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Estimation of effective atomic number in the Rayleigh to Compton scattering ratio using different methods

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ABSTRACT

The Rayleigh to Compton scattering ratio (R/C) is a very convenient parameter, which can be utilized in material analysis and estimating effective atomic number (Z_{eff}). In the case for a relatively low scattering angle, for which the energy of the Compton scattered photons is not very much different from that of incident photons, the corrections due to self-absorption for Rayleigh and Compton scattering will be roughly equal. Therefore, it enables a result to be obtained which is almost independent of X-ray attenuation inside the sample and it will depend only on the material under investigation. The most frequently used method for calculation of Z_{eff} available in literature is plotting R/C of elements as a function of atomic number and constituting the best fit curve. From this fit curve, the respective Z_{eff} can be determined using R/C of the material. In the present study, we report Z_{eff} of different materials using different methods such as interpolation and direct methods as possible alternatives to the most common fitting method. The results were compared with the experiments wherever possible. The agreement between interpolation method and the fitting method was found to be very satisfactory as relative changes (%) were always less than 9% while the direct method results with somehow significantly higher values of Z_{eff} when compared to the other methods.

1. Introduction

The Rayleigh to Compton scattering ratio has found to be a useful parameter in material analysis studies such as composition variations in alloys [1], mineral concentration estimation in trabecular bone [2], evaluation of the fat content in liver [3]. At relatively small scattering angle for which the energy of the Compton scattered photons is not very much different from that of Rayleigh scattered photons, the Rayleigh to Compton scattering ratio enables material to be characterized only by its atomic number, independent of the material density or of the attenuation inside the tested object [4]. If the material under study is a compound, mixture or a composite material, then this ratio is associated with a useful parameter called the "effective atomic number" Z_{eff}.

The most frequently used method for calculation of Z_{eff} available in literature is plotting R/C of elements as a function of atomic number and constituting the best fit curve. From this fit curve, the respective Z_{eff} can be determined using R/C of the material [5–9]. Duvauchelle et al. [4] have successfully compared different methods to calculate Z_{eff} and concluded that the method using R/C of the material should be most reliable as it takes into account both the photon energy (E_0) and the scattering angle (θ) [4]. A practical method was developed by İçelli [10] to calculate Z_{eff} using experimental linear differential scattering coefficients [10]. More recently, Vinaykumar and Umesh [11] have developed a power law relation based on the theoretical angle integrated small angle scattering cross-sections for calculation of Z_{eff} for some sugars and aminoacids [11]. However, Z_{eff} data for scattering of photons using interpolation and direct methods have not been reported yet. This prompted us to carry out this work. In the present study, we report Z_{eff} of 24 materials consisting of organic, inorganic compounds, alloys, polymers etc. using different methods such as interpolation and direct methods and then compared to the most common fitting method. The results were compared with the experiments wherever possible.

2. Computational method

2.1. Fitting method

At a given scattering angle of theta and energy, the number of Rayleigh (N_R) and Compton (N_C) photons and the R/C can be

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theoretically calculated using the following equation [7];

$$R/C(q,Z)=\frac{N_R}{N_C}=\frac{N_0.\eta_{at}.\left[\frac{d\sigma}{d\Omega}\right]_R.\Delta\Omega.V.\epsilon.A_R}{N_0.\eta_{at}.\left[\frac{d\sigma}{d\Omega}\right]_C.\Delta\Omega.V.\epsilon.A_C} \quad (1)$$

where, N_0 is the initial fluence, η_{at} is the number of atoms per volume of the sample, $\Delta\Omega$ is the solid angle subtended by the detector, ε is the detector efficiency, A_R and A_C are the self-attenuation factors for each scattering processes, $\left[d\sigma/d\Omega\right]_R$ and $\left[d\sigma/d\Omega\right]_C$ are differential cross-sections, respectively [7]. If N_R and N_C are measured in the same geometric conditions of irradiation and detection, then N_0, η_{at}, $\Delta\Omega$, V and ε become constant values. And Eq. (1) can be rewritten considering the Thomson, $\left[d\sigma/d\Omega\right]_{Th}$, and the Klein–Nishina, $\left[d\sigma/d\Omega\right]_{KN}$, differential cross-sections, the atomic form factor, F, and the incoherent scattering function, S, which are dependent on the momentum transfer ($q=\sin(\frac{\theta}{2})/\lambda$), as following [7];

$$R/C(q,Z)=\frac{[d\sigma/d\Omega]_R.A_R}{[d\sigma/d\Omega]_C.A_C}=\frac{\left[\left(\frac{d\sigma}{d\Omega}\right)_{Th}.F^2(q,Z)\right].A_R}{\left[\left(\frac{d\sigma}{d\Omega}\right)_{KN}.S(q,Z)\right].A_C} \quad (2)$$

