Refinement of Monte Carlo simulations of electron–specimen interaction in low-voltage SEM

Erik Kieft and Eric Bosch

Philips Research Laboratories Eindhoven, High Tech Campus 34, 5656 AE Eindhoven, The Netherlands

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Abstract
A Monte Carlo tool is presented for the simulation of secondary electron (SE) emission in a scanning electron microscope (SEM). The tool is based on the Geant4 platform of CERN. The modularity of this platform makes it comparatively easy to add and test individual physical models. Our aim has been to develop a flexible and generally applicable tool, while at the same time including a good description of low-energy (<50 eV) interactions of electrons with matter. To this end we have combined Mott cross-sections with phonon-scattering based cross-sections for the elastic scattering of electrons, and we have adopted a dielectric function theory approach for inelastic scattering and generation of SEs. A detailed model of the electromagnetic fields from an actual SEM column has been included in the tool for ray tracing of secondary and backscattered electrons. Our models have been validated against experimental results through comparison of the simulation results with experimental yields, SE spectra and SEM images. It is demonstrated that the resulting simulation package is capable of quantitatively predicting experimental SEM images and is an important tool in building a deeper understanding of SEM imaging.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
As feature sizes in the semiconductor industry continue to decrease, scanning electron microscopy is nowadays the method of choice for determination of critical dimensions (CDs). Feature sizes are now becoming so small that a detailed knowledge of the image contrast at the nanometre scale is essential in order to be able to accurately measure these dimensions from scanning electron microscope (SEM) or scanning transmission electron microscope (STEM) images. Computer simulations are a valuable tool for understanding how this image contrast is formed.

As many semiconductor structures contain non-conducting layers there is a trend to use low voltage SEM in order to be able to better control the effect of charging on image quality during imaging. At energies below 1 keV the main tool for high resolution imaging is to use secondary electron (SE) images, formed by electrons that leave the surface at energies that are typically below 10 eV. Understanding the contrast and resolution of the resulting SEM images necessitates the development of a simulation tool that is accurate down to these low energies.

There has been active research on models of the interactions of electrons with matter in the required energy range (0–30 keV) and this has led to the development of a number of software packages for simulating electron trajectories [1–8]. However, a survey of simulation tools that are publicly or commercially available showed that few of these packages are able to deal with energies below 100 eV and complex geometries combined with ray tracing through user defined electromagnetic fields. These are the ingredients necessary to make a quantitative comparison of simulations with actual SEM images.

In order to achieve our goal of obtaining quantitative predictions that can be directly compared with experimental SEM images, we built our own simulation tool using the Geant4 platform for Monte Carlo (MC) simulations developed for high-energy physics (HEP) at CERN [9]. This platform...
provides an infrastructure for generating and tracking particles, and defining complex geometries and detectors. We added the physical processes for the interaction of low-energy electrons with solids to the already existing models for higher energies (>250 eV). Furthermore the Geant4 platform allows integrating MC simulations of the electron–material interactions with ray tracing of backscattered and SEs through a realistic SEM column field. Hence simulations of the creation and the detection of secondary and backscattered electrons (BSEs) are combined in one package.

Our aim was not only to build a simulation tool but also to develop a procedure for validation of the model using experimental results. The end result is a software tool that can be used to make quantitative predictions on the result of experimental SEM images, especially using SE detection.

We start by introducing the physical models underlying our simulation tool. Then we describe the method for the experimental validation process that we developed, ending with a quantitative comparison between an actual experimental SEM image and simulations based on our tool.

2. Physical interaction models

With the main Monte Carlo simulator engine in place, only the models of the physical processes that are of interest in the energy range that is used in SEM imaging (i.e. from a few electronvolts up to 30 keV) need to be supplied. The Geant4 platform is highly modular, enabling flexibility in adding new physical processes and switching between different implementations of the same process. This makes the platform especially suited for detailed study of the effects of modelling choices. However, in what follows we only describe the ‘standard’ combination of models that is best suited for SEM imaging.

Our main focus has been to develop a tool that is flexible and universally applicable. From a physics point of view, this means we have chosen to adopt a pragmatic approach, i.e. to provide reasonable descriptions that work for a large range of materials rather than detailed interactions per material.

