is the electron density at distance r from the centre of the atom and $\hbar q = 2(h\nu_i/c)\sin(\theta/2)$ is the momentum transfer to the atom as the photon is scattered. The scattering cross-section in the form factor formulation is obtained from the Thomson formula as

$$\left(\frac{d}{d\Omega}\right)_{el} = \left(\frac{d}{d\Omega}\right)_{T} |f(q)|^2 \quad (3)$$

The form factor approximation gives generally good predictions for the total cross-sections for photon energies above the K-shell threshold. An improved version of Form factor (FF) includes electron binding energy corrections is commonly known as the modified form factor g(q) [5]. The modified form factor for a given electron is given by

$$g(q) = 4 \int \rho(r) \frac{\sin(qr)}{qr} \frac{mc^2}{E_i - V(r)} r^2 dr \quad (4)$$

where E_i is the total energy of the ith electron, V(r) is the atomic potential and ρ(r) is the charge distribution associated with the i^{th} electron. When non-relativistic and relativistic individual electron and total atom wavefunctions are used to derive the charge density, the resulting form factor is called non-relativistic (NF) [6] and relativistic (RF) [7] form factor, respectively. It has been found that of all form factors, modified form factor (MFF) is the best, while non-relativistic form factor (NFF) is found to be better than the relativistic form factor (RFF). In order to make the form factor valid at lower energies corrections known as the 'anomalous scattering factor' have been used. Cromer and Libermann [8] computed the anomalous scattering factor (non-relativistic) f' and f'' and tabulated them for all elements Z=3-98 I the photon energy range 1 to 70 keV. Henke *et al.* [9] also tabulated the anomalous scattering factor for all elements Z=1-92 and for photon energies 0.05 to 30 keV. Corrected form factor will be then $f(q,z) = f_o(q,z) + f' + if''$. It has been revealed initially from the S-matrix values energy limits $f'(\infty)$ used by Cromer and Libermann and by Henke is not correct. The correct values have been tabulated for all neutral atoms by Kissel and Pratt [10]. At large angle of scattering, the correction term improves the scattering cross-section by about 40% and it has been demonstrated that the use of correct high energy limit removes the discrepancy between values [11].

S-matrix approach

S-matrix approach is the best possible theoretical method to calculate the Rayleigh scattering cross-sections. The S-matrix is an operator that connects the final scattered state of a time dependent system with an initial state. In Rayleigh scattering, the matrix element $S_{ij} = < f|S|i >$ represents the amplitude of a specific stationary state $|j\rangle$ that evolved through scattering from the initial state $|i\rangle$. In this approach, the interaction of electrons and positrons with atomic field is included in the unperturbed Hamiltonian of the Feynman-Dyson formulation of quantum electrodynamics, while the interaction with radiation filed is treated as perturbation. The Feynman diagram for the absorption first, where the incident photon of energy $h\nu_i$ is first absorbed by the initial state of the electron at time t_1 and emission first in which the final photon of energy $h\nu_i$ is emitted at time t_1 is shown in figures.2(a) and 2(b). Tabulated values of Rayleigh scattering cross-sections [12] are available for the almost all the elements at seven selected photon energies of experimentalist choice in 65 angular set-ups in the energy range $0 \leq \theta \leq 180^o$.

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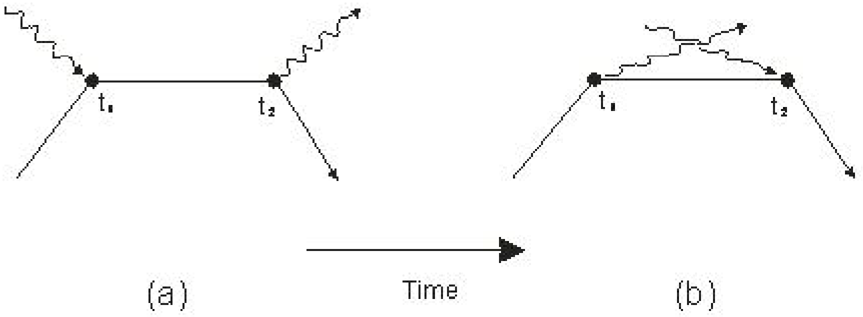

Figure 2: Feynman diagram for the Rayleigh scattering amplitude (a) absorption first (b) emission first contribution

The present study focuses on the measurements of the Rayleigh scattering cross-sections in the elementscovering the atomic region $1 \leq Z \leq 99$ at 141° for the 40keV photons. The results are given in the table1. The results are better presented in figure 3.

