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Technical note

Stopping powers and inelastic mean free path of 200 eV–50 keV electrons in polymer PMMA, PE, and PVC

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HIGHLIGHTS

- We used ELF from a previously published quantitative analysis of reflection electron energy loss spectroscopy (REELS) spectra.
- SP are lower by 10–15% from the National Institute of Standards and Technology (NIST) database for electron energies from 10 to 50 keV.
- IMFP for PE is similar with that of predictive IMFP-TPP2M formula with a root-mean-square (*rms*) of 7.01 Å.

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ABSTRACT

The stopping power (SP) and inelastic mean free path (IMFP) of three polymers: polymethyl methacrylate (PMMA), polyethylene (PE), and polyvinyl chloride (PVC) for electron energies from 200 eV to 50 keV have been determined based on dielectric models. The energy loss function (ELF) is the main input in the calculation of the SP and IMFP for the dielectric models. ELF in this study was determined from a previously published quantitative analysis of reflection electron energy loss spectroscopy (REELS) spectra. The SP of PMMA, PE and PVC decreases and the IMFP increases with increasing electron energies up to 50 keV. For comparison, data from the National Institute of Standards and Technology (NIST) database for electron energies from 10 to 50 keV were used and show that SP in this study is lowered by 10–15%. The obtained IMFP for PE was compared with those calculated using the TPP2M predictive equations and shows that a reasonable agreement with a root-mean-square (*rms*) is 7.01 Å. The present approach has high potential for the experimental determination of SP and IMFP from the REELS spectra.

1. Introduction

Polymer materials have become increasingly important because of their applications cover virtually all aspects in our daily life, such as clothing materials, furniture, optoelectronic devices, biomedical devices, and communication (Tahir and Tougaard, 2012a). In many cases, electronic properties such as electron stopping power (SP) and inelastic mean free path (IMFP) influence the performance of the polymer materials. However, we found few studies devoted to these properties of polymers for a wide range of energy loss function (ELF) up to 80 eV. The SP and IMFP also find importance in many other fields of research, such as radiobiology, biomedical applications, and modeling of electron transport for many other applications (Tan et al., 2009, 2004; Tahir et al., 2012; Akkerman et al., 2014; Varea and Arista 2014; Tanuma et al., 2005; Nagatomi and Goto, 2007, 2005; http://www.nist.gov/index.html; http://www.quases.com/products/quases-imfp-tpp2m/). For example, the SPs are required to calculate the radiation effects of energetic electrons passing through biological tissues (Tan et al., 2009, 2004; Tahir et al., 2012). The SP has also been used in Monte Carlo simulations for electron transport in electron-probe microanalysis, Auger-electron spectroscopy, and dimensional metrology in a scanning electron microscope (Tanuma et al., 2005; Nagatomi and Goto, 2007, 2005).

In this study, we report electron SPs and IMFPs calculated from the energy loss function (ELF) of PMMA, PE, and PVC for electron energies from 200 eV to 50 keV. The ELF in this study was obtained from quantitative analysis of experimental reflection electron energy loss spectroscopy (REELS) spectra which were published by Tahir and Tougaard (2012a). The calculated SPs were compared with the nonrelativistic Bethe equation from the National Institute of Standards and Technology (NIST) database (http://www.nist.gov/index.html) and the IMFP compared with Tanuma Powell Penn

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(TPP-2M) methods (Tanuma et al., 2005), which can be freely downloaded from http://www.quases.com/products/quases-imfp-tpp2m/. The aim of this work is to provide alternative basic data of SPs and IMFPs for the study on the energy deposition of low-energy electrons transport through PMMA, PE, and PVC.

