Effective atomic numbers and electron densities for some lanthanide oxide compounds using direct method in the energy region of 1 keV - 20 MeV

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Abstract

In this paper, the effective atomic numbers (Z_{eff}) and electron densities (N_{eff}) representing interaction of gamma rays with oxides of lanthanides were studied. The effective atomic numbers for photon energy-absorption (Z_{PEA_{eff}}), photon interaction (Z_{PI_{eff}}), relative to air Z_{eff} and N_{eff} for photon energy-absorption (N_{PEA_{eff}}) and photon interaction (N_{PI_{eff}}) were calculated using the values of the mass attenuation and energy absorption coefficients. In the continuous energy region, agreements and disagreements were observed between photon interaction and photon energy-absorption for Z_{eff} and N_{eff} of compounds in different energy regions. In addition, absorption edge effects on Z_{eff} leading more than a single value of Z_{eff} at a specific energy have been discussed for the given compounds. Comparisons with experiments wherever possible have been carried out for calculated values of Z_{eff} and N_{eff}.

Keywords: Lanthanides, Effective atomic number, Effective electron density, Radiation interaction.

1. Introduction

Radiation interaction with matter has become an important subject with the extensive use of X and/or gamma rays in various fields such as reactors, nuclear power plants, nuclear engineering and space technology, nuclear diagnostics, nuclear medicine, radiation dosimetry and radiation biophysics. Rapidly increasing use of radioactive materials in reactors, nuclear power plants, nuclear engineering leads to study of interaction parameters like attenuation coefficient, photon interaction cross-section, Z_{eff} and N_{eff}. Thus, precise knowledge of these parameters should be known before their application (Kawekhao et al. 2008; Kirdsiri et al. 2009; Demir and Han 2009).

The pure metals of the lanthanides have little use. Whereas, the alloys or compounds of the metals can be very useful. For example, the alloys of Cerium have been used for metallurgical applications due to their strong reducing abilities. In addition, the lanthanides can be used for nuclear purposes; oxides of lanthanides can be used as diluents in nuclear fields, can also be used for structural-alloy-modifying components of reactors. Thus, increasing usage of the radiations, it should be determined radiation matter interaction parameters of compounds such as total mass attenuation coefficient, Z_{eff} and N_{eff} (Petrucci et al. 2007).

The Z_{eff} and N_{eff} are employed in radiation studies, especially for the characterization of interaction processes in various multi-element materials. There are a lot studies in literature about Z_{eff} and N_{eff} for different materials, in different categories such as in different type of compounds (Shivaramu and V. Ramprasath 2000; Tengku Kamarul Bahr et al. 2014; Kurudirek 2014a, 2014b; Gowda et al. 2004; Onder et al. 2012; Kurudirek and Kurudirek 2015), in alloys (Kurudirek et al. 2010; Kaewkhao et al. 2008; İçelli et al. 2005; Murty 2004; El-Kateb et al. 2000), in glass and minerals (Kaewkhao and Limsuwan 2010; Manohara et al. 2009; Kirdsiri et al. 2009; Singh et al. 2002, 2005) in biological materials (Manohara et al. 2008; Manohara and Hanagodimath 2007; Gowda et al. 2005). However, studies about lanthanides on Z_{eff} and N_{eff} are very scarce (Içelli 2006; Singh et al. 2015). This motivated us to carry out the present study.

Niranjan et al. (2012) calculated Z_{eff} and N_{eff} (for total photon interaction) of these compounds using total and electronic cross-sections. But in the present work, the comparison between photon energy-absorption and photon interaction, and Z_{eff} (relative to air) has been made in addition to the calculation of electron densities for photon interaction and photon energy absorption.

In the present work, the effective atomic numbers for photon energy-absorption (Z_{PEA_{eff}}), for photon interaction (Z_{PI_{eff}}), the effective electron densities for photon energy-absorption (N_{PEA_{eff}}) and for photon interaction (N_{PI_{eff}}) of La_2O_3, Ce_2O_3, Pr_2O_3, Nd_2O_3, Sm_2O_3, Eu_2O_3, Gd_2O_3, Tb_2O_3, Dy_2O_3, Ho_2O_3, Er_2O_3, Tm_2O_3, Yb_2O_3 and Lu_2O_3 have been calculated using direct method. Wherever possible the results were compared with the experimental results available in the literature.