Table 1: Rayleigh Scattering Cross-sections for elements with 1 Z 99 at 40 keV at an angle of 141

Atomic number (z)	SM value (milli barn)	MFASF value (milli barn)	MF value (milli barn)
1	5.544E-07	0.0003651	0.0003641
2	0.0002747	0.1130783	0.1127269
3	0.0076357	2	2
4	0.069775	9	9
5	0.330606	23	23
6	1	43	42
7	3	64	63
8	5	84	82
9	9	101	98
10	15	119	113
11	21	138	130
12	29	163	150
13	38	197	180
14	61	246	230
15	55	313	279
16	80	404	357
17	73	522	458
18	82	667	583
19	91	837	728
20	123	1027	890

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21	113	1220	1052
22	155	1415	1214
23	176	1607	1372
24	158	1787	1517
25	178	1967	1662
26	552	2131	1793
27	626	2285	1917
28	493	2430	2034
29	412	2566	2149
30	472	2695	2264
31	494	2822	2383
32	613	2941	2510
33	691	3054	2651
34	774	3164	2811
35	1649	3260	2995
36	1302	3312	3210
37	1038	3331	3460
38	1129	3233	3750
39	899	2704	4080
40	1754	1969	4454
41	1375	3027	4871
42	1448	3786	5331
43	1188	4489	5833
44	1577	5187	6371
45	1632	5898	6942
46	1678	6626	7540
47	1717	7373	8157
48	1748	8130	8783
49	1771	8894	9412
50	1784	9655	10033
51	1771	10407	10641
52	1729	11144	11228
53	1525	11865	11793
54	1423	12566	12334
55	952	13250	12850

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56	770	13917	13346
57	1232	14575	13832
58	1372	15195	14286
59	1467	15821	14741
60	1796	16444	15190
61	2232	17065	15636
62	2232	17686	16084
63	2458	18313	16540
64	2699	18957	17014
65	1829	19575	17472
66	3185	20221	17855
67	3444	20877	18464
68	2430	21547	18988
69	3986	22227	19535
70	4267	22918	20108
71	4565	23652	20741
72	3284	24394	21419
73	5180	25201	22146
74	5494	25968	22926
75	5814	26783	23763
76	4254	27592	24661
77	6456	28388	25618
78	6778	29147	26637
79	7097	29836	27717
80	7411	30475	28863
81	7718	31029	30065
82	8022	31418	31317
83	8317	31451	32613
84	6404	30792	33946
85	6676	26872	35307
86	6942	24429	36693
87	7209	25834	38085
88	7466	28337	39489
89	7727	29771	40908
90	10175	30464	42335
91	8218	30250	43855
92	10639	27948	45360
93	8690	20042	46886
94	8914	27551	48466
95	11289	31567	50015
96	9339	34714	51524
97	11679	37520	53128
98	9728	40031	54689
99	12047	42410	56247

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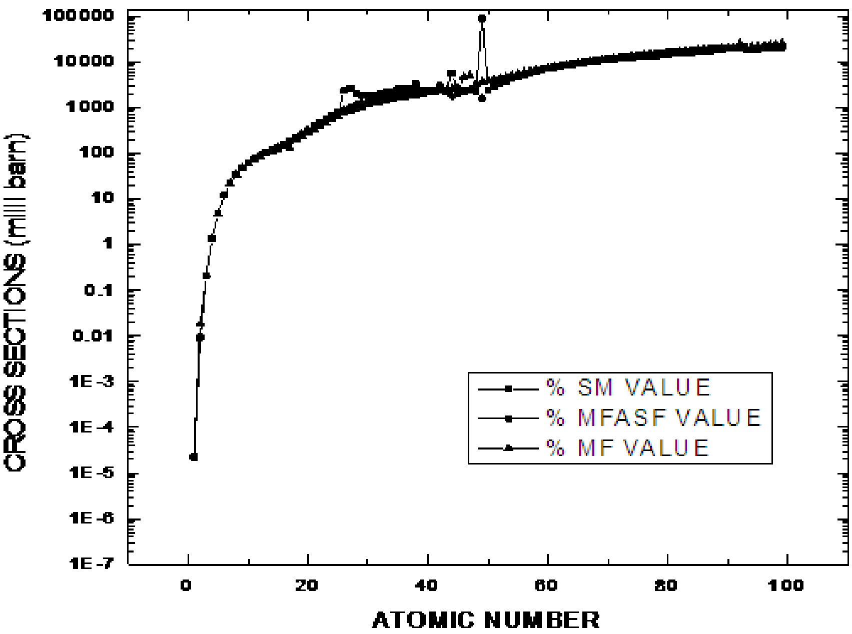

Figure3: Rayleigh Scattering Cross-sections for elements with 1 Z 99 at 40 keV at an angle of 141

The theoretical Rayleigh scattering cross-sections in different elementsexhibit almost linear angular dependence around 141. The average theoretical cross-section, evaluated by taking the weighted average of cross-sections at various scattering angles in proportion to the number of scattered photons agrees within 1% with the theoretical value at 141. The MF, MFASF and S-matrix Rayleigh scattering cross-sections are taken from Ref. [12]. Systematically computed second order S-matrix values are available for photon energies less than 300 times the *K*-shell binding energy on a 52-point grid of energies of experimental interest in the range 0.0543-2754.1 keV for the elements with $1 \leq Z \leq 103$ [12]. The MF, MFASF and S-matrix cross-sections for all the photon energies in all the elements under investigation have been interpolated from the values available assuming the same energy dependence as that for the MFASF values.

Conclusions

In the present results, it is observed that the Rayleigh scattering cross-sections at such low energy are significant enough even for the low-Z elements. The scattering information available in the energy dispersive X-ray fluorescence (EDXRF) measurements is useful for analytical applications related to the low-Z elements and hydrogen in the hydrogen-rich samples.

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