Monte Carlo modeling of low-energy electron-induced secondary electron emission yields in micro-architected boron nitride surfaces

https://escholarship.org/uc/item/5d99p79d

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 454

0168-583X

Chang, Hsing-Yin
Alvarado, Andrew
Weber, Trey
et al.

2019-09-01

10.1016/j.nimb.2019.05.079

Peer reviewed
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...
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]:

$$\sigma_{el} = \frac{3 \times 10^{-18} Z^2}{(E + 0.005 Z^2 / E^{1.5} + 0.0007 Z^2 / E^{1.5})} \ [\text{cm}^2],$$

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:

$$\lambda_{el} = \frac{1}{N \sigma_{el}} = \frac{AW}{Ne_{el}} \ [\text{cm}]$$

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:

$$R = \int_0^{\theta} \frac{d\sigma_{el}}{d\Omega} \ d\Omega \int_0^{\phi} \frac{d\sigma_{el}}{d\Omega} \ d\Omega$$

where $d\Omega = 2\pi \sin d\theta$ 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 $\theta$. Drouin [40] et al. (1994) gives a parameterized form of the function as

$$\cos (\theta_i) = 1 - \frac{2xR}{1 + z - R}$$

where $\theta_i$ is given in degrees. Then first parameter, $x$, as a function of the energy is obtained with

$$\log_{10}(x) = a + b \log_{10}(E) + c \log_{10}(E) + d \log_{10}(\log_{10}(E))$$

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 ($Z = 74$), $a = -0.2025, b = -1.2589, c = 0.271737, d = -0.695477$.

The second parameter, $\beta_i$, is calculated using the following equations:

$$\beta_i = a + b \sqrt{E} \ln(E) + c \ln(E) + \frac{d}{E}$$

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 ($Z = 74$), $a = 0.71392, b = 0.001179, c = -0.0172852, d = -0.0570799$.

The third parameter, $R_i$ is obtained as:

$$R_i = R \times R_{\text{max}}$$

where $R$ is a random number uniformly distributed between 0 and 1 and $R_{\text{max}}$ is the value of $R_i$ obtained when $\theta_i$ is set to 180° in Eq. (4), i.e.: $R_{\text{max}} = \cos(180°) + \alpha \cos(180°) - 1 - \frac{\alpha}{\cos(180°) - 1 - 2\alpha}$

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

$$\phi = 2\pi R$$

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, Br"{u}mstrahlung 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
energy, \( J \). However, this formula is not valid in the low energy regime (0.1–30 keV) or for high atomic number elements \((Z > 30)\). To resolve this, much effort has been devoted to modifying the Bethe formula, from which systematization of tabulated electron stopping powers for various elements and attempts to simplify the calculations have emerged. [45–49] In general, the use of these formulas for elements or compounds with fitting parameters requires a detailed and accurate supply of experimental data on which to base its physics and against which to test its predictions. [50] Nevertheless, the CSDA strategy may still become obsolete when an electron occasionally loses a large fraction of its energy in a single collision as well as when secondary electron emission distribution spectra are required. To develop a more comprehensive Monte Carlo approach, incorporating differential cross sections for each of the inelastic events seems necessary [51–54].

Ritchie et al. (1969) have demonstrated that the stopping power described by Bethe’s formula is obtained by the summation of theoretical stopping powers for conduction electron, plasmon and L-shell electron excitations for aluminum. [53] Fitting (1974) [55] has also shown that this stopping power derived by Ritchie et al. is in very good agreement with experimental investigation even in the energy range between 0.8 and 4 keV. Accordingly, the model of inelastic scatterings considered in the present approach are electron-conduction electron scattering, electron-plasmon scattering and electron-shell electron scattering as shown in Fig. 1.

2.3.1. Inner shell electron ionization

The classical formalism of Gryziński (1965) [56–59] has been adopted to describe inner-shell electron ionization. The differential cross section can be written as:

\[
\frac{d\sigma_i(\Delta E)}{d\Delta E} = \frac{\pi e^4 E_p}{(\Delta E)^3} \left( \frac{E}{E + E_p} \right)^{3/2} \left( 1 - \frac{\Delta E}{E} \right)^{1/2} \left( \frac{E_p}{E_p + \Delta E} \right) \frac{\Delta E}{E} \left[ 2.7 + \left( \frac{E - \Delta E}{E} \right)^{1/2} \right] \quad \text{(10)}
\]

where \( \Delta E, E \) and \( E_p \) are the energy loss, the primary electron energy, and the mean electron binding energy, respectively.