We distinguish three basic types of physical processes—elastic scattering, inelastic scattering and boundary crossing, which is responsible for interactions near interfaces between two materials. For a large part we build on existing descriptions of the processes involved that can be found in the literature, but we have added our own modifications as well. For instance, for elastic scattering we combine Mott cross-sections. We use the data provided by Czyzewski et al [11] and Ritchie [5]. Also Yue et al [6] apply Mott differential cross-section data but from different sources.

In an elastic scattering event, the electron experiences a tiny kinetic energy loss due to atomic recoil. We include this energy loss, although in most applications it is unnoticeable.

Figure 1 shows examples of the differential Mott cross-sections per scattering angle. Also shown are angular distributions of BSEs from a flat sample, as simulated using our Monte Carlo software. Some details of the Mott differential cross-sections correspond directly to features of the simulated angular distributions that might also be demonstrated in an experiment. Hence, in our opinion, it can be useful to apply the detailed, tabulated Mott cross-sections as discussed above, rather than an approximating analytical expression that ignores the finer details of the angular distributions, as, for example, proposed by Pasciak and Ford [12].

Below kinetic energies of approximately 100 eV, the Mott description breaks down. As Czyzewski et al point out, at such low energies the results become very sensitive to the precise choice of atomic potential. Furthermore, a more fundamental point is that the de Broglie wavelength of electrons becomes large compared with both the interatomic distances and the Mott mean free path (mfp). Hence, the picture of isolated scattering events on ions, which is the basis of the Monte Carlo procedure, is no longer valid. Instead, electrons at these low energies behave as Bloch waves with a much increased mfp [13, 14]. Within this picture electrons scatter only on thermal vibrations (phonons) and lattice imperfections.

The cross-section data are extended to lower energies in two different ways. The first applies to metals, the second to semiconductors and insulators.

2.1. Elastic scattering

For the physical description of elastic scattering, a distinction is made between high (100 eV–30 keV) and low (up to 100 eV) kinetic energies.

For the 100 eV–30 keV range we apply Mott cross-sections. We use the data provided by Czyzewski et al [10]. These Mott (differential) cross-sections are obtained by solving the Dirac equation for electrons deflected by the positively charged nucleus of an atom, as screened by the orbit electrons. The atomic potential in solids is approximated using the Bühring procedure. The same datasets were also applied by Drouin et al [11] and Ritchie [5]. Also Yue et al [6] apply Mott differential cross-section data but from different sources.

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The cross-section data are extended to lower energies in two different ways. The first applies to metals, the second to semiconductors and insulators.

2.1.1. Metals. In metals, the mobility $\mu$ of electrons at the Fermi level is easily derived from the material’s electrical conductivity combined with the conduction band electron density. The mobility is directly related to scattering rate $v_m$. This can be summarized as follows:

$$\mu = \frac{-1}{\rho n e} = -\frac{e}{m_e v_m},$$

so that

$$v_m = \frac{\rho n e^2}{m_e}.$$

Here $\rho$ is the resistivity of the metal, $n$ is the density of conduction electrons, $e$ is the elementary charge and $m_e$ is the electron mass.
the electron rest mass. The elastic mfp $\lambda$ now follows from

$$\lambda^{-1} = v_{\text{Fermi}} \frac{\hbar}{m_e}$$

where $v_{\text{Fermi}}$ is the electron velocity at the Fermi energy level.

This approach does not provide information on the angular scattering dependence. Therefore we have chosen to adopt the same angular dependence as in the model for semiconductors and insulators [15], which is discussed further below. The resulting scattering distribution is isotropic at the lowest energies, and forward peaked at higher energies.

The current method gives us the elastic mfp at only one energy, which is the Fermi energy. At energies between the Fermi energy and 100 eV we obtain the mfp by linearly interpolating between the resistivity-based value at the Fermi energy and the value based on the Mott cross-section at 100 eV.

As input, this method requires only the lattice constant, the sound velocity and an acoustic deformation potential for all relevant materials.