2. Calculation

The total mass attenuation coefficients of elements present in the compounds were obtained from the WinXCom computer program (Gerward et al. 2001, 2004). The total mass attenuation coefficients (\mu/p) for any compound or composite of elements is given by mixture rule:

\( (\mu/p) = \sum_i w_i (\mu/p)_i \)  \hspace{1cm} (1)

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where, $w_i$ and $(\mu/\rho)_i$ are the weight fraction and mass attenuation coefficient of $i$th constituent element, respectively (Jackson and Hawkes, 1981). These coefficients were then used to calculate the $Z_{\text{eff}}$ of compounds for photon interaction with the help of the following practical formula (Manohara et al. 2008):

$$Z_{\text{eff}} = \frac{\sum_i f_i A_i Z_i}{\sum_i f_i \mu_i}$$  \hspace{1cm} (2)

where $f_i$ is the fraction by mole of each constituent element provided $\sum_i f_i = 1$, $A_i$ is the atomic weight (IUPAC 2007), $Z_i$ is the atomic number and $(\mu/\rho)_i$ is the mass attenuation coefficient. This formula is known as "Direct method". And $Z_{\text{eff}}$ is given $Z_{\text{eff}} = Z_{\text{air}}$.

The effective atomic number, $Z_{\text{eff}}$, is closely related to the electron density, $N_{\text{eff}}$ which is expressed in number of electrons per unit mass. Also, the $N_{\text{eff}}$ is expressed by the following relation (Manohara et al. 2008):

$$N_{\text{eff}} = N A \frac{Z_{\text{eff}}}{\sum_i f_i A_i} = N A \frac{\langle A \rangle}{\langle Z \rangle} \text{ (electrons/g)}$$ \hspace{1cm} (3)

where $\langle A \rangle$ is the average atomic mass of the compound.

3. Results and Discussion

The variations of $Z_{\text{PIeff}}, Z_{\text{PEAeff}}, Z_{\text{Reff}}, N_{\text{PIeff}}$, and $N_{\text{PEAeff}}$ with photon energies are shown in Fig. 1 for all compounds.
Figure 1. (a), (b), (c), (d), (e), (f), (g), (h), (i), (j), (k), (l), (m), (n) $Z_{\text{PPI}}$, $Z_{\text{PI}}$, $Z_{\text{Reff}}$, $N_{\text{PPI}}$, and $N_{\text{PI}}$ for the given compounds in the energy range of 1 keV–20 MeV.
From the results, it can be clearly seen that the $Z_{eff}$ varies with energy. In the continuous energy range 1 keV-20 MeV, the variation of $Z_{eff}$ with energy is mainly dominated by different partial photon interaction processes namely photoelectric absorption, Compton scattering and pair production.

It can be seen clearly from Fig. 1 that the variation of $Z_{REcalc}$ and $Z_{eff}$ with energy is almost similar for all of compounds. In the energy region $E < 100$ keV (the first region), $Z_{eff}$ and $Z_{REcalc}$ of compounds increase as energy increases. In this region photoelectric process dominates for $Z_{REcalc}$ and maximum variation observed in $Z_{eff}$ due to variation of $(\mu/\rho)$ and $\mu_{en}/\rho$, and since attenuation cross section proportional to $Z^{6}$. The $Z_{eff}$ decreases rapidly with increasing energy in the energy region from 100 keV to 2 MeV where the importance of photoelectric absorption decreases and Compton scattering gradually becomes the main interaction process and $Z_{eff}$ depend on Z (the second region). In the immediate aftermath, the $Z_{eff}$ increases with increasing energy as pair production gradually becomes the main interaction process to 20 MeV (the third region). So in the energy region $0.1 < E < 20$ MeV there is no energy region where Compton scattering is totally dominating as mentioned before Manohara et al. (2008).

Generally, $(\mu/\rho)$ and $\mu_{en}/\rho$ take values close to each other, hence $Z_{REcalc}$ and $Z_{eff}$ take almost same values in the first energy region. Therefore, either $Z_{REcalc}$ or $Z_{eff}$ can be used in this energy region. While in the second region, $Z_{REcalc}$ values are higher than the values of $Z_{eff}$ in the third energy region the values of $Z_{REcalc}$ were found to be higher than the values of $Z_{eff}$.

One can see clearly from Fig. 1, $Z_{eff}$ has several discontinuous jumps in the low-energy range because of absorption edge effects of high elements. The values of $M_{s}$, $M_{a}$, $M_{b}$, $M_{c}$, $La$, $L_{a}$, $L_{s}$, $L_{b}$ and Kubas absorption edge energies are shown in Table 1 (the absorption edge of the low-Z element oxygen occurs at energies <1 keV and is therefore of no importance in the present work). These discontinuities make the concept of the $Z_{eff}$ somewhat problematic in the low-energy range.

