

Inelastic mean free path of swift electrons and stopping power in Ta_2O_5

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Abstract

Energy Loss Function (ELF) of Ta_2O_5 derived from optical limit and extended to the total part of momentum and their energy excitation region ELF plays an important function in calculating energy loss of electron in materials. The parameter Inelastic Mean Free Path (IMFP) is most important in quantitative surface sensitive electron spectroscopies, defined as the average distance that an electron with a given energy travels between successive inelastic collisions. The stopping cross section and single differential cross-section SDSCS are also calculated and gives good agreement with previous work.

Key words

Electron energy loss, stopping power, dielectric function.

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متوسط المسار الحر الغير مرن للالكترونات السريعة و قدرة الايقاف في الـ Ta_2O_5

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الخلاصة

دالة فقدان الطاقة للـ Ta_2O_5 تشتق من الحد البصري وامتدادات الأشتقاق تشمل الزخم ومنطقة الطاقة المتهيجة. وهذه الدالة تلعب دور مهم في حساب الطاقة المفقودة للالكترونات في المواد، كما يعتبر معامل متوسط المسار الحر غير المرن اكثر أهمية عند الحدود الطيفية للالكترونات والذي يعرف بأنه متوسط المسافة عندما يعطي الألكترون الطاقة اثناء انتقاله خلال التصادمات الغير المرنة الناجحة. وكذلك تم حساب المقطع العرضي لقدرة الأيقاف والمقطع العرضي التفاضلي تحسب والتي اعطت نتائج متوافقة مع الأعمال السابقة.

Introduction

The excitation spectrum of Ta_2O_5 has been studied theoretically and calculated by Reflection Electron Energy Loss Spectroscopy (REELS), which only covers a small region is improved and extended to the all of excitation region out of a suitable theoretical analysis that requires the investigation of physically motivated sum rules given in [1] and includes the contribution of intermediate and inner shell excitations.

Energy Loss Function (ELF) derive from several ways are based on experimental measurements, theoretical considerations, but the information provided by the former rarely covers the whole momentum and electronic excitation energy region, but the theoretical calculations many times lack of a direct experimental assessment [1]. The dielectric formalism used the resulting of ELF as input to evaluate the energy loss magnitudes to distinguish the passage of swift ions through matter.

These calculations are compared with the stopping cross section of Ta₂O₅ films for electron beams by means of Rutherford backscattering spectrometry.

ELF can be used as input function in the main formula which defined Stopping Cross Section (SCS) of swift ions through matter.

In solid state physics and electron spectroscopy there is an important material parameter known as (IMFP) Inelastic Mean Free Path of electrons. There are many number of papers published on the subject of IMFP evaluation. Only paper summarizes this problem [2].

In general, three experimental ways are applied to calculate the values of IMFP:

1- The method that can be confined to 1-2 peaks, where energy values are characteristic of the elements called x-ray photoelectron spectroscopy [3].

2- In this method the over layer must be perfectly regular in thickness and evident to electrons. Away from experimental difficulties in preparing thin layers, this method rather supplies the value of IMFP affected by multiple electron scattering. This way known as the over layer method [2].

3- Elastic peak electron spectroscopy (EPES) method [4, 5] a study of the development of EPES was given [6]. This method shows a possibility to calculate the value of IMFP for all solid surfaces.

Consider ELF given in the following equation [1]:

$$\text{Im} \left[\frac{-1}{\varepsilon(\omega, k)} \right] = \sum_i \frac{A_i}{\omega_i^2} \text{Im} \left[\frac{-1}{\varepsilon(\omega_i, u_i, k, \omega)} \right] \theta(\omega - \omega_{th,i}) = \sum_i \frac{A_i u_i \omega}{(\omega_i^2(k) - \omega^2)^2 + u_i^2(k) \omega^2} \theta(\omega - \omega_{th,i}) \tag{1}$$

where A_i, ω_i, u_i and $\omega_{th,i}$ are the intensity, position, width and threshold, respectively of Drude-ELF peaks, $\theta(\omega - \omega_{th,i})$ represents the Heaviside step function [7] and the extend from of Eq. (1) is [1].