We have implemented the energy loss per elastic scatter event as the average energy required to excite an acoustic phonon, $\bar{\hbar}\omega = \hbar u_s / a$, where $u_s$ is the sound velocity and $a$ the lattice constant. This also works for metals, if the values of $u_s$ and $a$ are available as input parameters. Note, however, that in metals this energy loss will normally be insignificant compared with inelastic scattering energy losses.

Finally, at low energies, especially in some semiconductors and many insulators, mfps for inelastic scattering go through a minimum when coming from higher energy, and then start to rise sharply. At the same time, elastic scattering can therefore become the strongly dominant scattering mechanism.

**Figure 1.** Angular differential Mott cross-sections (per unit solid angle) for carbon (a), copper (b) and gold (c) at two different energies: 500 eV (thick lines) and 1 keV (thin lines). $0^\circ$ and $180^\circ$ correspond to backward and forward scattering, respectively. Cross-sections are in arbitrary units. The graphs have been scaled such that the forward scattering peak (at $180^\circ$) falls outside the image but the other directions can be viewed more easily. Also shown are simulated angular distributions of BSEs from a flat, bulk sample with the primary beam at normal incidence (d) and tilted over $60^\circ$ (e) with respect to the normal of the sample surface. The horizontal scale indicates angle relative to the incident beam. Several features of these distributions correspond to features in the Mott cross-sections. As an example, the arrows indicate maxima in the angular distribution for the tilted Au sample at 500 eV incident electron energy; at roughly the same angles, the Au Mott cross-section at the same energy has readily distinguishable maxima as well.
This effect can be exploited for acceleration of the simulations, by replacing the description of elastic scattering as a series of discrete events, by a diffusion-like approach whenever elastic scattering is dominant. In this approach, the final position of the electron after many elastic scattering events is drawn directly from a near-Gaussian distribution, while the length of the path that the particle can travel is limited by inelastic scattering and geometric boundaries. At the same time, inelastic processes are still treated in a discrete manner.

2.2. Inelastic scattering

For the modelling of inelastic scattering events we apply DFT. Variants of this approach have been applied by different authors to calculate stopping powers [16, 17] and in Monte Carlo simulations [3, 6, 18–20].

DFT allows derivation of (differential) cross-sections for electron–atom interaction from optical data. The core of the theory is the extension of the material’s dielectric function to nonzero momentum transfer between the colliding particles. This is discussed by several authors [21–26]. The implementations differ partly in the choice of integration limits and the application of exchange correction. In other words, DFT provides only an approximation to detailed cross-sections, and there is some room in the choice of the details to match its results to those of other theories and experiments.

Its main advantage, however, is that optical data are readily available for a wide range of materials, and in the broad energy ranges that are relevant for electron–atom interaction in SEM. This makes it a very attractive candidate for application in a general-purpose Monte Carlo simulation tool for SEM. In the following the basic theory is outlined briefly, and our modifications are discussed.

The total inverse mfp for inelastic scattering is expressed as

$$\lambda^{-1} = \frac{1}{\pi E} \int d\omega \int_{q_0}^{q_1} \frac{dq}{q} \text{Im}[-1/\epsilon(q, \omega)],$$

(1)

where $\omega$ represents the total energy loss for the primary electron and $q$ the momentum transfer from the primary to the secondary electron. This expression contains the expanded dielectric function $\epsilon(q, \omega)$. It can be derived from optical data $\epsilon(0, \omega)$ in a plasmon-pole approximation as follows:

$$\text{Im}[-1/\epsilon(q, \omega)] = \frac{\omega'}{\omega} \text{Im}[-1/\epsilon(0, \omega')]$$

(2)

with the dispersion equation

$$\omega' = \omega - q^2/2.$$  

(3)

We call $\omega'$ the zero-momentum energy transfer.