At each inelastic scattering event, the energy loss of the primary electron resulting from an inelastic scattering with the shell is determined using a uniform random number \( R \) and by finding a value of \( \Delta E \) which satisfies the relation

\[
R = \int_{E_p}^{E_{\text{max}}} d\sigma_i(\Delta E) \frac{d\Delta E}{\sigma_i}
\]

The integral is given by the approximate expression [60]

\[
\int_{E_p}^{E_{\text{max}}} d\sigma_i(\Delta E) \frac{d\Delta E}{\sigma_i} = \left( \frac{\pi e^4 E_p}{(\Delta E)^3} \right) \left( \frac{E}{E + E_p} \right)^{3/2} \left( 1 - \frac{\Delta E}{E} \right)^{1/2} \left[ 2.7 + \left( \frac{E - \Delta E}{E} \right)^{1/2} \right]
\]

where \( n_i \) is the occupation number of electrons in the shell.

The total cross section of the inner electron excitation is obtained by integrating over all possible values of \( \Delta E \)

\[
\sigma_i(E) = \int_{E_p}^{E_{\text{max}}} d\sigma_i(\Delta E) \frac{d\Delta E}{\sigma_i} = 6.5141 \times 10^{-14} n_i E_p \left( \frac{E - E_p}{E + E_p} \right)^{3/2}
\]

where the maximum amount of energy that can be lost \( \Delta E_{\text{max}} \) is equal to \( E \).

When the random number selection gives an energy loss less than the binding energy \( E_p \), the actual energy loss is set to be zero. The scattering angle for an inelastic electron-electron event is calculated according to the binary collision approximation (BCA) as

\[
\sin \theta = \left( \frac{\Delta E}{E} \right)^{1/2}
\]

In tungsten, for primary energies \( E \leq 1 \) keV, inner shell electron ionization can be safely neglected, as the energy is insufficient to knock out inner shell electrons.

\[\phi = 2\pi R\]

![Fig. 1. Schematic diagram of the discrete collision model of electron scattering simulated using Monte Carlo calculation.](Image)
2.3.2. Conduction electron excitation

For metals bombarded by electrons, Streitwolf (1959) [61] has given the differential cross section for conduction electron excitation by using perturbation theory as

$$\frac{d\sigma_c(E_{\text{SE}})}{dE_{\text{SE}}} = \frac{e^4N_a\pi}{E} \frac{E - E_{\text{SE}} - \Phi}{\Phi(E - E_{\text{SE}})} \frac{\sqrt{\Delta E}}{E}$$ \hspace{1cm} (15)

The total energy loss cross section \(\sigma_c(E)\) can be obtained by integrating the above expression between the lower energy limit \(E_F + \Phi\) and the upper energy limit \(E\):

$$\sigma_c(E) = \frac{e^4N_a\pi}{E} \int_{E_F + \Phi}^{E} \frac{E - E_{\text{SE}} - \Phi}{\Phi(E - E_{\text{SE}})} \frac{\sqrt{\Delta E}}{E} \, dE$$ \hspace{1cm} (16)

The obtained relation samples the energy of the secondary electron with the random number \(R\):

$$E_{\text{SE}}(R) = [RE_F - A(E_F + \Phi)]/(E - A)$$ \hspace{1cm} (17)

where \(\Phi\) is the work function and \(A = (E - E_z)/(E - E_F)\). Once the energy of the secondary electron is known (equal to the energy lost by the primary electron), the next question is how the two electrons are oriented in space. More accurate results can be obtained if the classical BCA is used, which results from conservation of energy and momentum. The azimuthal angle is again assumed to be isotropic. For the incident electron, we then have:

$$\sin \theta = \sqrt{\frac{\Delta E}{E}}$$ \hspace{1cm} (18)
$$\phi = 2\pi R$$

where \(\Delta E\) is the energy lost by the incident electron. For the secondary electrons, scattering angles can be calculated as follow:

$$\sin \Theta = \cos \theta$$ \hspace{1cm} (19)
$$\varphi = \pi + \phi$$ \hspace{1cm} (20)

The above expression is applied to the inner shell electron as well as conduction electron excitations.