For a fixed experimental condition, when a small energy shift occurs between Rayleigh and Compton scattering and thus ratio of A_R and A_C becomes 1 ($A_R/A_C\approx 1$) [4,6,7,10]. In this case, Eq. (2) can be reduced. If molecular weight and elemental composition fractions of the given compound or composite material, R/C is calculated by weighting the atomic percentages α_j^{at} of elements as following equation [6];

$$R/C=\left[\frac{(d\sigma/d\Omega)_{Th}}{(d\sigma/d\Omega)_{KN}}\right].\left[\frac{\sum_{j=1}^{n}\alpha_j^{at}.[F(q,Z_j)]^2}{\sum_{j=1}^{n}\alpha_j^{at}.S(q,Z_j)}\right] \quad (3)$$

where α_j^{at} is defined by weight percentage w_j and atomic mass A_j of the *jth* element as [6]:

$$\alpha_j^{at}=\frac{(w_j/A_j)}{\sum_{j=1}^{n}(w_j/A_j)} \quad (4)$$

For a given energy and scattering angle, R/C is a function of only the Z of the sample [4,6,7,10]. Therefore, theoretical values of R/C can be calculated via Eq. (3) and when plotted in function of Z for pure elements, then the Z_{eff} of the material can be deduced using the best fit equation. The R/C values were plotted considering the F and S values and their corresponding q moments from Hubbell et al. [12,13]. A typical example has been shown for the best fit curve at momentum transfer $q=2.28$ Å^{-1} for elements $4\le Z\le 17$ (Fig. 1(a)). The equation satisfying the best fit condition is

$$y=0.061-0.032x+0.005x^2-6.23.10^{-5}x^3$$
$$-1.38.10^{-5}x^4+4.86.10^{-7}x^5$$

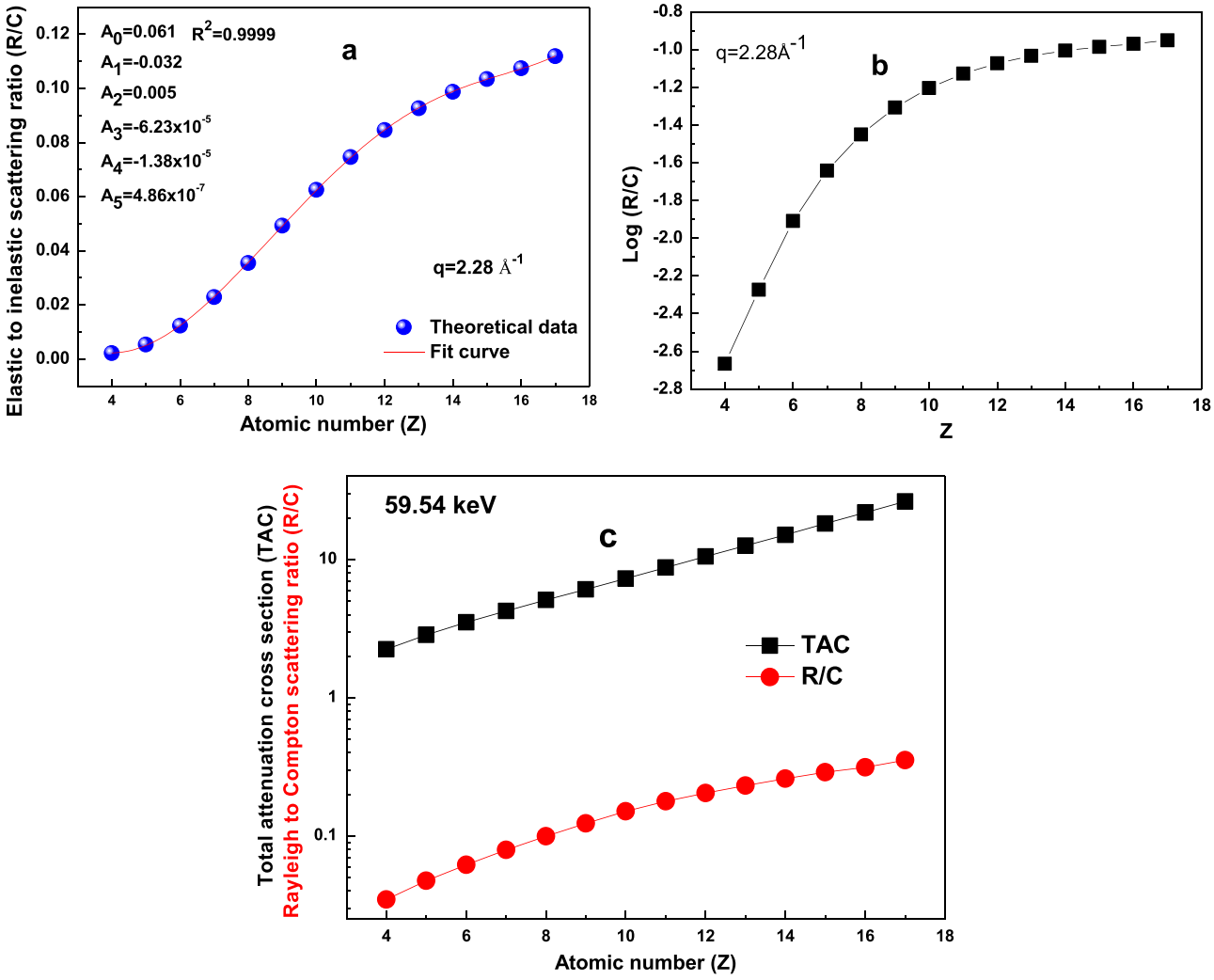

Fig. 1. (a and b) Variation of R/C with Z of elements at $q=2.28$ Å^{-1}. (c) Total attenuation cross section and Rayleigh to Compton scattering ratio vs. atomic number.