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Monte Carlo calculations of X-rays generation for electron beams with energies up to 500 keVolts

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ABSTRACT: The MC-SET Monte Carlo program for simulation of electron trajectories is being improved by adding X-rays generation calculation for each electron trajectory step. The method uses the 3D (N = 100 elements per dimension) energy deposition matrix and an additional equivalent matrix of average electron energies. These two matrixes provide us all information about an electron energy deposition in the specimen and allow us to carry generalized shell ionization computations and to obtain the 3D distribution of K shell ionization. Simulation results include the number of Kα photons per steradian per electron flying out from a spot of electron beam incidence in a specified direction, and information about the depth generation. The simulation can be used for individual elements with different tilt angles and with electron energies up to 500 keV, and for multi-layered specimens. Simulation results are in good agreement with experimental results and with other calculations.

1. INTRODUCTION

MC-SET (2003) is a computer program for the Simulation of Electron Trajectories using Monte Carlo methods. It simulates interactions of a large number of electrons travelling within a varied geometry specimen. From the calculated behaviour along the trajectories, details related to the electron transport can be evaluated. The program can use different scattering models based on different physical processes and mathematical models. It can estimate many of the observed signals encountered in electron beam experimental work, as that carried out with an electron microscope, such as backscattered electrons, transmitted electrons, secondary electrons, energy deposition and electron-hole pair formation. However, the program did not provide, until now, any information about ionization of the target material and about the resulting X-ray radiation.

X-ray generation and its evaluation was one of the driving forces for the original development of Monte Carlo methods as applied to electron microscopy and analysis. Increased computational power available now for personal computers allows calculations involving tens of thousand simulated electron trajectories to be carried out with in a matter of tens of seconds. It has now become possible to implement X-ray calculations into a generalized three-dimensional simulation, in which the resolution of the calculation can be in the range of the electron trajectory step.

This paper reports on the development of X-ray calculation capability using a three dimensional approach to the generation. With these new features the code is able to evaluate K-shell ionization of target atoms and Kα radiation, which can be measured in any specified direction. The first section will present the physical, mathematical and computing models used in the calculation, later sections present results obtained and compared with both experimental data and those from other simulation programs. The general nature of the calculation is further shown with some unique results for multi-layer specimens.

2. SIMULATION DETAILS

MC-SET provides a good description of the KeV electron transport and therefore, the generated electron trajectories can be considered as replicas of actual ones. According to this fact, the space distribution of K-shell ionization can be evaluated without altering the simulation routines. The information necessary for evaluation of K-shell ionization is stored in 3D matrixes that are simply actualized after each electron step. Each cell of these matrixes represents some small volume of the real target and the accuracy of the simulation results depends on their resolution. The first matrix contains information, about energy deposited by electrons in the target. Electrons are assumed to deposit their energy in the middle point of each trajectory step. Consequently, at every step the value in the energy deposition matrix corresponding to the middle point of the trajectory is increased by the difference of electron energy before and after the step. This matrix was already present in the MC-SET code and it was the starting point for our improvements. In the KeV energy range, in most cases the electron energy is lost mainly to ionization of target atoms. However, the fraction of this energy that corresponds to each atomic shell varies with electron energy. This is why two more matrixes of the same size were added. These were the matrix of electron energies and the matrix of numbers of electrons. The values of both are actualized only when electron leaves the volume corresponding to some cell, and enters a volume corresponding to the neighbouring cell, in other words when the electron crosses the boundary between cells in the matrix. The value of the former is increased by the actual electron energy and the value of the later is increased by one. If the resolution of these matrixes and the number of simulated electrons are sufficient, than at the end of the simulation one can extract from these two matrixes an average electron energy and a number of electrons with this energy, that were present during the simulation in every small volume of the target. Thus the matrixes together provide us for every small volume the total energy deposited by electrons and the average energy of electrons. The energy deposited in each volume element is calculated using the Joy and Luo modified Bethe expression for stopping power (Joy 1995).

The number of K shell ionizations is calculated using a formula similar to that used by Acosta et al (1998), which depends on the K shell ionization cross section. Three different analytical cross sections for K shell ionization are implemented in the simulation code: by Gryzinski (1965), the Bethe-Powell cross section (in Powell (1976)) and the semi-empirical cross section proposed by Casnati, Tartari and Baraldi (1982).

