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Study of photon interaction parameters in some newly developed superconductors

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The total mass attenuation coefficients, effective atomic numbers and electron densities in some recent and newly discovered non-centrosymmetric (NCS) and iron-based superconductors have been calculated for total and partial photon interactions in the wide energy range 1 keV-100 GeV. The values of these parameters have been found to change with composition of the superconductor and change in energy whereas their behaviour has been found to be identical with all energies. The variations of these parameters with energy are shown graphically for all photon interactions. The reported data could be useful for comparing these superconductors in terms of radiation sensitivity and radiation detection. The results of this work can stimulate research for other materials and different types of newly superconductors.

Keywords: Superconductors, Mass attenuation coefficients, Effective atomic numbers, Effective electron numbers

1 Introduction

Superconductors are very much attractive for future materials due to its potential applications in the field of electronics, energy efficient savers, magnetic resonance imaging scanners, nuclear power stations, satellites etc. Some of these devices made of superconducting materials which may be exposed to wide energy range of photons as in the case of nuclear reactors and satellites. So, it is important to study all possible interactions between photons and atomic nuclei in the superconductor materials. The mass attenuation coefficients, effective atomic numbers, effective electron densities, are basic quantities required to study all possible photon interactions, they depend on the incident photon energy and the nature of the absorbing material. In literature, a variety of work relevant to estimate mass attenuation coefficients, effective atomic numbers for different compounds or mixtures have been published by several researchers in different categories such as chemical compounds, alloys, glass, minerals and biological materials[1-10].

There are very few reports which measured the mass attenuation coefficients, effective atomic numbers and electron densities in superconducting materials[11,12] such as MgB_2 and YBaCuO. The non-centrosymmetric (NCS) superconductors which lack inversion symmetry in the respective crystal structures are one of the emerging topics in the condensed matter physics. This kind of superconductors cannot be strictly classified as spin-singlet or spin-triplet due to parity mixing. Frigeri *et al*[13]. reported that the lack of inversion symmetry reduces the effect of paramagnetic limiting for spin-singlet pairing in MnSi and $CePt_3Si$. A variety of novel superconducting properties can be predicted due to its unconventional characteristics. Many of unusual properties of NCS superconductors are still unknown as only few superconductors of these kinds are available currently and only two parameters pressure and temperature play an important role in the superconductivity creation[14,15]. NCS superconductors $CaMSi_3$ (M = Ir, Pt) were synthesized from the high purity raw materials of CaSi, Ir, Pt and Si by arc melting[16] while synthesis process of iron based superconductors $Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$ and $K_{0.8}Fe_{1.7}Se_2$ was reported elsewhere[17,18].

As NCS and iron based superconductors are expected to have good promise as future materials, it is very important to know all the unknown properties of these materials. Experimental study is also very important along with theoretical calculation. The objective of this study is to calculate mass attenuation coefficients, effective atomic numbers and electron densities of NCS superconductors $CaMSi_3$ (M = Ir, Pt) and iron-based superconductors $Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$ and

$K_{0.8}Fe_{1.7}Se_2$in the energy range 1 keV-100 GeV which may provide valuable insight for future experimental studies.

2 Method of Computation and Theoretical Basis

For materials composed of various elements, it is assumed that the contribution of each element of the material to total photon attenuation is additive[1,2]. In such cases, the total mass attenuation coefficient (μ/ρ) of any material with density ρ is related $(\mu/\rho)_i$ values of constituents by the mixture rule, $\Sigma_i c_i\ (\mu/\rho)_i$ where c_i is the proportion by weight of the i^{th} constituent element. The total molecular cross-section σ_m can be calculated from the knowledge of mass attenuation coefficient by using the following relation:

$$\sigma_m = \left(\frac{\mu}{\rho}\right)\frac{M}{N_A} \qquad \text{...(1)}$$

where $M=\Sigma_i n_i A_i$ is the molecular weight of the compound or mixture, N_A is the Avogadro number, A_i is the atomic weight of the i^{th} element and n_i is the number of formula units in the molecule. The average atomic cross-section σ_a can be obtained by dividing the molecular cross-section by the total number of formula units as follows:

$$\sigma_a = \sigma_m \frac{1}{\Sigma_i n_i} \qquad \text{...(2)}$$

Similarly, the average electronic cross-section σ_e is given by:

$$\sigma_e = \frac{1}{N_A}\Sigma_i \frac{f_i A_i}{z_i}\left(\frac{\mu}{\rho}\right)_i \qquad \text{...(3)}$$

where $f_i=n_i/\Sigma_j n_j$ and Z_i are fractional abundance and atomic number of constituent element, respectively. n_j is the number of atoms of the constituent element, $\Sigma_j n_j=n$ is the total number of atoms present in the molecular formula. The effective atomic number, Z_{eff} can now be defined through the relation:

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \qquad \text{...(4)}$$

The effective electron number or electron density N_{el} (number of electrons per unit mass) of the material can be derived from:

$$N_{el} = \frac{(\mu/\sigma)}{\sigma_e} = \left(\frac{Z_{eff}}{M}\right)N_A \Sigma_i n_i \qquad \text{...(5)}$$

3 Results and Discussion

Calculations of the mass attenuation coefficients (μ/ρ) of newly developed superconductors were carried out by the WinXCOM program[19]. The software can generate cross-sections and attenuation coefficients for elements, compounds or mixtures in the energy range between 1 keV and 100 GeV. High temperature iron-based superconductors $Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$ and $K_{0.8}Fe_{1.7}Se_2$were chosen in the calculation in addition to NCS superconductors $CaMSi_3$ (M = Ir, Pt). Calculations of (μ/ρ), Z_{eff} and $N_{el}$for Ca*M*Si_3 (*M* = Ir, Pt) are very close and this may return to similarity in the chemical compositions of the NCS superconductors.

The result of total mass attenuation coefficients of the studied superconductors is shown in Fig. 1. There are three energy ranges, where photoelectric absorption, Compton scattering and pair production, respectively, are the dominating attenuation processes (Fig. 1). In the low energy region, mass attenuation coefficients have the highest values, where the photoelectric absorption is significant[4,5] and its cross-section is proportional to Z. In the intermediate energy region, where the Compton scattering is significant there is a linear Z-dependence of incoherent scattering and the mass attenuation coefficient is found to be constant. In the high energy region, mass attenuation coefficients increase again,

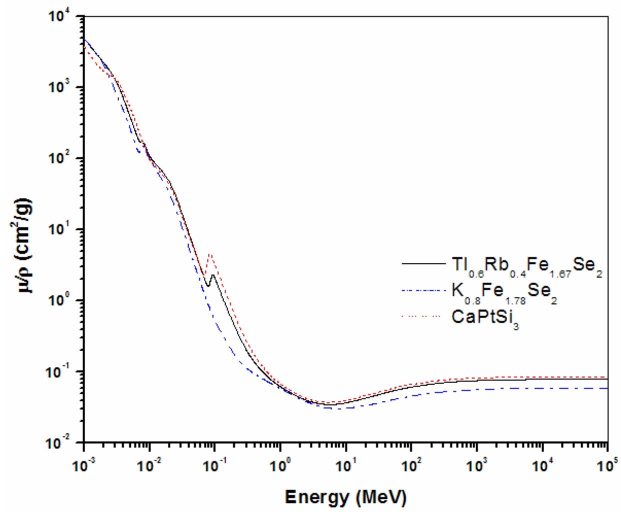

Fig. 1 — Variation of photon mass attenuation coefficient of some NCS and high temperature superconductors with photon energy for total photon interaction

where the pair production is significant and mass attenuation is proportional to Z^2. This fact has been verified experimentally by Medhat[6] who measured (μ/ρ) of some gemstones that used irradiation for improving their colours. The present theoretical results are similar to the observations of Medhat[6] for calculating (μ/ρ) for different types of solid state nuclear track detectors and the observations of Manhora and Hanagodimath[10] for calculating (μ/ρ) for different types of essential amino acids.