$$\omega_i(k) = \omega_i + g(k) \frac{\hbar k^2}{2m} \tag{2}$$

$$g(k) = 1 - \exp(-ck^d), \tag{3}$$

$$u_i(k) = u_i + ak + bk^2 \tag{4}$$

with $a=10$ eV, $b=6$ eV, $c=1.2$ and $d=0.4$ The parameters of dielectric for Ta₂O₅ are shown in Table 1.

Table 1: The parameters of Ta₂O₅ for the ELF [1].

i	$\hbar\omega_i$ (eV)	$\hbar u_i$ (eV)	A_i (eV ²)
1	8	3.5	4.23
2	15.5	6	43.3
3	22.5	11	123
4	30	9	131
5	39.5	5	25.8
6	42.5	5	25.8
7	52	16	240
8	54	8	37.7
9	80	30	94.1

Electronic excitation spectrum of Ta₂O₅

Electronic excitation spectrum is importance of a material like Ta₂O₅, but no experimental data are available

for it in a large range of excitation energies. There are spectrophotometric and transmittance measurements in a wavelength range that only permit obtaining the

absorptive and refractive index for energies that less than 6 eV. In the present work, we make use of an approximation which limits the IMFP calculation to electron energies greater than about 200 eV.

The dielectric formalism for non relativistic electron with kinetic energy T gives by Eq.(1) with its parameters given in Eq.(2) and Table 1, the stopping power S_e is given as follows [1]:

$$S_e = \frac{me^2}{\pi T} \int_0^{W_{max}} \omega d\omega \int_{k_1}^{k_2} \frac{dk}{k} [1 + f_{ex}(k)] \text{Im} \left[\frac{-1}{\epsilon(\omega, k)} \right] \quad (5)$$

where

$$K_{1,2} = (2m/\hbar) [\sqrt{T} \pm (T - \hbar\omega)^{1/2}] \quad (6)$$

The maximum energy transferred $\hbar W_{max} = \min(T/2, T - E_{gap})$

E_{gap} is target band gap energy.

f_{ex} is exchange term,

$$f_{ex}(k) = (\hbar k/mv)^4 - (\hbar k/mv)^2 \quad (7)$$

where v is the incident electron velocity.

Dielectric formalism gives also the inverse mean free path λ_e^{-1} in terms of kinetic energy for the interact of electron with solids [1],

$$\lambda_e^{-1} = \frac{me^2}{\hbar\pi T} \int_0^{W_{max}} d\omega \int_{k_1}^{k_2} \frac{dk}{k} [1 + f_{ex}(k)] \text{Im} \left[\frac{-1}{\epsilon(\omega, k)} \right] \quad (8)$$

Finally according to the dielectric function, the macroscopic single differential cross section (SDCS) to ejection of an electron with kinetic energy W_e from the electronic i-shell of the target by the electron of kinetic energy T ,

$$\frac{d\lambda_e^{-1}(T, W_e)}{dW_e} = \frac{me^2}{\pi T} \int_{k_1}^{k_2} \frac{dk}{k} \int \text{Im} \left[\frac{-1}{\epsilon(k, B_i + W_e)} \right] \quad (9)$$

B_i is the binding energy of i-shell.

Stopping power represents the mean energy loss per unit distance traveled by an energetic electron where IMFP indicates the average distance traveled by an energetic electron between two successive energy-loss events, there are many domains of research and applications such as, surface test with charged particles, micro dosimetry, and radiotherapy based on inelastic mean free paths, Inelastic interactions of energetic electron with condensed matter and stopping power describing the inelastic interactions of energetic electrons with condensed matter [8].