2. Calculation method

In the calculation of ELF from quantitative analysis of REELS spectra, Tahir and Tougaard (2012a, 2012b), Tahir et al. (2009, 2010b, 2010c, 2010a), Denny et al. (2012), and Shin et al. (2012) used the semi-classical dielectric response model proposed by Tougaard and Yubero (Yubero et al., 1996; Tougaard and Yubero, 2008; Romanyuk et al., 2011). The algorithms of this method have been implemented in the generally available QUEELS-$\varepsilon(k,\omega)$-REELS software package (Tougaard and Yubero, 2008). The validity and consistency of this method were extensively tested recently (Hajati et al., 2008) and the method was successfully used to obtain the ELF and optical properties of ultrathin dielectrics (Tahir et al., 2009, 2010b, 2010c) semiconductor (Romanyuk et al., 2011), polymer (Tahir and Tougaard, 2012a), metals (Tahir and Tougaard, 2012b; Hajati et al., 2008), and transparent oxide films (Tahir et al., 2010c, 2010a; Denny et al., 2012; Shin et al., 2012). In Ref. Hajati et al. (2008) there is a detailed discussion of experimental tests of the validity of the elastic scattering model.

In this model, the dielectric function $\varepsilon(k,\omega)$ (k is wave vector and ω is frequency) of the material is the only input in the calculation, which describes all the excitations. The dielectric function is given in terms of the energy loss function (ELF) Im $(-1/\varepsilon)$ which is parameterized as a sum of Drude–Lindhard type oscillators, as described in Tahir et al. (2009), Yubero and Tougaard (1992), Yubero et al. (1996), Tougaard and Yubero (2008), and Hajati et al. (2008):

$$\mathrm{Im}\left\{\frac{-1}{\varepsilon(k,\omega)}\right\}=\theta(\hbar\omega-E_g)\cdot\sum\frac{A_i\gamma_i\hbar\omega}{\left(\hbar^2\omega_{0ik}^2-\hbar^2\omega^2\right)^2+\gamma_i^2\hbar^2\omega^2} \tag{1}$$

where the dispersion relation is given in the form

$$\hbar\omega_{0ik}=\hbar\omega_{0i}+\alpha_i\frac{\hbar^2k^2}{2m}. \tag{2}$$

Here, A_i, γ_i, $\hbar\omega_{0i}$, and α_i are the oscillator strength, damping coefficient, excitation energy and momentum dispersion coefficient of the ith oscillator, respectively, and $\hbar k$ is the momentum transferred from the REELS electron to the solid. The dependence of ω_{0ik} on k is generally unknown, but we use Eq. (2) with α_i as an adjustable parameter. The values of the momentum dispersion coefficient α_i are related to the effective mass, e.g, $\alpha_I \approx 0$ for insulator and $\alpha_i \approx 1$ for metals (Yubero and Tougaard, 1992; Yubero et al., 1996; Tougaard and Yubero, 2008; Hajati et al., 2008). The step function $\theta(\hbar\omega - E_g)$ is included to describe the effect of the band gap energy E_g in semiconductors and insulators.

Table 1
The best fit oscillator parameters for PMMA, PE, and PVC to the experimental cross section at a primary energy of 500 eV from Tahir and Tougaard (2012a).

Polymer	$\hbar\omega_{0i}$ (eV)	A_i (eV^2)	$\hbar\gamma_i$ (eV)	E_g (eV) REELS
PMMA α_i=0.05	19.7	129.22	10.5	5.0
	23.8	60.45	7.2	
	30	159.60	13	
PE α_i =0.05	9	0.05	2	7.5
	22	315.18	12.8	
	29.8	47.13	8	
PVC α_i =0.05	20	137.36	11	8.0
	25.8	231.47	14.3	

Here, $\theta(\hbar\omega - E_g)=0$ if $\hbar\omega < E_g$ and $\theta(\hbar\omega - E_g)=1$ if $\hbar\omega > E_g$. The band gap was estimated from the onset value of REELS spectrum (see Ref. Tahir and Tougaard (2012a, Fig. 1)).