The $N_{eff}$ values for the present compounds were calculated using $< A >$ and $Z_{eff}$ and are given in Fig. 1. It is seen from this figure that $N_{eff}$ varies with photon energy. $N_{eff}$ is closely related to $Z_{eff}$ and has the same qualitative energy dependence as $Z_{eff}$. Thus, $N_{eff}$ values are proportional to $Z_{eff}$ values for the present compounds in the continuous energy range 1 keV - 20 MeV.

There is no experimental data on $\mu_{en}/\rho$ for comparison since it is not possible to measure $\mu_{en}/\rho$ experimentally, unlike $(\mu/\rho)$ which can be easily measured using the conventional gamma spectrometry system (Manohara et al. 2008). Thus, comparison was carried out for photon interaction only. The experimental results for $Z_{eff}$ and $N_{eff}$ (for photon interaction) of the given materials are given in Table 2.

### Table 1. K, L and M X-Ray absorption energies of lanthanides in keV.

<table>
<thead>
<tr>
<th>Elements</th>
<th>K_{ab}</th>
<th>L_{1ab}</th>
<th>L_{2ab}</th>
<th>L_{3ab}</th>
<th>M_{1ab}</th>
<th>M_{2ab}</th>
<th>M_{3ab}</th>
<th>M_{4ab}</th>
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<tr>
<td>La</td>
<td>38.941</td>
<td>6.283</td>
<td>5.894</td>
<td>5.489</td>
<td>1.361</td>
<td>1.204</td>
<td>1.123</td>
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<tr>
<td>Ce</td>
<td>40.449</td>
<td>6.561</td>
<td>6.165</td>
<td>5.739</td>
<td>1.437</td>
<td>1.273</td>
<td>1.185</td>
<td></td>
</tr>
<tr>
<td>Pr</td>
<td>41.998</td>
<td>6.846</td>
<td>6.443</td>
<td>5.968</td>
<td>1.511</td>
<td>1.337</td>
<td>1.242</td>
<td></td>
</tr>
<tr>
<td>Nd</td>
<td>43.571</td>
<td>7.144</td>
<td>6.727</td>
<td>6.215</td>
<td>1.575</td>
<td>1.403</td>
<td>1.297</td>
<td>1.005</td>
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<tr>
<td>Sm</td>
<td>46.846</td>
<td>7.754</td>
<td>7.281</td>
<td>6.721</td>
<td>1.723</td>
<td>1.541</td>
<td>1.420</td>
<td>1.106</td>
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<tr>
<td>Eu</td>
<td>48.515</td>
<td>8.069</td>
<td>7.624</td>
<td>6.983</td>
<td>1.800</td>
<td>1.614</td>
<td>1.481</td>
<td>1.161</td>
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<tr>
<td>Gd</td>
<td>50.229</td>
<td>8.393</td>
<td>7.940</td>
<td>7.252</td>
<td>1.881</td>
<td>1.688</td>
<td>1.544</td>
<td>1.217</td>
</tr>
<tr>
<td>Tb</td>
<td>51.998</td>
<td>8.724</td>
<td>8.258</td>
<td>7.519</td>
<td>1.968</td>
<td>1.768</td>
<td>1.611</td>
<td>1.275</td>
</tr>
<tr>
<td>Dy</td>
<td>53.789</td>
<td>9.083</td>
<td>8.621</td>
<td>7.850</td>
<td>2.047</td>
<td>1.842</td>
<td>1.767</td>
<td>1.332</td>
</tr>
<tr>
<td>Ho</td>
<td>55.615</td>
<td>9.411</td>
<td>8.920</td>
<td>8.074</td>
<td>2.128</td>
<td>1.923</td>
<td>1.741</td>
<td>1.391</td>
</tr>
<tr>
<td>Tm</td>
<td>59.335</td>
<td>10.144</td>
<td>9.628</td>
<td>8.652</td>
<td>2.307</td>
<td>2.090</td>
<td>1.885</td>
<td>1.515</td>
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<tr>
<td>Lu</td>
<td>63.304</td>
<td>10.876</td>
<td>10.345</td>
<td>9.241</td>
<td>2.491</td>
<td>2.263</td>
<td>2.024</td>
<td>1.639</td>
</tr>
</tbody>
</table>