2.3.3. Plasmon excitation

The Coulomb field of the primary electron can perturb electrons of the solid at relatively long range as it passes through the target. The primary electron can excite oscillations (known as plasmons) in the conduction electron gas that exists in a metallic sample with loosely bound outer shell electrons. The differential cross section for plasmon excitation is given by Ferrel (1956) [62–64], per conduction-band electron per unit volume

$$\frac{d\sigma_p(E, \theta)}{d\Omega} = \frac{1}{2\pi a_0} \frac{\theta_p}{\theta^2 + \theta_p^2}$$ \hspace{1cm} (21)

$$\theta_p = \frac{\Delta E}{2E} = \frac{\hbar c}{2E}$$ \hspace{1cm} (22)

where \(a_0\) is Bohr radius \((5.29 \times 10^{-11} \text{ cm})\). In plasmon scattering, primary electron energy loss is quantized and ranges from 3 to 30 eV depending on the target species, which is detected as strong features in electron energy-loss spectra (EELS). Plasmon scattering is so sharply peaked forward that the total plasmon cross section, \(\sigma_p\), can be found by setting \(d\Omega = 2\pi \sin \theta d\theta\) as \(2\pi \sin \theta d\theta\):

$$\sigma_p = \int d\sigma_p(\theta) = \frac{\theta_p}{2\pi a_0} \int_{0}^{\pi} \frac{2\pi \sin \theta d\theta}{\theta^2 + \theta_p^2}$$ \hspace{1cm} (23)

By assuming the upper integration limit as \(\theta_1 = 0.175\) rad, where \(\theta = \sin \theta\), and incorporating the factor \((n_a AW/N_{\text{atom}})\) to put the cross section on a per-atom/cm² basis gives the total cross section of the plasmon excitation as

$$\sigma_p = \frac{n_a AW\theta_0}{2N_{\text{atom}}D} \left[ \ln(\theta_0^2 + 0.175^2) - \ln(\theta_0^2) \right] \text{ cm}^2$$ \hspace{1cm} (24)

where \(n_a\) is the number of conduction-band electrons per atom. Essentially, the scattering of primary electrons due to plasmon excitations is restricted with \(\theta < \theta_{\text{max}}\), \(\text{k}\) being the cut-off wavenumber. Since \(\theta_{\text{max}}\) is so small, about 10 mrad in the energy range discussed here, the angular deflection due to plasmon excitation is neglected in this approach.

Again, the azimuthal angle \(\phi\) can take on any value in the range 0 to 2\(\pi\) selected by a random number \(R\) uniformly distributed in that range.

$$\phi = 2\pi R$$

3. Monte Carlo calculations

As indicated above, electron trajectories are simulated by generating a spatial sequence of collisions by randomly sampling from among all possible scattering events. The distance traveled by electrons in between collisions, \(\Delta s\), is assumed to follow a Poisson distribution defined by the total mean free path \(\lambda_t\) [35]:

$$\Delta s = -\lambda_t \log R$$ \hspace{1cm} (25)

where

$$\frac{1}{\lambda_t} = \frac{1}{\lambda_{el}} + \frac{1}{\lambda_p} + \frac{1}{\lambda_c} + \frac{1}{\lambda_s} = N(\sigma_{el} + \sigma_p + \sigma_c + \sigma_s)$$ \hspace{1cm} (26)

\(N\) is the number of atoms per cm³ and \(R\) is a random number uniformly distributed in the interval \((0,1)\). From this, we define the following probabilities:

$$P_{el} = \lambda_t/\lambda_{el}\text{: the probability that the next collision will be elastic}$$
$$P_p = \lambda_t/\lambda_p\text{: the probability that the next collision will cause a plasmon excitation}$$
$$P_c = \lambda_t/\lambda_c\text{: the probability that the next collision will cause a conduction electron excitation}$$
$$P_s = \lambda_t/\lambda_s\text{: the probability that the next collision will cause an inner shell electron excitation}$$ \hspace{1cm} (27)