For total photon interaction process, the variations of Z_{eff} and N_{el} with photon energy are shown in Figs 2 and 3. Although the dependence on the photon energy is dominant in interaction with low energies, it can be negligible at high energies. From Fig. 2, it is clear the value of Z_{eff} increases in the investigated superconductors, decreases up to 10 -100 MeV and then remains almost constant. It is observed also that the variation in Z_{eff} depends upon relative proportion and the range of atomic numbers of the elements of which superconductor is composed. The iron-based superconductor ($Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$) has the largest Z_{eff} with showing jump in low energy region due to the large range of Z than any other superconductors. The effective atomic numbers of almost all superconductors were found to lie within range 25.08-29.06 except in case of $Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$ for which value is 35.93-62.56 due to the presence of some high-Z constituent elements as presented in Table 1.

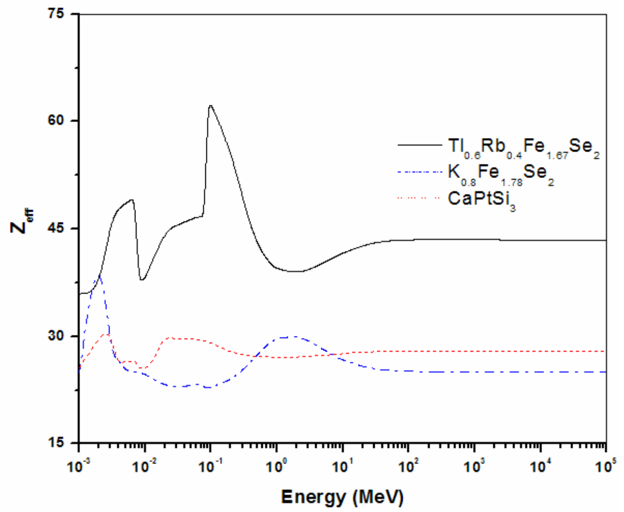

Fig. 2 — Variation of Z_{eff} with photon energy of the selected NCS and high temperature superconductors for total photon interaction

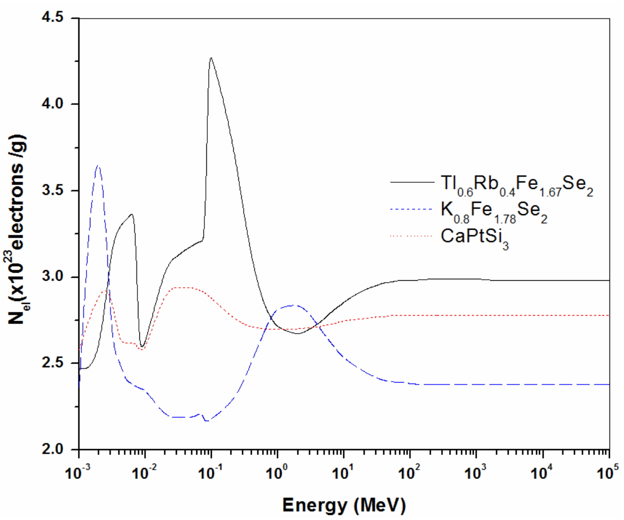

Fig. 3 — Variation of N_{el} with photon energy of the selected NCS and high temperature superconductors for total photon interaction (with coherent)

The behaviour of Z_{eff} for total interaction reflects the importance of the partial photon interaction processes. At low-energy range (0.01 MeV $< E <$ 0.1 MeV), the maximum value of Z_{eff} is found. At intermediate energies (0.05 MeV $<$ E $<$ 5 MeV), where Compton scattering is the main photon interaction process, Z_{eff} is approximately equal to the arithmetic mean of the atomic number calculated from the chemical formula of the molecule, $\langle Z \rangle = (1/n)\Sigma_i n_i Z_i$. At high energies, (E $>$ 100 MeV), Z_{eff} is again constant but smaller than in the low-energy range. This is due to the dominance of pair production and the cross-section has Z^2 dependence. It is seen from Table 1, there is a good agreement between Z_{eff} at 10 MeV and the mean atomic number, ⟨Z⟩, derived from the chemical formula of the molecule, where Compton scattering is the main photon interaction process.