Now, after a change of variables, we can introduce a new function $F$ and write

$$\lambda^{-1} = \frac{1}{2\pi E} \int d\omega' \int_{0}^{\omega} d\omega' \omega' \text{Im}[-1/\epsilon(0, \omega')] F(E, \omega', \omega)$$

(4)

after Ashley [23]. In order to find the integration limits in (1) we now apply conservation of momentum to the primary and secondary electron. This yields the following expression for the function $F$ in (4):

$$F(E, \omega', \omega) = \left\{ \begin{array}{ll} \frac{1}{\omega(\omega - \omega')} & \text{for } \omega' + q^2/2 < \omega < \omega' + q^2/2, \\ 0 & \text{otherwise}, \end{array} \right.$$  

(5)

where $q_\pm = \sqrt{2(\sqrt{E} \pm \sqrt{E - \omega})}$. One can now write

$$\lambda^{-1} \approx \frac{1}{2\pi E} \int_{0}^{E} d\omega' \text{Im}[-1/\epsilon(0, \omega')] L(\omega', E)$$

(6)

with

$$L(\omega', E) = \int_{\omega_\omega}^{\omega} d\omega \omega' F(E, \omega', \omega).$$

(7)

The lower integration limit follows from momentum conservation. Further, we limit the integration to cases where the final kinetic energy of the SE is smaller than that of the primary electron, so that $\omega_\omega = \frac{1}{2}(E + \omega')$.

In his work, Ashley now applies a correction to this result due to exchange and the indistinguishability of the primary and secondary electrons. After integration over $\omega$, he arrives at the approximate expression

$$L(\omega', E) \approx \left\{ \begin{array}{ll} (1 - a) \ln \frac{4}{a} - \frac{7}{4} a + a^{3/2} - \frac{33}{32} a^2 & \text{for } a < 1/2, \\ 0 & \text{with } a = \omega'/E. \end{array} \right.$$  

(8)

2.2.1. Model refinements. We, however, have made modifications to this approach, which will be discussed below. We make a distinction between interactions with outer shell electrons and plasmons on the one hand and with inner-shell electrons on the other hand. For practical reasons, the limit between the two cases is set at a fixed value of $\omega' = 50$ eV. For most materials, this energy is well above the centre of the plasmon peak but lower than the thresholds of relevant inner-shell ionization processes.

First of all, for $\omega' < 50$ eV we apply no exchange correction. The reasoning behind this is that plasmon excitation is the dominant energy loss mechanism in this regime. So no SE is excited directly (which would give rise to an exchange correction) but rather a plasmon is created that is subsequently assumed to decay under the creation of a single electron–hole pair. In the interaction, the plasmon behaves as a separate (boson) particle [27, 28] and hence the exchange correction does not apply. Therefore we use the basic expression (7) with $F$ as defined in (5).

Further, the primary electron cannot end up with a kinetic energy below the Fermi level. Therefore, we set $\omega_\omega = \frac{1}{2}(E - E_{\text{Fermi}} + \omega')$, where $E_{\text{Fermi}}$ is the kinetic energy of electrons at the Fermi level.
Through $\omega_a$, $L$ now depends explicitly on $\omega'$, $E$, as well as $E_{\text{Fermi}}$. The above considerations lead to the following expression for $a = \omega' / E < 1 / 2$:

$$
L(\omega', E, E_{\text{Fermi}}) = \int_{\omega_{\min}}^{\omega_{\max}} d\omega' F(\omega', \omega) = \left[ \ln \left( \frac{\omega - \omega'}{\omega} \right) \right]_{\omega=\omega_{\min}}^{\omega=\omega_{\max}} + \left( \frac{2}{\alpha} \left( 1 + \sqrt{1 - 2a} \right) - 1 \right) + \left( \frac{E - E_{\text{Fermi}} - \omega'}{E - E_{\text{Fermi}} + \omega'} \right)
$$

and $L = 0$ for $a > 1 / 2$ as before.

The above expressions predict trends in the (differential) inverse mfps rather well. However, we found that equation (6) with $L$ as defined in (8) tends to underestimate their absolute values, as compared with inverse mfps from other experimental and theoretical sources, such as presented in [29] for silicon, and the Lawrence Livermore National Laboratory Evaluated Electron Data Library [30] for various elements at energies above 1 keV. One cause may be the limited validity of the simple plasmon-pole approximation in equations (2) and (3); in particular, a more complex dispersion relation may lead to somewhat smaller mfps [31]. For this reason we introduce an adjusted $L_c = AL$ for $\omega' < 50$ eV with $L$ as in (8), where $A$ is an empirical parameter with a fixed, material-independent value of 1.5.