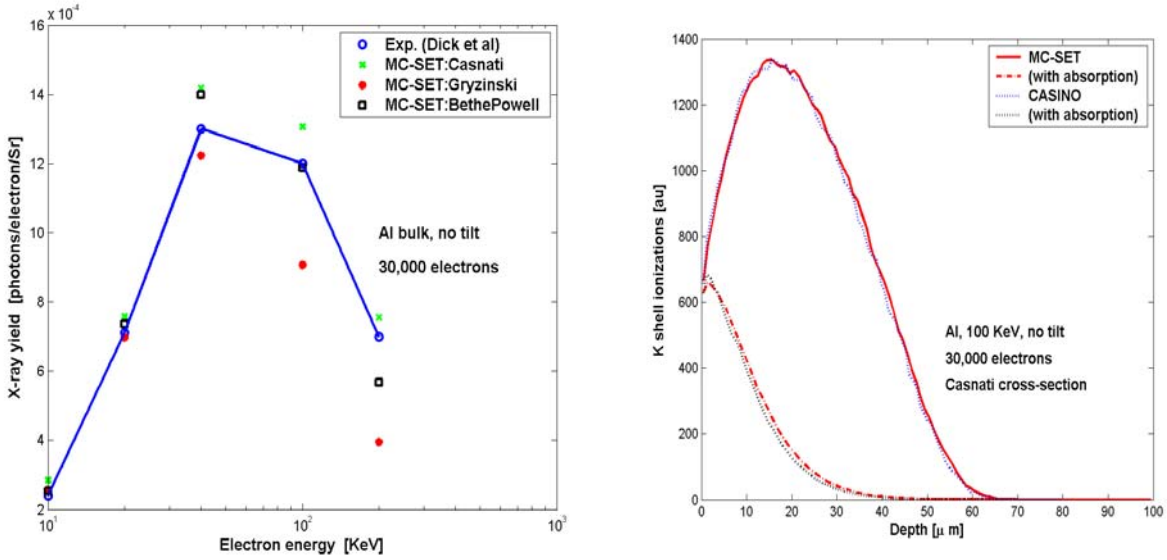
Atoms with a vacancy in the K shell relax to their ground states by migration of the vacancy to some outer electron shells, mostly to the L shell. This process is followed by emission of characteristic X-rays or Auger electrons. For K shell ionization, the most probable radiative transition is the one giving rise to Kα photons. Individual transition probabilities are described by fluorescent (radiative) yield, values for each material can be obtained from the Evaluated Atomic Data Library (EADL 2003. The emission of Kα photons is considered isotropic at each point.

The reduction of Kα intensity due to absorption during transport to the top target surface is calculated using Beer exponential law, with μ the mass attenuation coefficient taken from the NIST database (NIST 2003).

3. RESULTS AND DISCUSSION

Fig. 1(a) presents a comparison of results obtained using the simulation with the different X-ray ionization cross-sections against experimental data of Dick et al (1972). The comparison is made for a bulk Al sample, at normal beam incidence, for beam voltages up to 100 KeV, and measures the photon flux in the normal direction. The values calculated are based on the summation of all contributions in the energy deposition matrix, taking into account absorption by the specimen.

Fig. 1(b) presents a comparison between the depth-generation of X-rays calculated by the present simulation against data calculated by the CASINO (2003) simulation program, for a bulk Al specimen, with a 100 KeV electron beam at normal incidence. Both the depth generation and the absorbed depth generation of X-rays are presented, normalized to their original maximum values.



(a) (b)

Fig. 1. Comparison of results obtained with the present simulation against (a) experimental data from Dick et al (1972), using various algorithms for the ionization cross section, and (b) calculated results from the CASINO (2003) simulation program.

Fig.2 presents results calculated for a multi layer (2 μm Al on Si), at 25 KeV beam energy and normal incidence. The depth generation of X-rays is displayed, along with the same dose after absorption. In this figure, the K shell ionizations refer to the corresponding layers, i.e. up to 2 μm these are Al Kα photons, and for greater depths to Si Kα. The figure shows that it is possible to deal with different sources of X-rays in the same specimen. Integration of the absorbed intensity results in one value for the X-rays intensity for each of the component layers in this specimen.