The variations of N_{el} with photon energy for total interaction processes (Fig. 3) are similar to that of Z_{eff}

Table 1 — Effective atomic numbers (Z_{eff}) of investigated superconductors with their average atomic number <Z> at different energy (MeV) for total photon interaction

Energy (MeV)	NCS superconductors		Iron-based superconductors	
	$CaPtSi_3$	$CaIrSi_3$	$Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$	$K_{0.8}Fe_{1.7}Se_2$
10^{-3}	25.12	25.62	35.93	24.92
10^{-2}	24.97	25.61	37.98	24.72
10^{-1}	23.24	29.06	62.56	22.92
10^{0}	28.17	27.09	39.42	29.71
10^{1}	26.98	27.60	37.62	28.70
10^{2}	25.43	27.97	43.48	25.13
10^{3}	25.38	27.96	43.49	25.08
10^{4}	25.39	27.95	43.47	25.10
10^{5}	25.39	27.95	43.47	25.09
<Z>	28.00	27.80	37.43	28.27

and can be explained on the similar manner. It can be seen that the value of N_{el} is found to lie within range 2.19-2.84×10^{23}electron.g^{-1} except in case of $Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$ for which value is 2.47-4.29×10^{23} electron.g^{-1} as presented in Table 2. This expected behaviour for electron densities can be explained on the similar basis as for Z_{eff}.

For the photoelectric absorption process, the variations in Z_{eff} and N_{el} with photon energy are shown in Figs 4 and 5, respectively. It is clear that the most significant variations in Z_{eff} and N_{el} are due to chemical composition variations of the samples. Below 10 keV, the changes are more pronounced in superconductors containing high-Z elements. The behaviour for all the materials is similar after 10 MeV. The variation of calculated coherent to incoherent scattering ratio with all materials is almost constant with photon energy as shown in Fig. 6. For the pair production , the variations in Z_{eff} and N_{el} with photon energy are shown in Figs 7 and 8, respectively. There are slightly decrease with increase in photon energy from 1 to 200 MeV and then it is almost independent of energy. For total photon interaction process, the variations of Z_{eff} and N_{el} calculated atomic and electronic cross- section of the investigated superconductors is shown in Figs 9 and 10. Both the values of σ_a and σ_e are decreased sharply up to 10 MeV and then are increased slightly with photon energy.

Table 2 — Effective electron numbers (N_e × 10^{23} electrons/g) of investigated superconductors at different energy (MeV) for total photon interaction

Energy (MeV)	NCS superconductors		Iron-based superconductors	
	$CaPtSi_3$	$CaIrSi_3$	$Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$	$K_{0.8}Fe_{1.7}Se_2$
10^{-3}	2.36	2.37	2.47	2.58
10^{-2}	2.34	2.35	2.61	2.58
10^{-1}	2.19	2.17	4.29	2.88
10^{0}	2.81	2.84	2.71	2.69
10^{1}	2.54	2.53	2.86	2.74
10^{2}	2.39	2.38	2.98	2.78
10^{3}	2.39	2.38	2.99	2.78
10^{4}	2.39	2.38	2.98	2.78
10^{5}	2.39	2.38	2.98	2.78

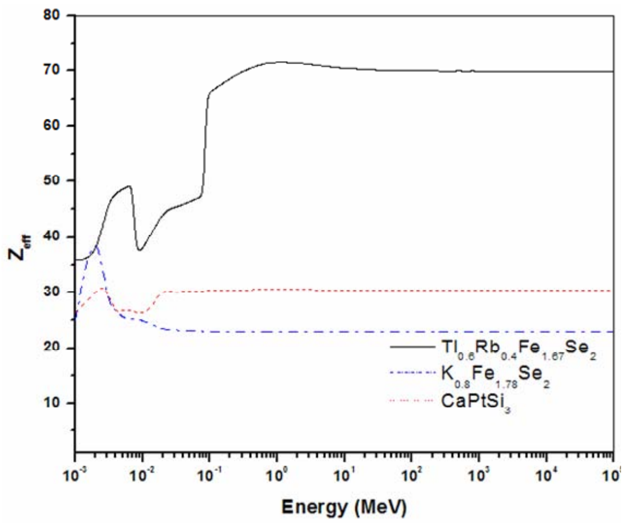

Fig. 4 — Variation of Z_{eff} of the selected NCS and high temperature superconductors with photon energy for photoelectric absorption

