Stopping power and inelastic mean free path of 300 eV–50 keV electrons for lanthanum aluminate

Dahlang Tahir*, Yulianti and Suarga

Department of Physics, Hasanuddin University, Tamalanrea, Makassar, 90245 Indonesia

*dtahir@fmipa.unhas.ac.id

Abstract. SP (Stopping Power) and IMFP (Inelastic Mean Free Path) of lanthanum aluminate (La$_2$O$_3$)$_x$ (Al$_2$O$_3$)$_{1-x}$ was varied with $x = 0.25$, $0.34$, and $0.5$ for electron energy from 300 eV to 50 keV have been determined by using composite Simpson from the equation of Born Ochkur correction. The main parameter in determining the SP and IMFP is Energy Loss Function (ELF) which was obtained from the experimental reflection electron energy loss (REELS) spectra. The method in this study is convenient methods for determining SP for binary compound lanthanum aluminate.

1. Introduction

Lanthanum aluminate is a compound alloy of Lanthanum Oxide (La$_2$O$_3$) and Aluminum Oxide (Al$_2$O$_3$). Dielectric constant of lanthanum aluminate is as high as about 30 compared to the HfO$_2$ and ZrO$_2$ that have dielectric constant is 25. Lanthanum Aaluminate has a large band gap values are from 5.75 to 6.35 eV when compared with the Hf-silicate that its value from 5.5 to 6.10 eV and Zr-silicate with a band gap value of 5.30 to 5.95 eV. In addition, lanthanum aluminate also have band offset of the conduction band is large at around 2.40 to 2.86 eV and a high thermal stability up to 1000 ° C [1]. Lanthanum aluminate is also used in the electronics industry.

There have been many reported for the experimental studies of the electronic properties, structural, surface layer, and dielectric properties of Lanthanum aluminate by using various methods including: X-ray Photoelectron Spectroscopy (XPS), reflection electron energy loss spectroscopy (REELS), X-ray diffraction (XRD), and also comparison with ab initio local density calculation.

The interaction between electrons with the material can be described by two main quantities, Stopping Power (SP) and Inelastic Mean Free Path (IMFP). A property of SP and IMFP of electrons passing through the electron describes a material through interactions with orbital electrons and atomic nuclei. Through this interaction, the electron will lose kinetic energy in the form of elastic or inelastic. Electron will lose their kinetic energy through inelastic scattering process which was described by the SP and the distance between two collisions is the IMFP. Both the fundamental quantity is very important in many fields of research, such as radiobiology, biomedical applications, radiation dosimeters, and the modeling of electron transport in materials for a variety of other applications. For example, to understand the effects of radiation in radiation dosimeters, SP is necessary for the calculation of the doses radiation through the biological tissue. SP also has been used the electron transport analysis, Auger electron spectroscopy, and dimensional metrology in the Scanning Electron Microscope [2].
In this study we report, the Stopping Power (SP) and inelastic Mean Free Path (IMFP) of electrons for Lanthanum aluminate materials in the energy range from 300 eV to 50 keV determined by using Born-Ochkur correction method.

2. Calculation Method

Effect of the exchange between the electrons incident and the target was included into account by using Born-Ochkur correction method based on dielectric response theory and statistical approach of Penn, resulting SP (-dE/dS) and IMFP (λ⁻¹) is expressed as [3]:

\[
SP = -\frac{dE}{dS} = \frac{1}{2\pi a_0 E} \int_0^{\frac{\alpha^2}{2}} \left( \frac{1}{\varepsilon(\omega)} \right) \left[ \frac{1}{\varepsilon(\omega)} \right] v(\alpha) d(h\omega)
\]  

\[
IMFP = \lambda^{-1} = \frac{1}{2\pi a_0 E} \int_0^{\frac{\alpha^2}{2}} \Im \left[ \frac{1}{\varepsilon(\omega)} \right] w(\alpha) d(h\omega)
\]  

Where \( E \) is the kinetic energy of the electrons incident, \( a_0 \) is the Bohr radius, \( h\omega \) is energy loss, \( \Im \left[ \frac{1}{\varepsilon(\omega)} \right] \) is the energy loss function (ELF), and \( v(\alpha) \) and \( w(\alpha) \) is given by:

\[
v(\alpha) = \frac{2s}{(1+\alpha)(1+\alpha+s)} + \ln \left[ \frac{(1-\alpha^2)(1+\alpha)}{(1-\alpha-s)(1+\alpha+s)} \right]
\]

\[
w(\alpha) = \frac{3\alpha^2 + 3\alpha + 1}{(1+\alpha)^2} \ln \frac{1+\alpha}{1+\alpha-s} + \frac{1}{1+\alpha-s} + \frac{2s}{(1+\alpha)^2(1+\alpha+s)}
\]

with \( \alpha = h\omega/E \) and \( s = \sqrt{1-2\alpha} \).