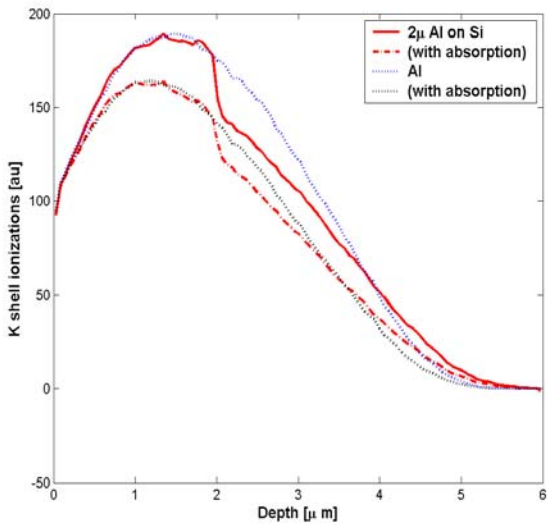


Fig. 2. K shell ionizations for a horizontally stacked multilayer specimen

By changing the electron beam voltage, and possibly the beam incidence angle, it is possible to study the variation in X-ray signals for all components of horizontally stacked layers. By scanning the beam along a direction normal to the layers of a vertically stacked specimen and calculating the resulting X-ray intensity it is possible to simulate an X-ray linescan across a boundary.

Both comparisons in Fig. 1 show a very good agreement between the current simulation results and those from the other sources. More work can be done in the selection of the cross section model, calculating for different materials at different beam conditions.

Fig. 3 presents calculated iso-contours of Kα photons generation for a bulk Al specimen at 100 KeV beam energy using 30,000 electrons, plotted from the 3-D X-ray generation matrix without

considering absorption. The profiles in Fig. 3(a) represent both the XZ and YZ planes for a zero beam tilt, while those in (b) and (c) represent the corresponding iso-contours for a beam incidence angle of 60 deg with respect to the specimen normal. The logarithmic ratio between each of the curves is fixed (equal to 3.455), the internal ones corresponding to the highest intensity. From these figures the variation of the generation volume with beam tilt can be evaluated, in planes normal to the specimen surface (figs. b and c). The reduction in the X-ray generation depth can also be found from these

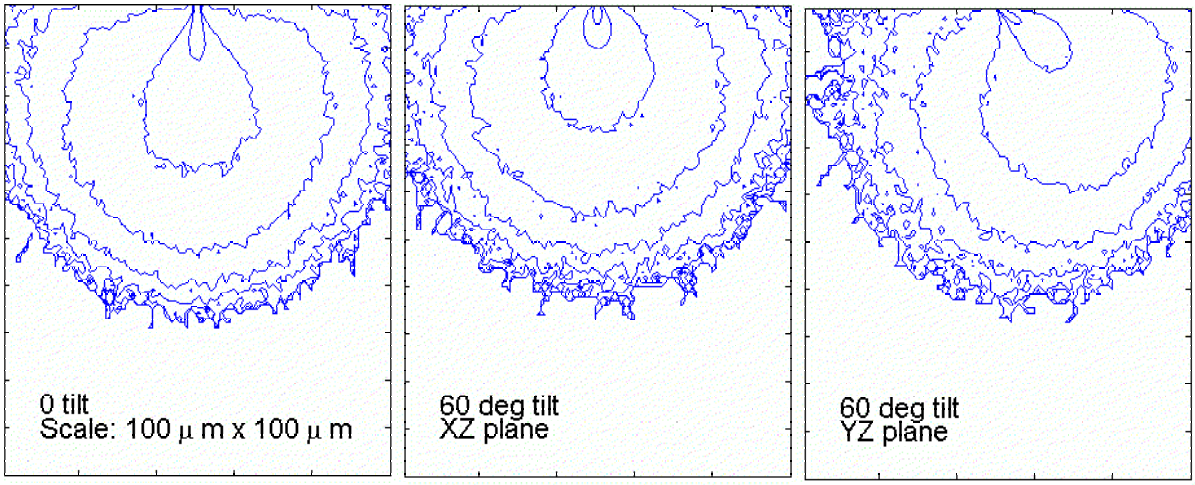


Fig. 3. Iso-contours of X-ray K photons generation for an Al bulk sample at 100 KeV electron beam energy. (a) for normal beam incidence (same profiles for both normal planes), and (b) and (c) for a 60 degree beam tilt for the corresponding normal planes

images.

4. CONCLUSIONS

First results of implementing X-ray calculation procedures into a Monte Carlo simulation of electron trajectories are presented. These compare well with experimental data, and with results from other simulation programs.

One of the characteristics of this simulation is the ability to evaluate electron beam dissipation, and thus inner shell ionizations in a 3-D geometry. Taking into consideration the electron beam penetration depth and the sample geometrical characteristics it is possible to have a spatial resolution approaching that of a single electron step in the trajectory calculation. This allows evaluating precise X-ray generation, as well as other SEM/TEM signals due to the beam energy deposition, in multi-layer or inhomogeneous specimens.

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