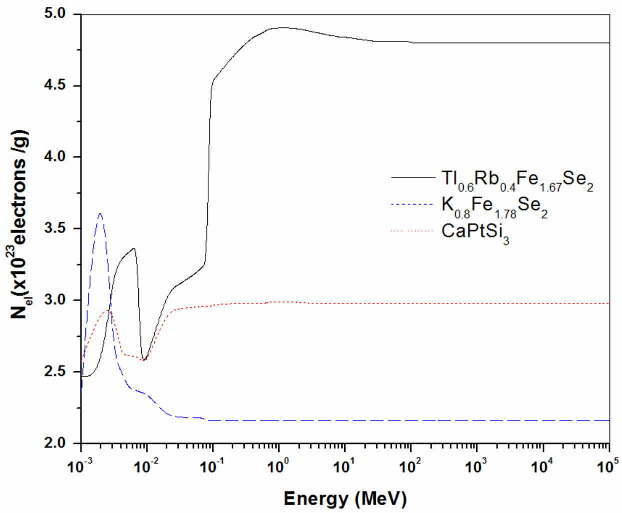

Fig. 5 — Variation of N_{el} of the selected NCS and high temperature superconductors with photon energy for photoelectric absorption

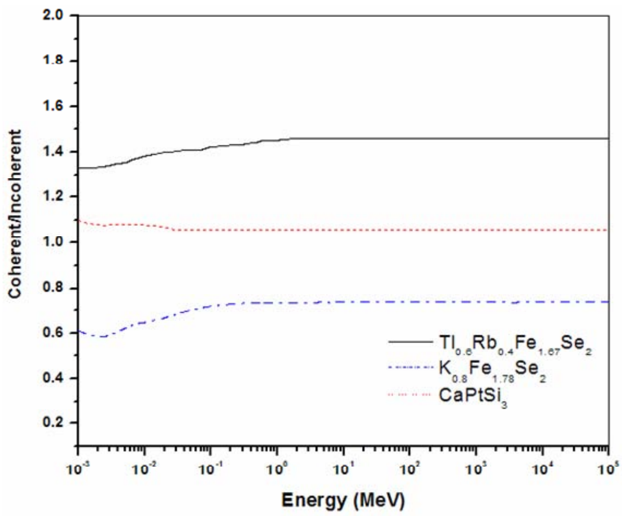

Fig. 6 — Variation of coherent to incoherent ratio for Z_{eff} of materials as a function of photon energy