The type of collision is then chosen based on the following partition of the value of \(R\):

$$0 < R \leq P_{el} \Rightarrow \text{elastic scattering}$$
$$P_{el} < R \leq P_{el} + P_p \Rightarrow \text{plasmon excitation}$$
$$P_{el} + P_p < R \leq P_{el} + P_p + P_c \Rightarrow \text{conduction electron excitation}$$
$$P_{el} + P_p + P_c < R \leq 1 \Rightarrow \text{inner shell electron excitation}$$ \hspace{1cm} (28)

The flow diagram corresponding to the implementation of the model just described is provided in Appendix C. Following this approach, electron trajectories are tracked in the energy-position space until a scattered electron either thermalizes, i.e. its energy follows below the surface escape threshold (Fermi level plus workfunction) within the material, or reaches the surface with a velocity having a component pointing along the surface normal with an energy larger than the escape threshold. In the latter case, the electron is tallied as a secondary electron and its energy and exit angle
are recorded.
Next we analyze the Monte Carlo calculations performed following this method and present results of secondary electron yield and emission energies as a function of primary electron energy and angle of incidence.

4. Results

The total secondary electron yield for perfectly-flat tungsten surfaces is calculated for primary incident angles of $0^\circ$, $30^\circ$, $45^\circ$, $60^\circ$, $75^\circ$ and $89^\circ$ measured off the surface normal, and incident energies in the range 100–1000 eV. In this work, the typical number of primary particles simulated ranges between $10^4$ and $10^5$, which generally results in statistical errors around 3%. Our first set of results includes the energy and angular distributions of emitted secondary electrons for normal incidence and 100 eV and a primary electron energy of 100 eV. The normalized distributions are given in Fig. 2a and b, where the characteristic energy decay of $1/\epsilon$ and cosine angular distribution of collisional processes can be appreciated in each case. One of the advantages of using a discrete event method for simulating electron scattering processes is that useful information of discrete nature can be extracted from the data. For example, in Fig. 3a we show the depths from which secondary electrons are emitted (last scattering collision inside the material) as well as the depth distribution of thermalized (non-emitted) electrons, i.e. the depth at which electrons attain an energy less than the threshold. Both cases are for normal incidence and $E = 100$ eV. In Fig. 3b we break the total number of collisions down into the main scattering

---

**Fig. 2.** Normalized distributions for 100-eV primary electrons incident at $0^\circ$: (a) Energy distribution of secondary electrons; (b) Angular distribution of secondary electrons.

**Fig. 3.** (a) Depth distribution of both emitted and thermalized (captured) electrons for a primary electron energy and incident angle of 100 eV and $0^\circ$. (b) Relative occurrence of the main scattering mechanisms as a function of primary energy for normal incidence.
modes as a function of primary energy and normal incidence. It can be seen that scattering with conduction electrons is always the dominant mechanism, although its relative importance reduces with $E$.

Next, we plot the SEE yields as a function of primary electron energy for angles of incidence of 0 and 45° to facilitate comparison with existing experimental data and other published Monte Carlo simulation results. The results are shown in Fig. 4a and b, respectively, with error bars provided in each case. In general, the simulation results are found to agree reasonably well with experimental data. The agreement is slightly worse for 45° than for 0° incidence, which we rationalize in terms of the higher incidence direction. It is well-known that the fraction of reflected particles increases with the angle of incidence [71]. In addition, the roughness of ‘real’ experimental surfaces compared to the ideally-smooth ones in the model likely plays a significant role in the comparison. SEE yields as a function of $E$ for all angles of incidence considered here are given in Fig. 5.

Surface plots of both SEE energy distributions and the yields are given in Fig. 6a and b. As mentioned earlier, these data will be used in ray-tracing Monte Carlo simulations of SEE in arbitrary surface geometries. In these simulations, primary rays are generated above the material surface with the corresponding incident energy $E$. Intersections of these primary rays with surface elements determine the corresponding angle of incidence $\alpha$. $E$ and $\alpha$ are then used to sample from the data shown in, e.g., Fig. 2, after which secondary rays with appropriate energies $E_{SE}$ and exit angles (sampled from a cosine distribution) are generated. These ‘daughter’ rays are themselves tracked in their interactions with other surface elements, after which the sequence is repeated and subsequent generations of rays are produced. This process goes on until rays either escape the surface with an upward velocity –in which case the event is tallied as a successful SEE event– or until their energy is below the threshold escape energy (Fermi level plus workfunction). However, directly interpolating from our data tables potentially hundreds of thousands of times can slow down the simulations considerably. To avoid that, it is more efficient to fit the data to suitable analytical expressions that can be evaluated very fast on demand. To this end, we fit our raw data to bivariate mathematical functions obtained using symbolic regression (SR), which is a type of genetic evolutionary algorithm for machine learning which utilizes evolutionary searches to determine both the parameters and the form of the fitting expressions simultaneously, to speed up our calculation. We have used the trial version of Eureqa [72,73], a commercial SR engine, to generate a catalog of potential candidate expressions for mathematical fitting. We then select the final expression by capping the fitting errors to be no higher than the intrinsic statistical errors of the Monte Carlo simulations.
Distributions from an ideally-flat W as a function of primary electron energy and angle of incidence.