### Table 2. Total mass attenuation coefficient $(\mu/\rho)$ (cm$^2$/g), effective atomic number and electron density (electrons/g) of oxides of lanthanides in 59.54 keV.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$(\mu/\rho)$</th>
<th>Z_{eff}^{a}</th>
<th>Z_{eff}^{b}</th>
<th>Z_{eff}^{c}</th>
<th>Z_{eff}^{d}</th>
<th>N_{eff}^{a}</th>
<th>N_{eff}^{b}</th>
<th>N_{eff}^{c}</th>
</tr>
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<tbody>
<tr>
<td>PrO_{3}</td>
<td>8.459</td>
<td>56.95</td>
<td>57.57</td>
<td>57.57</td>
<td>5.709</td>
<td>5.770</td>
<td>5.770</td>
<td>5.768</td>
</tr>
<tr>
<td>NdO_{3}</td>
<td>9.058</td>
<td>58.19</td>
<td>58.84</td>
<td>58.85</td>
<td>50.03</td>
<td>55.39</td>
<td>5.208</td>
<td>5.270</td>
</tr>
<tr>
<td>GdO_{3}</td>
<td>10.427</td>
<td>62.24</td>
<td>62.93</td>
<td>62.93</td>
<td>5.170</td>
<td>5.230</td>
<td>5.225</td>
<td></td>
</tr>
<tr>
<td>TbO_{7}</td>
<td>10.637</td>
<td>63.07</td>
<td>63.78</td>
<td>63.77</td>
<td>5.589</td>
<td>5.650</td>
<td>5.648</td>
<td></td>
</tr>
<tr>
<td>HoO_{3}</td>
<td>11.683</td>
<td>65.24</td>
<td>65.99</td>
<td>65.99</td>
<td>5.200</td>
<td>5.260</td>
<td>5.257</td>
<td></td>
</tr>
<tr>
<td>ErO_{3}</td>
<td>12.163</td>
<td>66.23</td>
<td>67.01</td>
<td>67.01</td>
<td>5.214</td>
<td>5.280</td>
<td>5.273</td>
<td></td>
</tr>
<tr>
<td>LuO_{3}</td>
<td>7.827</td>
<td>55.77</td>
<td>54.33</td>
<td>51.57</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$^{a}$Experimentally measured values from G. Singh et al. (2015).

$^{b}$Calculated values of the present work by using Direct method.

$^{c}$Experimentally measured values by using coherent to Compton scattering ratio method from Içelli (2006).

$^{d}$Calculated values by using coherent to Compton scattering ratio method from Içelli (2006).
In general, the agreement is good between experiments and our presented results except for values of İçelli (2006) because of that the used (coherent to Compton scattering ratio) method for calculation of $Z_{\text{eff}}$. Thus $Z_{\text{eff}}$ may have significantly different values in different energy regions. Coherent to Compton scattering ratio method is based on directly proportional to the areas of the measured spectrum ($R/C$ method) and For a fixed momentum transfer, $R/C$ is a function of only the $Z_{\text{eff}}$ of the sample (Duvauchelle et al. 1999; Del Lama et al. 2015). On the other hand, ratio method is based on proportional of the total atomic cross-section to total electronic cross-section of sample (Demir and Han 2009).

4. Conclusions

Below conclusions can be deduced from the present study:

- $Z_{\text{RED}}$, $Z_{\text{RED}}$, $N_{\text{RED}}$ and $N_{\text{RED}}$ of compound of oxides of lanthanides have been calculated for total photon interaction and photon energy-absorption in an extended energy range 1 keV–20 MeV.
- Because of the high element present in compounds (lanthanide elements of compounds), the $Z_{\text{eff}}$ show strong energy dependence.
- In the low energy region, where photoelectric absorption is more dominant, significant variations and maximum values were observed for $Z_{\text{eff}}$. The minimum values of $Z_{\text{eff}}$ have been observed in intermediate energies where Compton scattering is dominant, but there is no energy region where Compton scattering is totally dominating.
- At the K, L, M-absorption edge energies of lanthanide elements of compounds, more than a single value of $Z_{\text{eff}}$ could be obtained due to the non-uniform variation of mass attenuation coefficients.
- The $N_{\text{RED}}$ is closely related to the $Z_{\text{eff}}$ and has the same qualitative energy dependence as $Z_{\text{eff}}$.
- We have shown that $Z_{\text{RED}}$ and $N_{\text{RED}}$ for both photon energy-absorption and photon interaction are useful parameters for compounds at all energies greater than 1 keV.
- In the second region, significant differences exist between $Z_{\text{RED}}$ and $Z_{\text{RD}}$ and it is preferable to use $Z_{\text{RED}}$ or $Z_{\text{RD}}$ in the radiation dosimetry according to the purpose. Thus the results of the present work may be useful for applications of the compounds in the fields where radiation is used.

Highlights

(i) Effective atomic number and electron density of some lanthanide oxide compounds were calculated in continuous energy range using direct method.

(ii) The significant differences for $Z_{\text{eff}}$ and $N_{\text{eff}}$ were determined in different energy region.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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