Finally, momentum conservation between the interacting electrons in general does not apply to inner-shell ionizations. This follows from the experimental observation that ionization of electrons in general does not apply to inner-shell ionizations. For this reason we introduce an adjusted $L_c = AL$ for $\omega' < 50$ eV with $L$ as in (8), where $A$ is an empirical parameter with a fixed, material-independent value of 1.5.

2.2.2. Input data. Given the model as described above, what is still needed to complete the description of inelastic scattering events in MC simulations, is to provide (tabulated) data on the energy loss function $\text{ELF}(\omega') = \text{Im}[-1/\epsilon(0, \omega')]$ for each relevant material and for all energies $\omega'$ up to the highest kinetic energy in the simulation. This follows from the fact that (6) contains an integration over $\omega'$ from zero up to the kinetic energy $E$.

The ELF can be constructed from any sufficiently complete and accurate set of optical data. Useful compilations of optical data can be found in the handbooks edited by Palik [32–34] and on the CXRO website [35].

Furthermore, the kinetic energy at the Fermi level is a required parameter. In the case of metals this information is readily available in the form of tabulated data [14, 36]. In the case of semiconductors and insulators it needs to be approximated from band structure data; it can be either zero or larger than zero, depending on the shape of the first conduction band.

2.2.3. Implementation. In our implementation of the inelastic scattering model, total (inverse) mfps are determined as described in equations (6) and (7) above. The integration over $\omega'$ in (6) is done numerically. The intermediate results, i.e. the cumulative differential inverse mfps,

$$
\int_0^{\omega'} \frac{\partial \lambda}{\partial \omega}^{-1} d\omega' = \frac{1}{2\pi E} \int_0^{\omega'} d\omega' \text{Im}[-1/\epsilon(0, \omega')] L,
$$

are stored in separate data tables. This facilitates drawing the values of $\omega'$ in inelastic scattering events.

A number of steps is taken when an individual inelastic scattering event is processed. The parameters that need to be determined for each event include the total energy transfer from the primary to the secondary electron, the effective binding energy of the SE and the final momentum directions of both particles.

The first step is to determine the zero-momentum energy transfer $\omega'$ using tabulated data as stated above. However, the SE’s binding energy $E_{\text{bind}}$ does not follow directly from $\omega'$ and the optical input data alone. Instead binding energies and relative cross-sections need to be provided separately. Fortunately, there is existing code in Geant4 that can provide these for electron-induced ionization of the inner shells of individual atoms, based on data from Perkins et al [30]. In our code we assume that these data are applicable also to atoms in solids for binding energies above 50 eV and $\omega' > 100$ eV.

At lower energies, the bandgap $E_g$ (if any) of the material serves as a lowest binding energy, and any interaction with $\omega' > E_g$ is assigned at least that binding energy. Additional binding energies can be defined per material in the input data files. Note, however, that for most materials the interaction in the $\sim 10$–$50$ eV range is dominated by the plasmon peak which does not have any associated binding energy (other than perhaps the bandgap for the subsequent creation of an electron–hole pair).

Next, the total energy transfer $\omega$ from the primary to the secondary electron is determined following a distribution similar to (5) for given $E$ and $\omega'$. Note that an upper bound for $\omega$ is applied as in (8) for the reasons given above.

The case of zero binding energy now deserves some additional attention. In the case of a metal, this corresponds to an electron being excited from the partially filled conduction band. The probability distribution for this is $p \sim \sqrt{E_s(E_s + \omega)}$ where $E_s$ is the initial kinetic energy of the secondary electron [6]. In the case of a semiconductor or insulator, any interaction with $\omega' < E_g$ is treated as a longitudinal optical (LO) phonon loss. The total energy loss is equal to $\omega'$. No SE is generated and momentum change is considered negligible and therefore not taken into account.