196

Ding et al. [69] use Penn’s dielectric function [74] for electron own differential cross sections, corresponding to valence, inner
tions thereof). For their part, inelastic scattering processes in this
els treat elastic interactions within Mott’s formalism [34] (or adap-
approximations introduced in the model are described. Most mod-
Monte Carlo simulations depends directly on how precisely the
theoretical treatment of electron scattering a tractable analyt-
Physics behind SEE and are just intended for efficient numerical
calculations (≈ 3%). This ensures that the fitted functions always
provide solutions to within the natural variability of the fitted data. Beyond that, we generally try to use functions that are well
behaved numerically in as wide an energy range as possible, e.g.
discarding those with logarithmic terms, etc. The final expressions
for the total SEE yield and energy distributions are

\[
\begin{align*}
\gamma(E, \alpha) &= 3.05288 + 1.7949 \times 10^{-3} a^2 + 6.15912 \times 10^{-7} E^2 \\
&\quad + (3.71317 \times 10^{-2} - \exp(4.8259 \times 10^{-2} a))/(-8.760195 \times 10^{-1} - E) \\
&\quad - 1.974 \times 10^{-4} E - 1.0971 \times 10^{-1} \cos(1.20187 \times 10^{-1} + 2.469421 a) \\
\end{align*}
\]

(29)

\[
E_{\text{ef}}(E, \alpha) = 1.95 \times 10^{-1} E + 1.69 \times 10^{-6} E^2 + 1.48 \times 10^{-1} a \sin(E) \\
+ 3.44 \times 10^{-15} E a^2 - 6.54
\]

(30)

We note that these expressions do not necessarily reflect the
physics behind SEE and are just intended for efficient numerical
evaluations strictly in the ranges shown in the figures.

5. Discussion and conclusions

Electron-matter interactions are complex processes. To make
the theoretical treatment of electron scattering a tractable analytical
problem, it is assumed that elastic scattering occurs through the
interatomic potential, while inelastic scattering only through
electron–electron interactions. Evidently, the accuracy of the
Monte Carlo simulations depends directly on how precisely the
approximations introduced in the model are described. Most mod-
els treat elastic interactions within Mott’s formalism [34] (or adap-
tations thereof). For their part, inelastic scattering processes in this
work are considered individually, each one characterized by its
own differential cross sections, corresponding to valence, inner
shell, conduction, and plasmon electron excitation. In contrast,
Ding et al. [69] use Penn’s dielectric function [74] for electron
inelastic scattering obtained from a modification of the statistical
approximation. Many other models for metals account for valence
interactions only [35,75,76]. Here, we improve in these models,
although we do not capture the generation of SE from plasmon
decay, backscattered electrons, reflected electrons, and transmitted
electrons (coming out from the back side of the sample). This must
be kept in mind when comparing the simulation results with
experimental data (cf. Fig. 4). In this sense, it can be said that our
results provide a first-order check of the importance of internal
scattering processes, which helps us understand the governing
physics behind SEE.