For the polymers in this work, we used ELF data from Ref. Tahir and Tougaard (2012a) in which parameters are obtained by fitting the inelastic electron scattering cross section $\lambda K_{th}(\hbar\omega)$ spectrum simulated with the QUEELS-$\varepsilon(k,\omega)$–REELS software to an experimental inelastic scattering cross section $\lambda K_{exp}(\hbar\omega)$. The parameters A_i, γ_i, $\hbar\omega_i$, and α_i, of the oscillators are varied until good agreement between the calculated and experimental inelastic cross sections is obtained. The oscillator strengths are adjusted to make sure that $\varepsilon(k,\omega)$ fulfills the well-established Kramers–Kronig sum rule (Yubero and Tougaard, 1992; Yubero et al., 1996; Tougaard and Yubero, 2008; Hajati et al., 2008))

$$\frac{2}{\pi}\int_0^\infty \mathrm{Im}\left\{\frac{1}{\varepsilon(k,\omega)}\right\}\frac{d(\hbar\omega)}{\hbar\omega}=1-\left(\frac{1}{n_0{}^2}\right) \tag{3}$$

Here, n_0 is the refractive index of the materials in the optical limit $\hbar\omega \to 0$. These parameters are listed in Table 1 and in Ref. Tahir and Tougaard (2012a) for all considered polymers.

The ELF is the main input parameter for determining SP and IMFP based on the Born Ochkur correction in Ref. (Tan et al., 2009, 2004; Tahir et al., 2012) as follows:

$$SP=-\frac{dE}{dS}=\frac{1}{2\pi a_0E}\int_0^{E/2}(\hbar\omega)\mathrm{Im}[-1/\varepsilon(k,\omega)]v(\alpha)d(\hbar\omega) \tag{4}$$

$$\lambda^{-1}=\frac{1}{2\pi a_0E}\int_0^{E/2}\mathrm{Im}[-1/\varepsilon(k,\omega)]w(\alpha)d(\hbar\omega) \tag{5}$$

where E is the kinetic energy of the incident electron, a_0 is the Bohr radius, $\hbar\omega$is the energy loss, Im$[-1/\varepsilon(k,\omega)]$is the energy loss function (ELF), $v(\alpha)$ and $w(\alpha)$are, respectively:

$$v(\alpha)=\frac{2s}{(1+\alpha)(1+\alpha+s)}+\ln\left\{\frac{(1-\alpha^2)(1+\alpha)}{(1-\alpha-s)(1+\alpha+s)^2}\right\} \tag{6}$$

$$w(\alpha)=\frac{3\alpha^2+3\alpha+1}{(1+\alpha)^2}\ln\frac{1+\alpha-s}{1+\alpha}+\ln\frac{1-\alpha}{1-\alpha-s}+\frac{2\alpha^2+\alpha}{(1+\alpha)^2}\ln\frac{1+\alpha}{1+\alpha+s}+\frac{2\alpha s}{(1+\alpha)^2(1+\alpha+s)} \tag{7}$$

with $\alpha=\hbar\omega/E$ and $s=\sqrt{1-2\alpha}$.

3. Results and discussion

Fig. 1 shows that the SP decrease and the IMFP increase with increasing electron energy. SP and IMFP values are similar for the

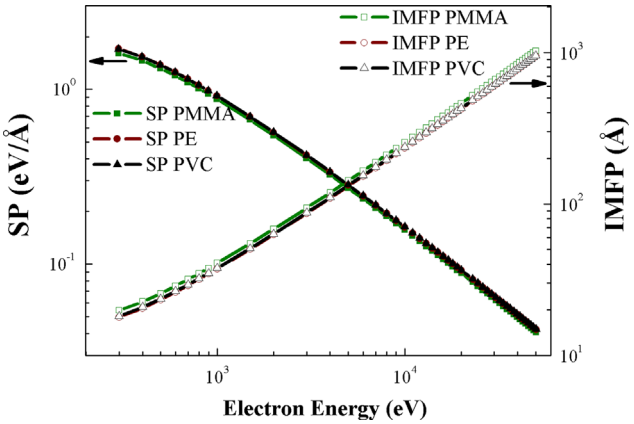

Fig. 1. Stopping power (SP) and inelastic mean free path (IMFP) determined in this study as a function of electron energy for PMMA, PE, and PVC.