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Full Length Article

Calculation of secondary electron emission yields from low-energy electron deposition in tungsten surfaces

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ABSTRACT

We present calculations of secondary electron emission (SEE) yields in tungsten as a function of primary electron energies between 100 eV and 1 keV and incidence angles between 0 and 90°. We conduct a review of the established Monte Carlo methods to simulate multiple electron scattering in solids and select the best suited to study SEE in high-Z metals. We generate secondary electron yield and emission energy functions of the incident energy and angle and fit them to bivariate fitting functions using symbolic regression. We compare the numerical results with experimental data, with good agreement found. Our calculations are the first step towards studying SEE in nanoarchitected surfaces for electric propulsion chamber walls.

1. Introduction

Secondary electron emission (SEE) is the emission of free electrons from a solid surface, which occurs when these surfaces are irradiated with external (also known as *primary*) electrons. SEE is an important process in surface physics with applications in numerous fields, such as electric propulsion [1–5], particle accelerators [6], plasma-walls in fusion reactors [7–11], electron microscopy and spectroscopy [12,13], radio frequency devices [14–16], etc. In Hall thrusters for electric propulsion, a key component is the channel wall lining protecting the magnetic circuits from the discharge plasma. These channel walls are a significant factor in Hall thruster performance and lifetime through its interactions with the discharge plasma. These interactions are governed by the sheath formed along the walls, and so the properties of the sheath determine the amount of electron energy absorbed by the wall, which in turn affects the electron dynamics within the bulk discharge [1,17–19]. Furthermore, the energy imparted by the sheath to the ions within the discharge determines the impact energy and incident angle of ions upon the surface, thus affecting the amount of material sputtered and consequently the wall erosion rate [20,21]. Thus, understanding how SEE affects sheath stability is crucial to make predictions of channel wall lifetime.

Recently, a new wall concept based nano-architected surfaces has been proposed to mitigate surface erosion and SEE [22–25]. Demonstration designs based on high-Z refractory materials have been developed, including architectures based on metal nanowires and nanofoams [26–30]. The idea behind these designs is to take advantage of very-high surface-to-volume ratios to reduce SEE and ion erosion by internal trapping and redeposition. Preliminary designs are based on W, W/Mo, and W/Re structures, known to have intrinsically low sputtering yields secondary electron emission propensity. A principal signature of electron discharges in plasma thrusters is the low primary electron energies expected in the outer sheath, on the order of 100 eV, and only occasionally in the several hundred eV regime. Accurate experimental measurements are exceedingly difficult in this energy range due to the limited thickness of the sheath layer, which is often outside the resolution of experimental probes [31–33]. Modeling then suggests itself as a complementary tool to experiments to increase our qualitative and quantitative understanding of SEE processes.

To quantify the net SEE yield from these surfaces, models must account for the explicit geometry of these structures, which requires high spatial resolution and the capacity to handle large numbers of degrees of freedom. However a precursor step to the development of these descriptions is the characterization of the SEE yield functions as a function of incident electron energy and angle of incidence in flat surfaces. Once defined, these functions can then be implemented at the level of each surface element to create a spatially-dependent emission picture of the SEE process. This is the subject of the present paper: to calculate SEE yield functions from flat W surfaces in terms of primary electron energy and incidence angle. To this end, we carry out Monte Carlo calculations

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of electron scattering processes in pure W using a series of scattering models specifically tailored to high-Z metals.

The paper is organized as follows. First we discuss the theoretical models employed to study electron scattering in W. This is followed by a discussion of the implementation of these models under the umbrella of a Monte Carlo framework. Our results follow, with emphasis on emission yield and energy functions. We finalize with the conclusions and the acknowledgments.

2. Theory and methods

2.1. Electron scattering theory

The present model assumes that electrons travel in an isotropic homogeneous medium undergoing collisions with bulk electrons. Each collision results in a trajectory change with an associated energy loss, which depend on the nature of the electron-electron interaction. As well, collisions may result in secondary electron production. We classify interactions into two broad categories: elastic and inelastic, each characterized by the corresponding collision mean free path and an angular scattering function. These processes are then simulated using a Monte Carlo approach, where collisions are treated stochastically and trajectories are tracked as a sequence of scattering events until the resulting secondary electrons are either thermalized or emitted back from the surface.

Scattering theory provides formulas for the total and the differential scattering cross sections, from which the mean free path and polar scattering angle can be obtained, respectively. Next, we provide a brief description of the essential theory behind each of the distinct collision processes considered here. Our implementation accounts for the particularities of low-energy electron scattering in high-Z materials. The validity range of the present approach in Z, which is for atomic numbers up to 92, and in primary electron energy, from 100 eV to 30 keV.