In any case, discrete event simulations—e.g. as the Monte Carlo
model implemented in this paper—present the advantage that they
provide a measure of the statistical errors associated with a given
formulation. This is not just a numerical matter because experi-
mental measurements themselves correspond to averages of a
given realization of the scattering process. In the discrete approach
the energy loss of electrons traveling through a solid is determined
by considering different inelastic scattering processes—including
conduction electron excitation, plasmon decay, and inner shell
electron ionization—are considered individually, whereas within
the so-called continuous slowing down approximation (CSDA),
the overall inelastic scattering mechanisms are averaged out by
using the total stopping power. From this point of view, the CSDA
and the discrete-event simulation method would formally con-
verge in the limit of an infinite number of events. Discrete simula-
tions also allow a better physical and spatial dissection of electron
scattering processes, providing spatial distributions and break-
downs among the different scattering mechanisms. This informa-
tion is important to ascertain what scattering events dominate
the secondary electron emission process in each material. This is
what is shown in Fig. 3b, where the partition of scattering mecha-
nisms for normal incidence and 100 eV primary energy is given. A
disadvantage of discrete vs continuous simulations is, however, the
longer computational cost required to obtain acceptable statistics.
Modelers, therefore, must weigh in each of these factors (better
spatial resolution and statistical information vs worse computa-
tional efficiency) and decide what approach to use.

To summarize, in this work we have carried out Monte Carlo
calculations of low energy electron induced SE emission from flat
tungsten surfaces. Our model includes multiple elastic and inelas-
tic scattering processes, implemented via a discrete energy loss
approach. We compare predictions of our model with other Monte
Carlo techniques as well as experimental data, with generally good
agreement found. We have calculated the total SEE yield and
egin{figure}
(a) Surface plot of the total SEE yield from an ideally-flat W as a function of primary electron energy and angle of incidence. (b) Surface plot of the SEE energy distributions from an ideally-flat W as a function of primary electron energy and angle of incidence.

Fig. 6.
secondary electron energy spectrum for primary electron beams at incident angles of 0°, 30°, 45°, 60°, 75° and 89°, in the range 100–1000 eV. We have used SR to obtain analytical expressions that represent the numerical data. These functions are currently being used in ray-tracing Monte Carlo simulations of SEE in arbitrary surface geometries.

Acknowledgement

The authors acknowledge support from the Air Force Office of Scientific Research (AFOSR), through award number FA9550-11-1-0282 with UCLA.

Appendix A. List of Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>a₀</td>
<td>Bohr radius</td>
</tr>
<tr>
<td>AW</td>
<td>atomic weight</td>
</tr>
<tr>
<td>Z</td>
<td>atomic number</td>
</tr>
<tr>
<td>N₀</td>
<td>Avogadro’s number</td>
</tr>
<tr>
<td>ρ</td>
<td>density of the target</td>
</tr>
<tr>
<td>N = ρNₑ/AW</td>
<td>atomic number density</td>
</tr>
<tr>
<td>rₑ</td>
<td>number of electrons in shell or subshell</td>
</tr>
<tr>
<td>nₑ</td>
<td>number of conduction-band electrons per atom</td>
</tr>
<tr>
<td>e</td>
<td>electron charge</td>
</tr>
<tr>
<td>ε</td>
<td>permittivity of vacuum</td>
</tr>
<tr>
<td>mₑ</td>
<td>mass of electron</td>
</tr>
<tr>
<td>h</td>
<td>reduced Planck constant</td>
</tr>
<tr>
<td>ωₑ</td>
<td>plasma frequency</td>
</tr>
<tr>
<td>Eₑ</td>
<td>primary electron energy</td>
</tr>
<tr>
<td>E_SE</td>
<td>secondary electron energy</td>
</tr>
<tr>
<td>E_F</td>
<td>Fermi energy</td>
</tr>
<tr>
<td>k_F</td>
<td>Fermi wave number</td>
</tr>
<tr>
<td>E_B</td>
<td>binding energy of the shell</td>
</tr>
<tr>
<td>E_pl</td>
<td>plasmon energy</td>
</tr>
<tr>
<td>ΔE</td>
<td>energy loss of primary electron</td>
</tr>
<tr>
<td>Φ</td>
<td>work function</td>
</tr>
<tr>
<td>J</td>
<td>mean ionization potential</td>
</tr>
<tr>
<td>z</td>
<td>incident angle of primary electron</td>
</tr>
<tr>
<td>σₑl</td>
<td>elastic scattering cross section</td>
</tr>
<tr>
<td>σ_p</td>
<td>plasmon excitation cross section</td>
</tr>
<tr>
<td>σ_c</td>
<td>conduction electron ionization cross section</td>
</tr>
<tr>
<td>σ_s</td>
<td>inner shell electron ionization cross section of differential scattering cross section with respect to direction</td>
</tr>
<tr>
<td>dσ/dΩ</td>
<td>differential scattering cross section with respect to direction</td>
</tr>
<tr>
<td>λₑl</td>
<td>elastic mean free path</td>
</tr>
<tr>
<td>λ_p</td>
<td>plasmon excitation mean free path</td>
</tr>
<tr>
<td>λ_c</td>
<td>conduction electron excitation mean free path</td>
</tr>
<tr>
<td>λ_s</td>
<td>inner shell electron excitation mean free path</td>
</tr>
<tr>
<td>λ_F</td>
<td>total mean free path</td>
</tr>
<tr>
<td>θₑl</td>
<td>polar scattering angle of the primary electron</td>
</tr>
<tr>
<td>θ_p</td>
<td>plasmon loss scattering angle</td>
</tr>
<tr>
<td>d</td>
<td>depth</td>
</tr>
</tbody>
</table>