SP and IMFP in this study were determined by using integral composite Simpson. Composite Simpson method is requires the integration area is divided into small area (h) of a region as can be seen in Figure 1 and Eq. (5). The interval area is uniform and applied from the lowest (\( x_0 \)) part to the highest (\( x_n \)) part of horizontal axis (see Figure 1) resulting number of integral as outcomes as expressed by [4-5]:

\[
\int_a^b f(x)dx = \sum_{j=1}^{n} \int_{x_{j-1}}^{x_j} f(x)dx = \sum_{j=1}^{n} \left\{ \frac{h}{3} \left( f(x_{j-2}) + 4f(x_{j-1}) + f(x_{j}) \right) \right\}
\]

Where \( h = (b-a)/n \) and \( x_j = a + jh \), for \( j = 1, ..., n/2 \), with \( x_0 = a \) and \( x_n = b \). Equation (5) expressed as [6]:

![Figure 1. Interval for the integration area of composite Simpson method](image-url)
\[
\int_{a}^{b} f(x) \, dx = \frac{h}{3} \left[ f(x_0) + 2 \sum_{j=1}^{(n-1)/2} f(x_{2j}) + 4 \sum_{j=1}^{(n-2)/2} f(x_{2j-1}) + f(x_n) \right]
\]

\[= -\frac{h^5}{90} \sum_{j=1}^{n} f^{(4)}(\xi_j) \quad (6)\]

As shown by equation (1) and (2), required for the calculation of SP and IMFP are ELF, which is described the inelastic scattering event. A key problem for the calculation of the SP and IMFP is how to determine ELF.

Dielectric response theory is usually used to describe the inelastic scattering based on a semi classical description of the dielectric response of the interaction between the electron incident and the target in solids. It can be used for quantitative analysis of REELS to evaluate the dielectric function of solids and to determine the inelastic scattering cross section. Theory of scattering cross sections inelastic \( K_{sc}(E_0, \hbar \omega) \) can be calculated if the dielectric function \( \varepsilon(k, \omega) \) is known. Energy loss function (ELF) obtained through trial and error system (trial and error) where the function is successful if the corresponding ELF with \( K_{sc}(E_0, \hbar \omega) \)obtained from experimental results for some electron energy levels come \( E_0 \).

All types of excitation is described by the material dielectric function \( \varepsilon(k, \omega) \), which is the only input parameter in the calculation of inelastic scattering cross sections in theory. Usually is described by the theory of inelastic scattering cross section \( K_{th}(E_0, \hbar \omega) \) for all electrons REELS. \( E_0 \) is the primary electron energy and \( \hbar \omega \) is the energy lost by the electrons in the scattering. To model the ELF on the material, we use the expansion involving Drude - Lindhard types oscillator [7-8]:

\[
Im\left\{\frac{1}{\varepsilon(\omega)}\right\} = \theta(\hbar \omega - E_g) \sum_{l} \frac{\alpha_l \hbar \omega}{(\hbar^2 \omega_{li}^2 - \hbar^2 \omega^2 + \gamma_l^2 \hbar^2 \omega^2)} \quad (7)
\]