Energy loss function derived from reflection electron energy loss measurements only accounts for contributions of outer-shell electrons to the target ($\hbar\omega \leq 80$ eV) to optical (i.e., $k = 0$) excitations. Used the Mermin Energy Loss Function–Generalized Oscillator Strength (MELF-GOS) this method to obtain an ELF that covers the all momentum and energy transfers region. This procedure supported by its effective application to describe the electron excitation spectra of elemental and compound targets.

Results and discussion

Fig.1 shows (a) the 2D of optical ELF $\text{Im} \left[\frac{-1}{\epsilon(\omega, k=0)} \right]$ of Ta_2O_5 as a function the transferred energy function $\hbar\omega \leq 100$ eV and (b) the 3D of $\text{Im} \left[\frac{-1}{\epsilon(\omega, k)} \right]$ as a function of the transferred momentum $\hbar k$ and energy $\hbar\omega \leq 100$ eV functions. ELF of Ta_2O_5 has five peaks which agree with previous work presented in [1].

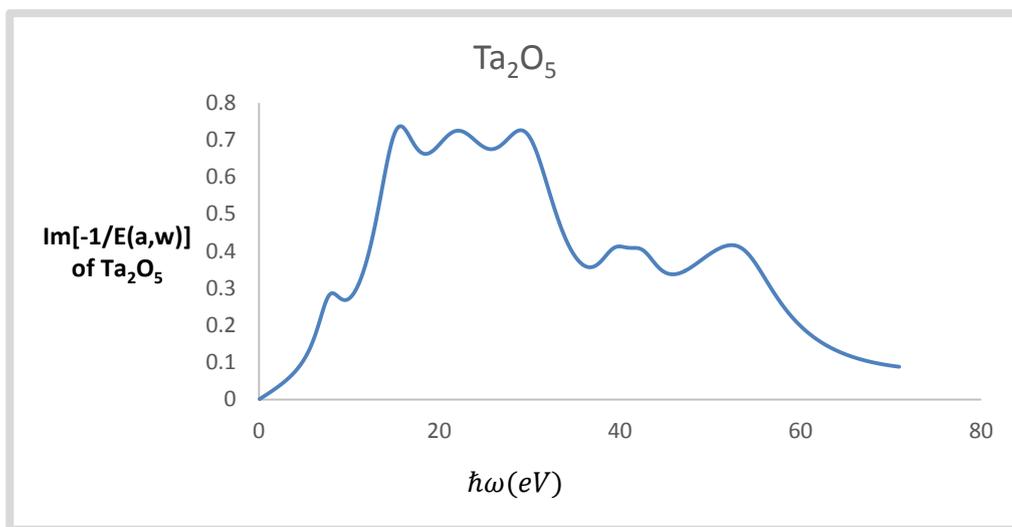
Fig.2 shows the stopping power S in $(eV.cm^2 \times 10^{-15} / atom)$ with incident electron energy T_e in eV calculated from the results of ELF given in Eqs. (1-4), and its solution given in Eq. (5) for interact of electron with Ta_2O_5 . ELF applied to obtain the inelastic

mean free path of electrons and the stopping power of in Ta_2O_5 which is consider relevant for description and modification of solid media by means of electron beam techniques like as electron microscopy-ray photoelectron, auger electron spectroscopy and other techniques. The variation of electron stopping power agree very well with previous work [1]. The range of incident electron energy between ((10-10000)eV) the maximum stopping power, S_e ($Mev.cm^2/gm$) (i.e Bragg