Finally, if an SE is generated, the new momenta of both particles are determined in a semi-classical way according to momentum and energy conservation evaluated at the potential of the atomic orbit (i.e. $2E_{\text{bind}}$) that the primary electron is interacting with. A randomly oriented motion of the target electron prior to the collision is taken into account. This implementation is essentially that of V Ivanchenko in the Geant4 G4LowEnergyIonisation class (unpublished).
It should be noted that SEs, after having been generated in the simulation, are not treated any differently from primary particles—be it in their transportation or their capability to create further SEs (cascade generation).

In the inelastic scattering part of the code a reduction of simulation time is achieved by applying a so-called ‘range cut’ as a function of energy. The range is the typical distance an electron of a certain energy can travel in the material before its energy drops below the vacuum energy. Hence any electron below the vacuum energy by definition has zero range.

Before a simulation starts, upper bounds to the ranges for all materials are calculated and tabulated as a function of energy. An electron is removed from the simulation once its distance to the nearest volume boundary is more than five times its estimated range at the given kinetic energy.

2.3. Boundary crossing

A third type of process has been implemented to describe what happens when an electron reaches a boundary, either between two solids or between a material and vacuum. We use a quantum mechanical expression for transmission and reflection at a potential step [26] where the potential difference is the change in ‘inner potential’ when going from one material to another. This ‘inner potential’ is defined as the sum of the kinetic energy at the Fermi level (as discussed above) and the work function of the material.

When the electron is not transmitted, it is assumed to be either absorbed (for energies in the SE range) or specularly reflected (for high kinetic energies—this is quite rare but may occur if an electron approaches a surface or interface at a very low grazing angle).

3. Integrated SEM simulator

Capitalizing on the available facilities in Geant4 we have completed an integrated simulation tool for SEM operation including the final detection and (optionally) also SE3 generation and detection. Through its GDML interface, the geometry of an actual SEM column is modelled. The corresponding 3D electromagnetic fields that govern the probe formation as well as the final detection of the image were precomputed using a finite element model and imported via a custom interface between the finite element model and Geant4.

Several detectors can be defined in this virtual SEM column and we typically include one virtual detector, located just above the sample, and a through the lens detector (TLD). The latter is the standard detector in the electron column for all high-end SEM and Dual beam systems of FEI Company, which we use as our default SEM column.

In principle it would be possible to compute the electron traces starting from the gun and ending on this detector. As we are not concerned with the probe formation in the SEM (which is modelled independently during column design) we start our traces in a focused spot just above the sample. Using the built-in Geant4 general particle source, it is possible to define a realistic spot (including e.g. chromatic and spherical aberrations) for the computation of virtual SEM images.

4. Experimental validation

The aim of our modelling effort is to obtain a better quantitative understanding of the image formation process in an SEM. As a validation of our models we have defined three progressive steps that enable us to build confidence in the models incrementally based on the availability of experimental data. First we test whether the total numbers of SEs and BSEs agree with experimental data. Next we compare the energy spectrum of the emitted secondaries with available experiments and finally, we check the complete tool using an SEM image taken from a known sample in a known microscope.

4.1. Total SE and BSE yield

The first step is to use the BSE and SE yields as a function of the kinetic energy of the primary electron $U_0$. Experimental data have been collected by Joy [37] for a wide variety of materials. E Napchan is maintaining an internet-accessible database based on this original collection. Figure 2 shows the results of our comparison for carbon, silicon and gold. For carbon the comparison is based on the optical properties of both glassy carbon and highly oriented pyrolytic graphite (HOPG). The data are plotted on a logarithmic energy scale in order to emphasize the low-energy range which is becoming increasingly important in SEM imaging.

From this comparison we conclude that our simulation tool predicts SE yields that are, at least to within experimental uncertainty, in agreement with the available data. The computed backscatter yields at primary energies between 1–10 keV for gold are somewhat higher than in the experimental data, while the SE yields are slightly lower below 1 keV.

An interesting case is that of aluminium. In figure 3 we show the SE yield as a function of landing energy for aluminium compared with data from the same database as above. The dashed line shows the results from our simulations assuming a clean aluminium surface. This result seems to correspond to only one of the datasets [39].

