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Energy loss of electrons impinging upon glassy carbon, amorphous carbon, and diamond: Comparison between two different dispersion laws

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ABSTRACT

In this paper, we compare and discuss calculated inelastic mean free path, stopping power, range, and reflection electron energy loss spectra obtained using two different and popular dispersion laws. We will present and discuss the results we obtained investigating the interaction of electron beams impinging upon three allotropic forms of carbon, *i.e.* solid glassy carbon, amorphous carbon, and diamond. We will compare numerical results with experimental reflection electron energy loss spectra.

1. Introduction

Carbon can be found in various allotropic forms. The crystalline ones (graphite, diamond) are very well understood both theoretically and experimentally. Much less is known on the properties of amorphous and glassy phases. Due to the extreme variability of these materials, the interpretation of the experimental reflection electron energy loss (REEL) spectra is far from trivial. In this paper, we will present theoretical calculations and compare them to available experimental data, in order to better understand the features observed in the spectra. In particular, we will consider electron spectra, which can be generally described using the dielectric theory for inelastic scattering and the Mott theory for the elastic interactions. The dielectric theory was firstly suggested by Fermi [1], and subsequently developed by various authors [2–5]. In the present paper the Ritchie's dielectric theory is utilized [5].

In the theoretical framework of the Ritchie's dielectric theory, the calculation of the differential inverse inelastic mean free path (DIIMFP) of electrons traveling in solids can be calculated in different ways. The two simplest ones are represented by the electron gas statistical model (EGSM) and by the extended dielectric model (EDM).

The EGSM is based on the assumption that the response of the medium to the perturbation represented by the passage of the incident electrons is that of a system constituted by a set of independent and non-interacting electrons [6–9].

The other simple approach, the EDM, is an efficient alternative to the EGSM and consists in the extension of the optical dielectric function, obtained from empirical data, to non-zero values of the momentum transfer q. It was first proposed by Powell [10] and then developed and used by Ritchie and Howie [11], Liljequist [12], Penn [13], Ashley [14] and Tanuma et al. [15].

In this paper we adopt the EDM as well. The extension to $q \neq 0$ required by this model depends on the selected dispersion law. For recent discussions about this topic, see Kyriakou et al. [16,17], Emfietzoglou et al. [18] and Calliari et al. [19].

We compare and discuss the calculations of inelastic mean free path (IMFP), stopping power, range, and reflected electron energy loss spectra obtained using two different and popular dispersion laws.

These two laws were selected because they are both widely used in the literature with a considerable success in explaining the principle features of REEL spectra. As a consequence, a comparison of their effect on the mean free paths, ranges, and electron energy loss spectra seems to be quite important. By comparing them, we additionally obtain an estimate of the uncertainty in the calculations.

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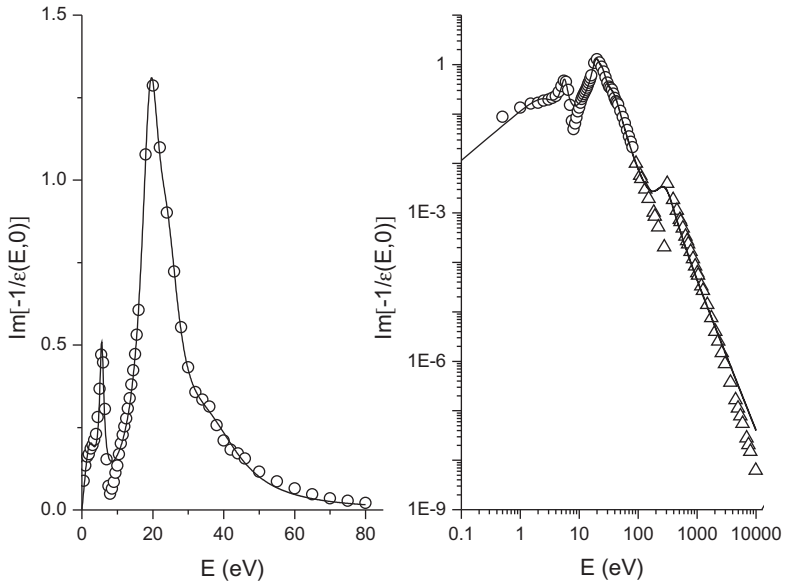

Fig. 1. Energy loss function of glassy carbon in the optical limit. Left panel: energies up to 80 eV. Right panel: energies up to 10000 eV. Circles: Williams and Arakawa experimental data [21] (energies lower than 80 eV). Triangles: Henke et al. experimental data [22] (energies higher than or equal to 80 eV). Line: best fit (parameters can be found in Table 1).