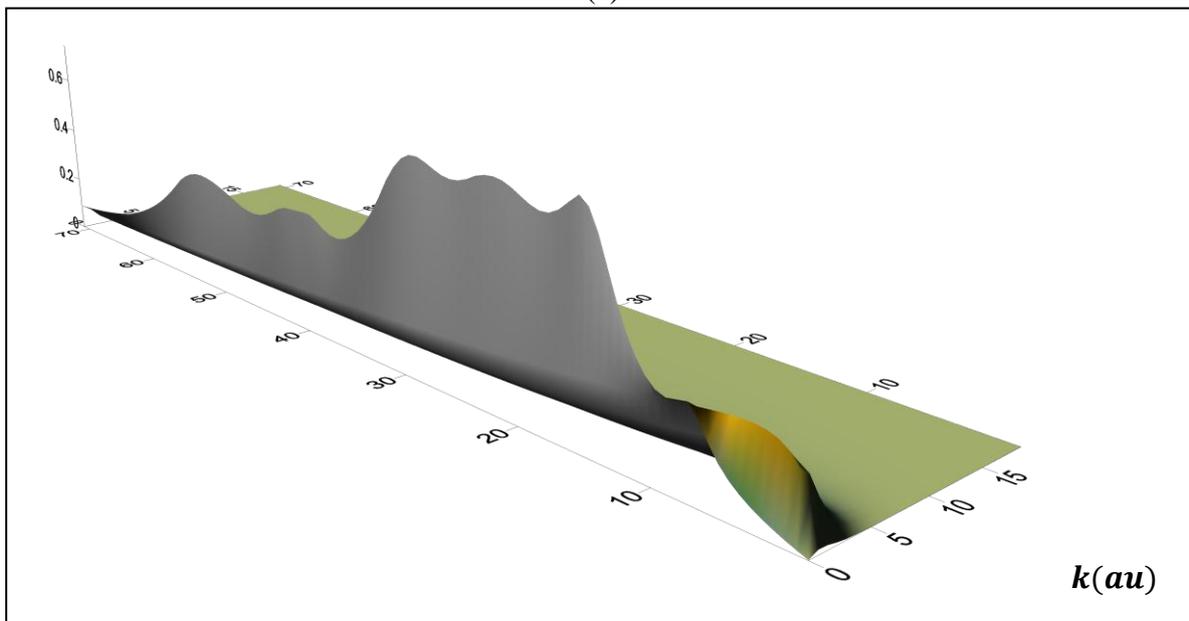
peak) is at energy ≈ 700 eV which is agree with [1].

Fig.3 shows the IMFP λ_e^{-1} in \AA^{-1} for the interaction of electrons with Ta_2O_5 and kinetic energy T_e in eV.

Fig.4 shows the single differential cross section SDCS ($A.eV$) $^{-1}$ for ionization of Ta_2O_5 by electrons with kinetic energy $T(eV)$ (0.01 to 10) as a function to the ejection electron W_e in (eV).



(a)



(b)

Fig.1: Function of the transferred (a) 2D of optical ELF (Energy Loss Function) of Ta_2O_5 (b) 3D of optical ELF at energy $\hbar\omega \leq 100eV$.