This can be understood by realizing that it was never the intention of Joy to include only the results of ideal experiments into his database. Therefore, it contains both references for ideal conditions and for conditions that could occur in standard SEM operation, including oxide layers, which is an explanation for the large spread in SE yields observed in figure 3.

When we add a thin oxide (Al$_2$O$_3$) layer on top of the sample in our simulation, it turns out that a thickness of 1.6 nm gives a satisfactory match over the whole energy range for the topmost set of experimental data, as shown by the solid line in figure 3.

While adding this layer is easy, the fact that the result is corresponding so well to several sets of experimental data is surprising, as there are several modelling uncertainties involved. First of all, one could question whether the ‘jellium’ approach (i.e. ignoring crystal lattice effects), assumed in our Monte Carlo modelling, still holds at these small length scales. As the experiments for determining yields by necessity average over relatively large areas, the numerical results are still
expected to give correct predictions for this average. It would be a different matter as soon as position resolved measurements are done with a resolution close to the interatomic distances involved.

Secondly, the material properties of a thin oxide layer probably differ significantly from the bulk parameters used in the simulations. Therefore, the uncertainty in the observed thickness of 1.6 nm is unknown and hence, it cannot be taken as a fitted value for the oxide layer thickness.

Finally, it is surprising that a match is found over the whole energy range, corresponding to at least two different sets of experimental data, using only one value for the thickness of the oxide layer. This suggests that the oxide layer thickness is constant for all of these experiments.

In conclusion, these results clearly demonstrate the usefulness of our simulation tool as an aid in the interpretation of experimental results.

4.2. Energy spectrum

In the second step of our validation process we consider the energy spectra of the emitted SEs and BSEs.

In figure 4(a) the computed SE spectrum of silicon is shown together with experimental data from Joy et al [40]. The numerical result is obtained using $10^6$ primary electrons incident normally to a bulk silicon sample with 1 keV kinetic energy. The energies of the electrons emitted from the sample are binned into 1 eV intervals. The resulting histogram is first scaled such that its integral over all energies is equal to the total yield, and subsequently multiplied by the energies of the emitted electrons analogous to the results reported by Joy. Because the experimental data do not have an absolute intensity scale, they are scaled to give the same peak height as the simulated spectrum. In our opinion, the correspondence of the simulation result to the experimental data is quite convincing.

In figure 4(b) the energy loss spectrum of the BSEs is displayed for the same simulation. The data are compared with
Figure 4. (a) Comparison between the simulated SE spectrum based on our models and experimental results of Joy et al [40]. The primary energy is 1 keV in both cases. The simulated SE spectrum is based on 10^6 primaries and is binned in 1 eV intervals. (b) Simulated energy loss spectrum for the same model parameters (solid line). Dashed line: experimental result from Werner et al [41], including the effect of surface plasmons. The curve was rescaled to match the integrated intensity from 960 up to 999 eV to the simulation result.

Figure 5. (a) Cross-section through the sample showing the silicon in dark grey. The lighter parts on top of the silicon are a platinum deposit used to make the FIB cut (image courtesy Steve Reyntjens). (b) SEM images of the line structure before (top half) and after (lower half) plasma cleaning (images courtesy Ingo Gestmann). From left to right the image starts and ends with a groove and shows two complete lines with one groove in between. (c) Perspective view of the geometry of the sample as used in the simulations.

4.3. Comparison with experimental SEM images

Finally, the complete imaging process was simulated using both the physical models for electron–sample interaction and a model for the SEM column including the detector as described in section 3. The resulting numerical images are therefore directly comparable to actual SEM images and provide a useful validation for our complete code.

We used a silicon sample containing a surface pattern consisting of repeating lines with 500 nm pitch. The individual lines are 250 nm wide and 120 nm high. The sample was obtained from NTT-AT. Figure 5 shows SEM images of both a focused ion beam (FIB) cross-section (a) and a top view (b) of the sample. From the cross-section image we obtained the shape of the line as input for our sample model. It is clearly not completely flat inside the groove, and the edges of the line are slightly rounded. These features were taken into account in the numerical model of the sample, of which a graphical representation is shown in figure 5(c).