Table 1
Parameters used to fit the optical energy loss function of glassy carbon.

n	E_n (eV)	Γ_n (eV)	A_n (eV^2)
1	2.94	4.25	1.78
2	5.64	1.48	3.39
3	19.58	6.14	119.62
4	24.49	8.76	109.68
5	37.28	23.36	176.81
6	284.2	200.0	169.75

As a case study, we will present the results we obtained investigating the interaction of electron beams impinging upon solid glassy carbon, amorphous carbon, and diamond.

2. Theoretical framework

The DIIMFP is given by

$$\frac{d\lambda_{\text{inel}}^{-1}}{dE} = \frac{1}{\pi a_0 T}\int_{q_-}^{q_+}\frac{dq}{q}\text{Im}\left[-\frac{1}{\varepsilon(E,q)}\right], \tag{1}$$

where

$$q_\pm = \sqrt{2m}\left(\sqrt{T}\pm\sqrt{T-E}\right), \tag{2}$$

a_0 is the Bohr radius and T is the incident electron kinetic energy. It depends on the energy loss function $\text{Im}\left[-\frac{1}{\varepsilon(E,q)}\right]$, that can be represented as a linear combination of Drude-type functions, that is [11]

$$\text{Im}\left[-\frac{1}{\varepsilon(E,q)}\right] = \sum_n A_n D(\Gamma_n(q), E_n(q), E), \tag{3}$$

where

$$D(\Gamma_n, E_n, E) \equiv \frac{\Gamma_n E}{\left(E_n^2 - E^2\right)^2 + (\Gamma_n E)^2}. \tag{4}$$

As a function of the energy loss E, a Drude function $D(\Gamma_n, E_n, E)$ has a maximum located at $E \sim E_n$ (representing the excitation energy) and a full width at half maximum $\Delta E \sim \Gamma_n$ (representing the damping constant). The excitation energies E_n, the damping constants Γ_n and the relative strength parameters A_n are determined, in the $q = 0$ limit, by a best fit with the experimental optical data of the material under investigation, requiring that certain sum-rules are fulfilled [20]. The extension from the optical limit to $q \neq 0$ is obtained by extrapolation, introducing proper dispersion relations for the excitation energy E_n and the damping constant Γ_n.

In this paper, we will consider two different recipes to calculate the dependence of $E_n(q)$ and $\Gamma_n(q)$ on q. For each n, the first recipe (DL1) is given, according to Emfietzoglou et al. [18], by

$$\Gamma_n(q) = \Gamma_n, \tag{5}$$

$$E_n(q) = \sqrt{E_n^2 + \frac{12E_F}{5}\frac{q^2}{2m} + \left(\frac{q^2}{2m}\right)^2}, \tag{6}$$

where E_F is the Fermi energy and m the electron mass. The second recipe (DL2) is provided by the following equations, proposed by Ritchie and Howie [11]

$$\Gamma_n(q) = \sqrt{\Gamma_n^2 + \frac{q^4}{4m^2}}, \tag{7}$$

$$E_n(q) = \left[E_n^p + \left(\frac{q^2}{2m}\right)^p\right]^{1/p}, \tag{8}$$

where $p = 2/3$.

3. Energy loss function in the optical limit

The energy loss function of glassy carbon in the optical limit is presented in Fig. 1. Circles represent the Williams and Arakawa experimental data [21], triangles the Henke et al. experimental data [22]. The solid line is the best fit of the two sets of experimental optical data. The values of the parameters obtained from the best fit of the optical data can be found in Table 1. The reported values are close to those proposed by Ritchie and Howie [11] and by Garcia-Molina et al. [23]. The differences are mainly due to the different ranges of E and the number of oscillators utilized in the fitting function.