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\textsuperscript{1-10}.

There are very few reports which measured the mass attenuation coefficients, effective atomic numbers and electron densities in superconducting materials\textsuperscript{11,12} such as MgB\textsubscript{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\textsuperscript{13} reported that the lack of inversion symmetry reduces the effect of paramagnetic limiting for spin-singlet pairing in MnSi and CePt\textsubscript{3}Si. 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\textsuperscript{14,15}. NCS superconductors CaMS\textsubscript{1} (\textit{M} = Ir, Pt) were synthesized from the high purity raw materials of CaSi, Ir, Pt and Si by arc melting\textsuperscript{16} while synthesis process of iron based superconductors Tl\textsubscript{0.8}Rb\textsubscript{0.2}Fe\textsubscript{1.67}Se\textsubscript{2} and K\textsubscript{0.3}Fe\textsubscript{1.7}Se\textsubscript{2} was reported elsewhere\textsuperscript{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 CaMS\textsubscript{1} (\textit{M} = Ir, Pt) and iron-based superconductors Tl\textsubscript{0.8}Rb\textsubscript{0.2}Fe\textsubscript{1.67}Se\textsubscript{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. In such cases, the total mass attenuation coefficient ($\mu/\rho$) of any material with density $\rho$ is related to its constituent by the mixture rule, $\Sigma c_i (\mu/\rho)$, where $c_i$ is the proportion by weight of the $i^{th}$ constituent element. The total molecular cross-section $\sigma_m$ can be calculated from the knowledge of mass attenuation coefficient by using the following relation:

$$\sigma_m = \left( \frac{\mu}{\rho} \right) \frac{M}{N_A}$$

where $M=\Sigma n_i A_i$ 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 $\sigma_a$ can be obtained by dividing the molecular cross-section by the total number of formula units as follows:

$$\sigma_a = \frac{1}{\Sigma n_i} \sigma_m$$

Similarly, the average electronic cross-section $\sigma_e$ is given by:

$$\sigma_e = \left( \frac{\mu}{\rho} \right) \frac{1}{N_A} \sum_i f_i A_i \left( \frac{\mu}{\rho} \right) z_i$$

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

$$Z_{eff} = \frac{\sigma_a}{\sigma_e}$$

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

$$N_{el} = \frac{(\mu/\sigma)}{\sigma_e} = \left( \frac{Z_{eff}}{M} \right) N_A \sum n_i$$

3 Results and Discussion

Calculations of the mass attenuation coefficients ($\mu/\rho$) of newly developed superconductors were carried out by the WinXCOM program. 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 CaMnS$_3$ ($M=\text{Ir}, \text{Pt}$). Calculations of ($\mu/\rho$), $Z_{eff}$ and $N_{el}$ for CaMnS$_3$ ($M=\text{Ir}, \text{Pt}$) 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 regions, 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 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,
where the pair production is significant and mass attenuation is proportional to $Z^2$. This fact has been verified experimentally by Medhat\textsuperscript{6} who measured $(\mu/\rho)$ of some gemstones that used irradiation for improving their colours. The present theoretical results are similar to the observations of Medhat\textsuperscript{6} for calculating $(\mu/\rho)$ for different types of solid state nuclear track detectors and the observations of Manhora and Hanagodimath\textsuperscript{10} for calculating $(\mu/\rho)$ for different types of essential amino acids.

For total photon interaction process, the variations of $Z_{\text{eff}}$ and $N_{\text{el}}$ 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 $Z_{\text{eff}}$ increases in the investigated superconductors, decreases up to 10 -100 MeV and then remains almost constant. It is observed also that the variation in $Z_{\text{eff}}$ depends upon relative proportion and the range of atomic numbers of the elements of which superconductor is composed. The iron-based superconductor ($\text{Tl}_{0.6}\text{Rb}_{0.4}\text{Fe}_{1.67}\text{Se}_2$) has the largest $Z_{\text{eff}}$ 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 $\text{Tl}_{0.6}\text{Rb}_{0.4}\text{Fe}_{1.67}\text{Se}_2$ for which value is 35.93-62.56 due to the presence of some high-Z constituent elements as presented in Table 1.

The behaviour of $Z_{\text{eff}}$ 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 $Z_{\text{eff}}$ is found. At intermediate energies (0.05 MeV $< E < 5$ MeV), where Compton scattering is the main photon interaction process, $Z_{\text{eff}}$ is approximately equal to the arithmetic mean of the atomic number calculated from the chemical formula of the molecule, $\langle Z \rangle = (1/n)\sum n_i Z_i$. At high energies, (E $> 100$ MeV), $Z_{\text{eff}}$ 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 $Z_{\text{eff}}$ at 10 MeV and the mean atomic number, $\langle Z \rangle$, derived from the chemical formula of the molecule, where Compton scattering is the main photon interaction process.