The SEM images were taken using the FEI Helios electron column operating at a beam energy of 1 keV and a working
Figure 7. (a) Horizontal line scan taken from figure 5. Negative $x$-values correspond to the lower part of the edge, positive values to the higher part. Both a left and a right edge (mirrored around the edge) are shown in order to visualize the experimental variation. The bold line shows the result of the corresponding numerical simulation, which includes the complete column and detector. (b) The effect of adding a 2 nm thick layer of carbon in the numerical simulation, the experimental curve is the average of the two curves in (a). (c) The effect of plasma cleaning on the experimental line scans. (d) Comparison of line scans taken from a virtual detector placed just above the sample and the simulated through the lens detector (TLD). The signal from the virtual detector is rescaled.

distance of 4 mm in ultra-high resolution (UHR) mode. The fields of this microscope configuration were included in the model. Care was taken to ensure that the black level in the image corresponds to zero detector count such that experimental and numerical results differ only by a scaling factor.

The simulated image of figure 6 is obtained from a virtual detector located at the actual position of the through the lens detector in the Helios column. A 100% detection efficiency is assumed for this simulated detector. Note that the column fields provide a selection of both emission energy and angle of the SE leaving the surface, which is properly taken into account in this way.

In order to make a more quantitative comparison between the experimental and numerical results, we obtain horizontal line scans from both the simulated and the experimental images. Figure 7 shows such a comparison in detail.

First, we compare the experimental line scan from the sample as received with our numerical simulation in the top left part of the figure. In order to make the comparison we scaled the intensity of the experimental signal to match the simulation in the region $x > 50$ nm (i.e. on the ‘high’ side of the edge).

Although most of the experimental features are captured qualitatively, the simulation does not seem to predict the height of the peak correctly. The agreement improves dramatically, however, when we assume that a thin layer of carbon is present on top of the silicon surface as shown in figure 7(b).

The layer consists of glassy carbon and extends 2 nm in the vertical direction along the whole profile. No carbon is present on the side walls of the steps. The same issues regarding the validity of bulk material parameters as discussed in section 4.1 hold in this case and therefore the thickness of the layer is only indicative.

In order to obtain experimental evidence for a possible contamination effect we repeated the SEM imaging after plasma (N$_2$) cleaning of the sample for about 30 s. The SEM images before and after cleaning are displayed in figure 5(b). Figure 7(c) shows the corresponding line scans.

Clearly the effect of cleaning the sample is indeed to reduce the magnitude of the peak. However, the amount of cleaning was apparently not enough to obtain the result for the bare silicon sample as shown in the top left part of figure 7.

Finally, figure 7(d) shows the result for a virtual detector placed directly above the sample and compares it with the result from the simulated TLD. The virtual detector scan contains some contrast between the low and the high side of the edge (cf the dashed line in the figure 7(d)), which is not observed in either the simulated signal from the TLD or the experimental SEM images. Although the effect is limited, we believe that being able to incorporate the complete column is a useful feature that increases the understanding of the complete SEM imaging process.

5. Conclusions

We have built a numerical tool that is capable of simulating the complete SEM imaging process. We put special emphasis on the low-energy processes, to include simulation
of the behaviour of electrons in the SE part of the energy spectrum. Furthermore, the integration of an electromagnetic field raytracer allows incorporating realistic SEM column geometries into the model.

For validation of our models against experimental data we have proposed and executed a three step procedure, consisting of comparisons of total SE and BSE yields, BSE and SE energy spectra, and finally a quantitative comparison of a numerical image with an experimental SEM image.

As part of this work we found that in order to make a quantitative comparison between simulations and experiments it is crucial that the properties of the sample are accurately known. Experimental issues such as contamination and detector positioning have to be considered in detail. Our simulation tool is flexible enough to take such factors into account. The simple test case of the silicon lines shows that satisfactory agreement between experimental and numerical results can be achieved.

Understanding the effects of contamination and surface oxidation on image results is especially important in applications where the exact locations of edges need to be determined. The filtering of SEs in the SEM column by angle and/or energy can also play a significant role. The above analysis shows that having an accurate and flexible Monte Carlo simulation tool that incorporates the complete SEM imaging process can be of great help in the interpretation of SEM images.

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