Appendix B. Constants & kinematical quantities

- N₀ = 6.022 × 10²³, Avogadro’s number
- ε = 8.85 × 10⁻¹² [F/m], permittivity of vacuum
- mₑ = 9.1 × 10⁻³¹ [kg]
- e = 1.6 × 10⁻¹⁹ [C], electron charge
- h = 6.58 × 10⁻¹⁶ [eV · s/rad], reduced Planck constant
- Eₑ = mₑe⁴/ℏ² = 2Ry = 27.2114 [eV], Hartree energy
- Ry = 13.6 [eV], Rydberg energy
- α₀ = ℏ²/(mₑe²) = 5.29177 × 10⁻⁹ [cm], Bohr radius
- πe⁴ = π(a₀Eₑ)² = 6.5141 × 10⁻¹⁴ [cm² eV²]
- mc² = 510.999 [keV], rest energy of the electron

The Fermi energy can be estimated using the number of electrons per unit volume as

\[ E_F = \frac{\pi}{3} \frac{\hbar^2}{m_ec^2} n^{2/3} [eV] = 1.69253 n_0^{2/3} [eV] \]

where n and n₀ are in the units of [cm⁻³] and n = n₀ × 10²². The Fermi wave number is calculated as

\[ k_F = 6.66511 \times 10^7 n_0^{1/3} [cm^{-1}] \]

The Fermi velocity is calculated as

\[ v_F = 7.71603 \times 10^7 n_0^{1/3} [cm/s] \]

Appendix C. Program flowchart

Fig. 7.

Appendix D. Definition of coordinate system

The basic geometry for the simulation assumes that the electron undergoes an elastic scattering event at some point P₀, having traveled to P₀ from a previous scattering event at Pₙ₋₁ as shown in Fig. 8. To calculate the position of the new scattering point Pₙ₊₁, we first require to know the distance Δₙ₋₁ between Pₙ₋₁ and the preceding point Pₙ.

The path is described using direction cosines, ca, cb and cc. The coordinates at the end of the step at Pₙ₋₁, xₙ₋₁, yₙ₋₁, and zₙ₋₁, are then related to the coordinates x₀, y₀, and z₀ at P₀ by the formulas [65]

\[ x_{n+1} = x_n + \Delta s_{n+1} \cdot ca \]
\[ y_{n+1} = y_n + \Delta s_{n+1} \cdot cb \]
\[ z_{n+1} = z_n + \Delta s_{n+1} \cdot cc \]

The direction cosines ca, cb, cc are found from the direction cosines cx, cy and cz with which the electron reached P₀. The result is

\[ ca = (cx \cdot \cos \theta) + (V_1 \cdot V_3) + (cy \cdot V_2 \cdot V_4) \]
\[ cb = (cy \cdot \cos \theta) + (V_4 \cdot (cz \cdot V_1 - cx \cdot V_2)) \]
\[ cc = (cz \cdot \cos \theta) + (V_2 \cdot V_3) - (cy \cdot V_1 \cdot V_4) \]

where

\[ V_1 = AN \cdot \sin \theta \]
\[ V_2 = AM \cdot AN \sin \theta \]
\[ V_3 = \cos \phi \]
\[ V_4 = \sin \phi \]
and

$$AM = -\frac{CX}{CZ}$$

$$AN = \frac{1}{\sqrt{1 + AM \cdot AM}}$$

References