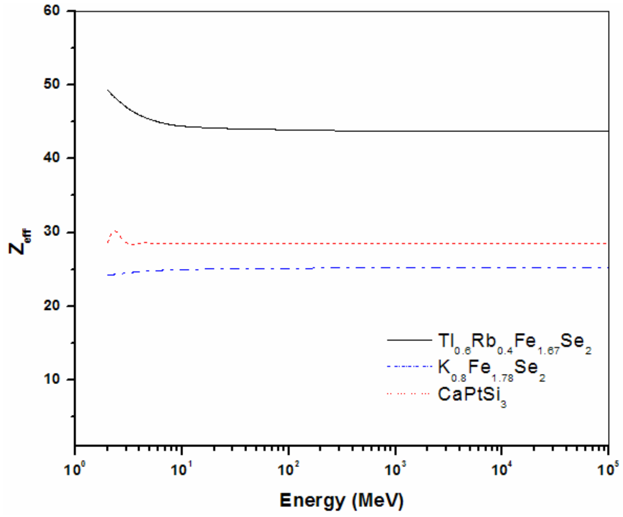

Fig. 7 — Variation of Z_{eff} with photon energy for pair production

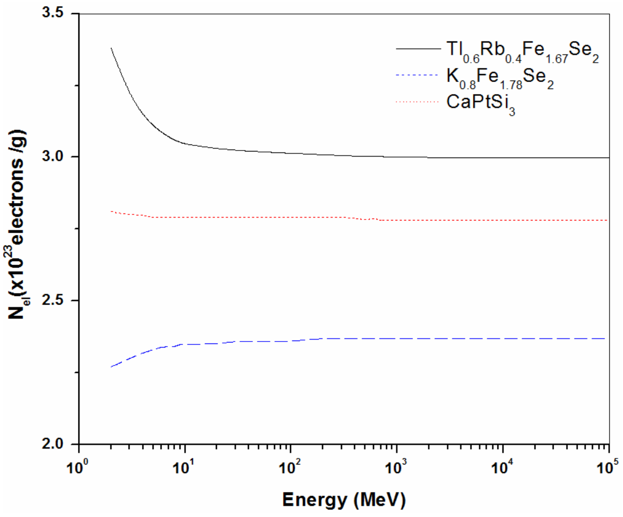

Fig. 8 — Variation of N_{el} with photon energy for pair production in nuclear field

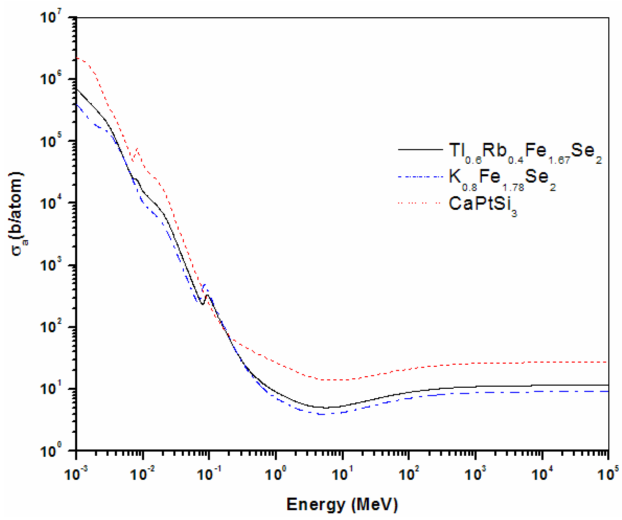

Fig. 9 — Variation of atomic cross sections σ_a (*b*/atom) with photon energy

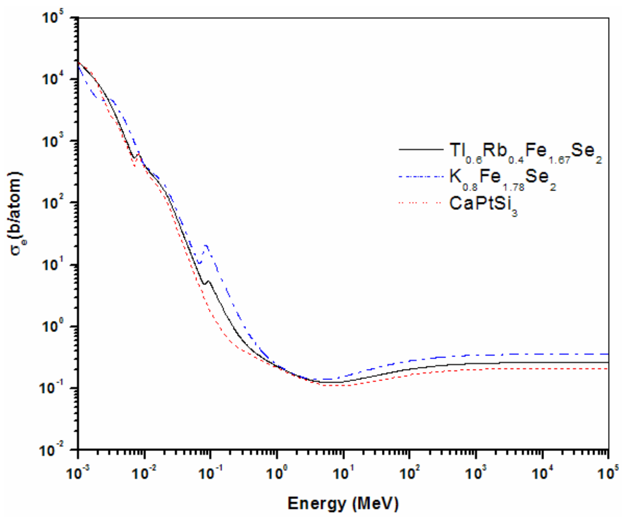

Fig. 10 — Variation of electronic cross - sections σ_e (b/atom) with photon energy

4 Conclusions

The present study has been undertaken to get some information on the mass attenuation coefficients and related parameters, effective atomic numbers and electron densities for some newly discovered non-centrosymmetric and iron-based superconductors. The obtained values of (μ/ρ) are varied with photon energy regions (photoelectric absorption, Compton scattering and pair production). The electron density and effective atomic number are closely related and they are qualitative energy dependence. The dependence on the atomic number indicates that superconductor having high Z_{eff} absorbs powerfully incoming photons. The minimum value is found in the intermediate region, where Compton scattering is dominating and Z_{eff} is approximately equal to the mean atomic number of the superconductor. The maximum value of Z_{eff} is found in the low energy range, where photoelectric absorption is dominating.

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