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

### Table 1 — Effective atomic numbers ($Z_{\text{eff}}$) of investigated superconductors with their average atomic number $\langle Z \rangle$ at different energy (MeV) for total photon interaction

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>CatoSi$_3$</th>
<th>CalSi$_3$</th>
<th>Tl$<em>{0.6}$Rb$</em>{0.4}$Fe$_{1.67}$Se$_2$</th>
<th>K$<em>{0.8}$Fe$</em>{1.7}$Se$_2$</th>
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<tbody>
<tr>
<td>$10^{-1}$</td>
<td>25.12</td>
<td>25.62</td>
<td>35.93</td>
<td>24.92</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>24.97</td>
<td>25.61</td>
<td>37.98</td>
<td>24.72</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>23.24</td>
<td>29.06</td>
<td>62.56</td>
<td>22.92</td>
</tr>
<tr>
<td>$10^{0}$</td>
<td>28.17</td>
<td>27.09</td>
<td>39.42</td>
<td>29.71</td>
</tr>
<tr>
<td>$10^{1}$</td>
<td>26.98</td>
<td>27.60</td>
<td>37.62</td>
<td>28.70</td>
</tr>
<tr>
<td>$10^{2}$</td>
<td>25.43</td>
<td>27.97</td>
<td>43.48</td>
<td>25.13</td>
</tr>
<tr>
<td>$10^{3}$</td>
<td>25.38</td>
<td>27.96</td>
<td>43.49</td>
<td>25.08</td>
</tr>
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<td>$10^{4}$</td>
<td>25.39</td>
<td>27.95</td>
<td>43.47</td>
<td>25.10</td>
</tr>
<tr>
<td>$10^{5}$</td>
<td>25.39</td>
<td>27.95</td>
<td>43.47</td>
<td>25.09</td>
</tr>
<tr>
<td>$\langle Z \rangle$</td>
<td>28.00</td>
<td>27.80</td>
<td>37.43</td>
<td>28.27</td>
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</table>
and can be explained on the similar manner. It can be seen that the value of $N_{\text{el}}$ is found to lie within range $2.19-2.84 \times 10^{23}$ electron.g$^{-1}$ except in case of Tl$_{0.6}$Rb$_{0.4}$Fe$_{1.67}$Se$_2$ for which value is $2.47-4.29 \times 10^{23}$ electron.g$^{-1}$ as presented in Table 2. This expected behaviour for electron densities can be explained on the similar basis as for $Z_{\text{eff}}$.

For the photoelectric absorption process, the variations in $Z_{\text{eff}}$ and $N_{\text{el}}$ with photon energy are shown in Figs 4 and 5, respectively. It is clear that the most significant variations in $Z_{\text{eff}}$ and $N_{\text{el}}$ 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 $Z_{\text{eff}}$ and $N_{\text{el}}$ 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 $Z_{\text{eff}}$ and $N_{\text{el}}$ calculated atomic and electronic cross-section of the investigated superconductors is shown in Figs 9 and 10. Both the values of $\sigma_a$ and $\sigma_e$ are decreased sharply up to 10 MeV and then are increased slightly with photon energy.

Table 2 — Effective electron numbers ($N_{\text{el}} \times 10^{23}$ electrons/g) of investigated superconductors at different energy (MeV) for total photon interaction

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>NCS superconductors</th>
<th>Iron-based superconductors</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CaPtSi$_3$</td>
<td>CaIrSi$_3$</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>2.36</td>
<td>2.34</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>2.37</td>
<td>2.35</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>2.47</td>
<td>2.61</td>
</tr>
<tr>
<td>$10^{0}$</td>
<td>2.71</td>
<td>2.74</td>
</tr>
<tr>
<td>$10^{1}$</td>
<td>2.98</td>
<td>2.78</td>
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<tr>
<td>$10^{2}$</td>
<td>2.99</td>
<td>2.78</td>
</tr>
<tr>
<td>$10^{3}$</td>
<td>2.98</td>
<td>2.78</td>
</tr>
<tr>
<td>$10^{4}$</td>
<td>2.78</td>
<td>2.78</td>
</tr>
</tbody>
</table>

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

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

Fig. 6 — Variation of coherent to incoherent ratio for $Z_{\text{eff}}$ of materials as a function of 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 $\left(\frac{\mu}{\rho}\right)$ 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 $Z_{\text{eff}}$ absorbs powerfully incoming photons. The minimum value is found in the intermediate region, where Compton scattering is dominating and $Z_{\text{eff}}$ is approximately equal to the mean atomic number of the superconductor. The maximum value of $Z_{\text{eff}}$ is found in the low energy range, where photoelectric absorption is dominating.

References