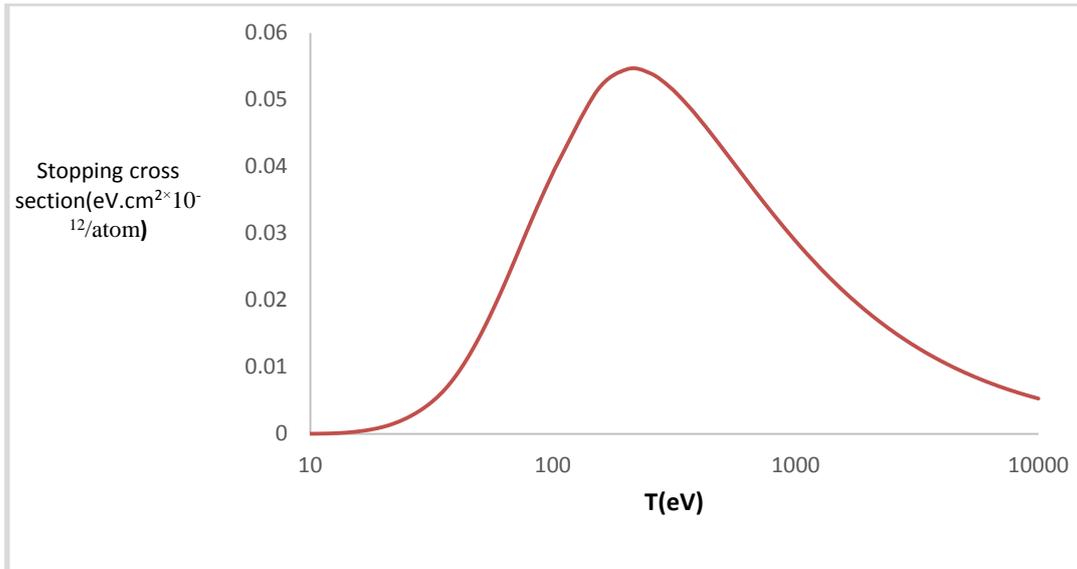


Fig.2: Stopping cross section SCS of electrons in Ta_2O_5 with the incident electron energy T .

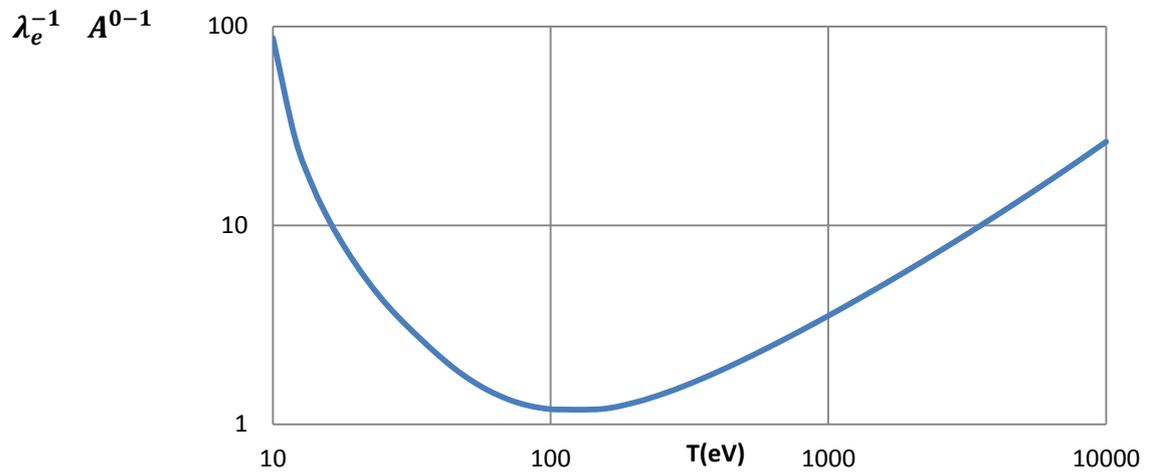


Fig.3: Inelastic mean free path (IMFP) with the incident electron energy T (eV).