2.2. Elastic scattering

Elastic scattering takes place between electrons and atomic nuclei, which–due to the large mass difference–results in no net energy loss for the electron, only directional changes [34]. A widely used electron-atom elastic scattering cross section is the screened Rutherford scattering cross section [35,36], which provides a simple analytical form and is straightforward to implement into a Monte Carlo calculation. However, the screened Rutherford scattering is generally not suitable for low-energy electron irradiation of high-Z metals.

In this work, we use an empirical total elastic scattering cross section proposed by Browning et al. (1994), which is obtained via fitting to trends in tabulated Mott scattering cross section data set described by Czyżewski *et al.* [37] using the relativistic Hartree-Fock potential. This is amenable to fast Monte Carlo computations at a high degree of accuracy. The equation for the total elastic scattering cross section is [38,39]:

$$\sigma_{el} = \frac{3.0\times10^{-18}Z^{1.7}}{(E + 0.005Z^{1.7}E^{0.5} + 0.0007Z^2/E^{0.5})} \quad [\mathrm{cm}^2], \tag{1}$$

which is valid for atomic numbers up to 92 and for energies from 100 eV to 30 keV. From this, the elastic mean free path can be derived:

$$\lambda_{el} = \frac{1}{N\sigma_{el}} = \frac{AW}{N_a\rho\sigma_{el}} \quad [\mathrm{cm}] \tag{2}$$

where N is the number of atoms per cm^3. For its part, the polar scattering angle can be obtained by a random number R uniformly distributed between 0 and 1:

$$R = \frac{\int_0^{\theta}\left(\frac{d\sigma_R}{d\Omega}\right)d\Omega}{\int_0^{\pi}\left(\frac{d\sigma_R}{d\Omega}\right)d\Omega} \tag{3}$$

where $d\Omega = 2\pi\sin\theta d\theta$ is the infinitesimal solid angle.

Solving the above equation for the Mott cross section requires numerical integration, as there is no simple analytical form for the polar scattering angle θ. Drouin [40] et al. (1994) gives a parameterized form of the function as

$$\cos\left(\theta_i^{\beta}\right) = 1 - \frac{2\alpha R^*}{1+\alpha-R^*} \tag{4}$$

where θ_i is given in degrees. Then first parameter, α, as a function of the energy is obtained with

$$\log_{10}(\alpha) = a + b\log_{10}(E) + c\log_{10}^2(E) + \frac{d}{e^{\log_{10}(E)}} \tag{5}$$

where E is the energy in keV, a, b, c and d are constants that have been calculated using the least-square method, and $e = 2.7813$. A tabulation form of a, b, c and d for the first 94 elements of the periodic table is found in Table 2 in Ref. [40]. For tungsten ($Z = 74$), $a = -2.0205, b = -1.2589, c = 0.271737, d = -0.695477$.

The second parameter, β, is calculated using the following equations:

$$\begin{aligned} \beta^* &= a + b\sqrt{E}\ln(E) + \frac{c\ln(E)}{E} + \frac{d}{E} \\ \beta &= \begin{cases} 1 & \text{if} \quad \beta^* > 1 \\ \beta^* & \text{if} \quad \beta^* \le 1 \end{cases} \end{aligned} \tag{6}$$

where E is the energy in keV, a, b, c and d are constants that have been obtained using the least-squares fitting. A tabulation form of a, b, c and d for the first 94 elements of the periodic table is found in Table 3 in reference [40]. For tungsten ($Z = 74$), $a = 0.71392, b = 0.00197916, c = -0.0172852, d = -0.0570799$.

The third parameter, R^* is obtained as:

$$R^* = R \times R_{max} \tag{7}$$

where R is a random number uniformly distributed between 0 and 1 and R_{max} is the value of R^* obtained when θ_i is set to 180° in Eq. (4), i.e.:

$$R_{max} = \frac{\cos(180^{\beta}) + \alpha\cos(180^{\beta}) - 1 - \alpha}{\cos(180^{\beta}) - 1 - 2\alpha} \tag{8}$$

The azimuthal angle ϕ can take any value in the range 0–2π as determined by a random number R uniformly distributed in that range.

$$\phi = 2\pi R \tag{9}$$

2.3. Inelastic scattering

In contrast to elastic scattering, inelastic scattering implies collisional energy loss. There are several distinct inelastic interaction processes to be considered, including phonon excitation, secondary electron excitation, *Bremsstrahlung* or continuum X-ray generation, and ionization of inner electron shells. Each mechanism is described by a model that provides expressions for the scattering cross section, scattering angle, and mean free path. The physics behind some of these processes is complex, and detailed expressions for the associated cross sections are often unavailable [41,42].

In conventional Monte Carlo approaches, Bethe's theory of stopping power based on a continuous slowing-down approximation (CSDA) [35,43,44] is used to describe the average energy dissipation rate of a penetrating electron along its path, in which the contribution of all possible excitation processes to the energy loss has been represented by a factor called the mean ionization