With \( \alpha_l = \) oscillator strength, \( \gamma_l = \) damping coefficient, and \( \hbar \omega_{li} = \) excitation energy. The effect of the energy band gap \( (E_g) \) in semiconductors and insulators is \((\hbar \omega - E_g)\). Where result of \( \hbar \omega - E_g = 0 \) if \( \hbar \omega < E_g \) and \( \hbar \omega - E_g = 1 \) if \( \hbar \omega > E_g \). Energy Loss Function (ELF) in this study as shown in figure 2 from Ref. [1] for Lanthanum Aluminate with composition were varied between \( \text{La}_2\text{O}_3 \) and \( \text{Al}_2\text{O}_3 \); \( \text{La}_2\text{O}_3\text{Al}_{0.5} \), \( \text{La}_2\text{O}_3\text{Al}_{0.34} \), \( \text{La}_2\text{O}_3\text{Al}_{0.25} \), and \( \text{La}_2\text{O}_3\text{Al}_{0.75} \). Band Gap for composition \( \text{Al}_2\text{O}_3 \) 50%, 66%, and 75% respectively is 5.75 eV, 6.04 eV, and 6.35 eV and \( \alpha-\text{Al}_2\text{O}_3 \) is 8.4 eV. In figure 2, we can see clearly the difference between ELF of \( \text{La}_2\text{O}_3\text{Al}_{0.5} \) with \( \alpha-\text{Al}_2\text{O}_3 \). For ELF lanthanum aluminate shows similar peaks at energy loss \( \sim 15 \text{ eV} \), \( \sim 20 \text{ eV} \), \( \sim 23 \text{ eV} \), and \( \sim 28 \text{ eV} \) but for \( \alpha-\text{Al}_2\text{O}_3 \) have only two peaks, at the energy loss \( \sim 25 \text{ eV} \) and \( \sim 32 \text{ eV} \). These results indicated that the strong effect of \( \text{La}_2\text{O}_3 \) on lanthanum aluminate even the amount of \( \text{Al}_2\text{O}_3 \) up to 75%. Energy Loss Function (ELF) is used as input parameter in Born-Ockel correction method to calculate the Stopping Power (SP) and inelastic Mean Free Path (IMFP).
3. Results and Discussion

Stopping Power (SP) and inelastic Mean Free Path (IMFP) of Lanthanum aluminate at energy 300 eV - 50 keV obtained by equation (1) and (2) using integral composite Simpson. SP in this study compared with a database derived from the National Institute of Standards and Technology (NIST) and IMFP compared with the data TPP2M IMFP which can be freely downloaded from Ref. [10].

Figure 3 shows the relationship between the SP and the electron energy is clear that the value of SP for lanthanum aluminate has almost the same value so that if drawn will overlap. This is due to the value of the Energy Loss Function (ELF) it is almost the same as well. When compared with the $\alpha$-$\text{Al}_2\text{O}_3$ has good agreement with the SP generated for lanthanum aluminate. Meanwhile, when compared with the total Stopping Power of NIST database, it has a big different value. This is likely caused by the calculation of Total Stopping Power of NIST using Bethe theory is only used for bulk materials and apply at high energy [11]. Whereas in this study, the data used ELF is the result of a quantitative analysis of REELS experiments using thin film materials with 7 nm thick. In the SP calculation, we use the correction method of Born-Ochkur by considering the effect of the exchange between the electrons targets and incident electron.

Figure 4 shows a graph of relationship where the IMFP on energy electron IMFP resulting value is almost the same due to its ELF are almost the same anyway. If any described IMFP results for Lanthanum aluminate will overlap. Figure 5 shows a graph of the relationship IMFP for $\text{Al}_2\text{O}_3$ electron energy obtained in this study and compared with values obtained TPP2M where IMFP value of these results for $\alpha$-$\text{Al}_2\text{O}_3$ approaching TPP2M value.

Figure 2. Energy loss function (ELF) for $(\text{La}_2\text{O}_3)_x(\text{Al}_2\text{O}_3)_{1-x}$ [1] and $\alpha$-$\text{Al}_2\text{O}_3$ [9]
Figure 3. Stopping Power of $\alpha$-$\text{Al}_2\text{O}_3$ and Lantanum Aluminate. We included data from NIST database for comparison.

Figure 4. IMFP on of Lantanum Aluminate.
Figure 5. IMFP $\alpha$-$\text{Al}_2\text{O}_3$ in this study compared with the value TPP2M.

4. Conclusion
Stopping Power (SP) of Lanthanum Aluminate decreased while IMFP increases with increasing electron energy of 300 eV to 50 keV and SP value for $\text{Al}_2\text{O}_3$ in this study in contrast to the value of the Bethe theory but IMFP value nearly equal to the value of TPP2M.

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