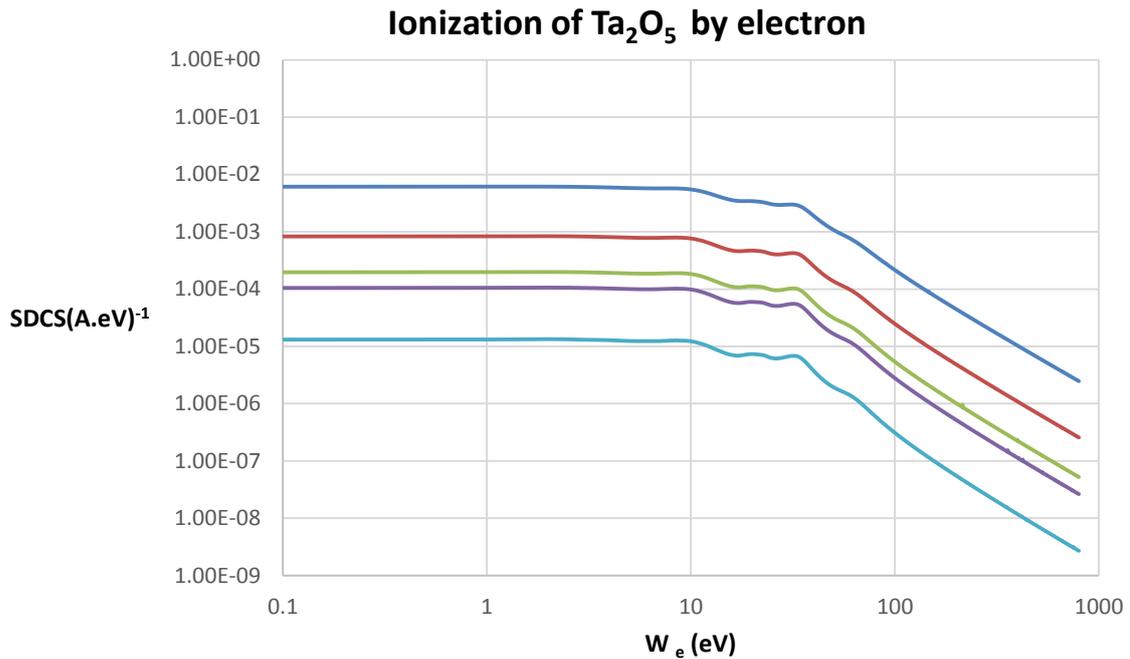


Fig.4: Single differential cross section $SDCS (A.eV)^{-1}$ for ionization of Ta_2O_5 by electrons with kinetic energy $T (eV)$ as a function to the ejection electron W_e in (eV) .

Conclusions

In this work a theoretical study performed to calculate ELF energy loss function of Ta_2O_5 which magnitude that enters as a main ingredient in numerous areas of materials science, outer shell electron of the target excitations contribution to the ELF was derived from reflection electron energy loss spectroscopy measurements, phase and chemical effects have been taken into account to derive a realistic ELF for Ta_2O_5 , for all momentum and energy transfer measurements.

The inelastic mean free path and the stopping cross section of swift electron in Ta_2O_5 was calculated, both has relevance in more studies of this material in the microelectronics industry.

According to Fig. 4

- (i) The most ejected electron are generated in the low energy region.
- (ii) The number of ejected electrons increases with incident proton energies decreases.

- (iii) The influence of target energy loss function in the ionization of secondary differential cross section is larger for lower proton energies.

Quantitative surface sensitive electron spectroscopies the parameter Inelastic Mean Free Path IMFP is most important that defined as the average distance that an electron with the transportation energy between successive inelastic collisions. The stopping cross section is calculated and gives good agreement with previous work given in [1].

At intermediate and high electron energies we need these two parameter in order to elucidate the discrepancy between ELF models of the target electron excitations.

References

- [1] C. Raul, Fadanelli, Moni Behar, Luiz C. C. M. Nagamine, Maarten Vos, Néstor R. Arista, Chiara D. Nascimento, Rafael Garcia-Molina,

Isabel Abril, *J. Phys.-Chem.*, 119, 35 (2015) 20561-20570.

[2] C. J. Powell, *Scanning Electron Microscopy, IV*, Ed. 237, (1984).

[3] S. Evans, R. G. Pritchard, J. M. Thomas, *J. Phys. C., Sol. St. Phys.*, 10, 2483 (1977).

[4] G. Gergely, *Surface Interface Anal.* 3 (1981) 201-205.

[5] A. Jablonski, P. Mrozek, G. Gergely, M. Menyhard, A. Sulyok, *Surface Interface Anal.*, 6 (1984) 291-294.

[6] G. Gergely, *Scanning*, 8 (1986) 203-214.

[7] Rafael Garcia-Molina, Isabel Abril, Santiago Heredia-Avalos, Ioanna Kyriakou, Dimitris Emfietzoglou, *Phys. Med. Biol.*, 56, 19 (2011) 6475-6493.

[8] Zhenya Tan, *Elsevier*, 82 (2013) 325-331.