

CASINO V2.42—A Fast and Easy-to-use Modeling Tool for Scanning Electron Microscopy and Microanalysis Users

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Summary: Monte Carlo simulations have been widely used by microscopists for the last few decades. In the beginning it was a tedious and slow process, requiring a high level of computer skills from users and long computational times. Recent progress in the microelectronics industry now provides researchers with affordable desktop computers with clock rates greater than 3 GHz. With this type of computing power routinely available, Monte Carlo simulation is no longer an exclusive or long (overnight) process. The aim of this paper is to present a new user-friendly simulation program based on the earlier CASINO Monte Carlo program. The intent of this software is to assist scanning electron microscope users in interpretation of imaging and microanalysis and also with more advanced procedures including electron-beam lithography. This version uses a new architecture that provides results twice as quickly. This program is freely available to the scientific community and can be downloaded from the website: www.gel.usherbrooke.ca/casino. SCANNING 29: 92–101, 2007. © 2007 Wiley Periodicals, Inc.

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Introduction

The motivation of this work was to provide an easy-to-use and accurate simulation program of electron

beam–sample interactions in a scanning electron microscope (SEM). It can be used to assist scanning electron microscopy users in planning and interpreting their routine SEM-based imaging and analysis and also in more advanced topics such as electron-beam lithography. On the basis of a single-scattering algorithm, this software is specially designed for modeling low-energy beam interactions in bulk and thin foil samples. The initial version of CASINO (Hovington *et al.* 1997) was developed for expert users and presented some limitations in data handling capabilities. These aspects have been addressed in the present version by the development of a new user interface. This paper presents the simulation models used, the main features of the program, and some example applications.

CASINO v2.42 Structure and Principles

This software has been developed using C++ object oriented programming language. It therefore takes full advantage of the native PC operating environment. The graphical interface used was the MFC library. The following section describes the details of program operation: sample modeling, electron trajectory calculations, output and other special features.

Sample Modeling

Two basic geometries for sample representation are handled by CASINO v2.42: vertical planes and horizontal planes. These simple models can be used to reproduce a large number of real samples such as multilayers, heterostructures and grains boundaries. Using the *Simulation/Modify Sample* dialog box, the appropriate type of geometries for the desired sample modeling, the total number of regions with different chemical composition, and the thickness or width of each region are set. The substrate option extends the thickness of the bottom region in the case of horizontal planes, or

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the width of both first and last regions in the case of vertical planes, to a value much larger than the electron penetration depth in the sample.

Each of the added layers then needs to be matched to a chemical composition. This operation is easily done by “double-clicking” on the layer and then entering directly the chemical formula (SiO₂ for SiO₂) or the atomic or weight fraction of each element present. The software will calculate an average density based on the weight fraction of each element, but it is recommended to use known density values in g/cm³, if available. A library function allows the user to store special compositions, for uncommon alloys and compounds.

Electron Trajectory Calculation

The main part of a Monte Carlo program is the simulation of a complete electron trajectory. This section describes the different steps and physical models used by CASINO to calculate electron trajectories.

Different physical models are preprogrammed, so expert users can set them using the *Simulation/Change Physical Models* according to their different preferences. The present work uses the default values.

The tool is intended to represent, as accurately as possible, the actual interaction conditions in SEMs. Modern electron optics and advanced electron sources such as field emission can achieve subnanometer image resolution on the sample. CASINO assumes a Gaussian-shaped electron beam, where the user can specify the electron-beam diameter of their instrument, d , representing 99.9% of the total distribution of electrons. The actual landing position of the electron on the sample is thus calculated using eq(1):

$$\begin{aligned} X_0 &= \frac{d\sqrt{\log(R_1)}}{2 \times 1.65} \times \cos(2\pi R_2) \\ Y_0 &= \frac{d\sqrt{\log(R_1)}}{2 \times 1.65} \times \cos(2\pi R_3) \end{aligned} \quad (1)$$

where R_x are random numbers uniformly distributed between 0 and 1.

The initial penetration angle is fixed by the user, and no scattering angle is initially calculated. The distance between two successive collisions is evaluated using the equations:

$$L = -\lambda_{ed} \log(R_4) [\text{nm}] \quad (2)$$

$$\frac{1}{\lambda_{ed}} = \rho N_0 \sum_{i=1}^n \frac{C_i \sigma_d^i}{A_i} \quad (3)$$

where C_i , A_i are the weight fraction and atomic weight of element i , respectively, ρ is the density of the region (g/cm³) and N_0 the Avogadro's constant. The value of the total cross-section (Mott and Massey

1949, Czyzewski *et al.* 1990), σ_i (nm²), for each chemical element of the region is determined using the precalculated and tabulated value (Drouin *et al.*, 1997).

This program neglects the effect of inelastic scattering on electron deviation and groups all the electron energy loss events in a continuous energy loss function (Joy and Luo, 1989). With this assumption, the energy, in keV, between collisions can be calculated using the following equations:

$$E_{i+1} = E_i + \frac{dE}{dS} L \quad (4)$$

$$\begin{aligned} \frac{dE}{dS} &= \frac{-7.85 \times 10^{-3} \rho}{E_i} \\ &\times \sum_{j=1}^n \frac{C_j Z_j}{F_j} \ln \left(1.116 \left(\frac{E_i}{J_j} + k_j \right) \right) [\text{keV/nm}] \end{aligned} \quad (5)$$

where Z_j and J_j are atomic number and mean ionization potential of element j , respectively. k_j is a variable only dependant of Z_j (Gauvin and L'Espérance 1992).

The elastic collision angle is determined using precalculated values of partial elastic cross-section and a random number (Drouin *et al.*, 1997). For regions containing multiple chemical elements, the atom responsible for the electron deviation is determined using the total cross-section ratio (Hovington *et al.* 1997).

These steps are repeated until the electron energy is less than 50 eV or the electron escapes the surface of the sample and is recorded as a backscattered electron (BE). The default minimum energy can be adjusted using *Simulation/Options*; however, it is not recommended to use a value lower than 50 eV. Most of the default physical models used are not accurate below 50 eV, but higher values can be set by the user in order to speed up the calculation.

As the electron travels within the sample, the program will correct the trajectories while crossing the interface between two regions. In this case, no angular deviation is calculated and a new random number is generated to calculate the distance, L , in the new region. Using the same random number to calculate L when the electron trajectory is crossing an interface will introduce an artifact within the electron trajectory compared to the green line, where a new random number was used when an electron trajectory was crossing an interface. This method produces a more reliable distribution of the maximum depth of electrons in homogeneous and multilayer samples of the same chemical composition compared to using the same random number to calculate L in each new region.

Representation of Collected Data

Once the electron trajectories are simulated in the material, a large amount of information can be derived

from these raw data. The physical models behind CASINO give information about the absorbed energy in the sample and the electrons escaping the surface of the sample with energy higher than 50 eV. From such information, different representations of the data, depending on users requirements, can be generated by the program. This section gives a brief overview of the options.

Figure 1 shows an example of the overview distribution panel display for a thin 35 nm silicon film simulated using 200,000 electrons of 1 keV. This display gives the user a quick overview of all the distributions being generated while the simulation is still running and also once completed. Figure 1(a) shows the maximum penetration depth in the sample of the electrons,

(b) the maximum penetration depth in the sample of electron trajectories that will escape the sample surface (BE), (c) the energy of BEs when escaping the surface of the sample, (d) the energy of the transmitted electrons when leaving the bottom of the thin film sample, (e) the radial position of BEs calculated from the primary beam landing position on the sample, and (f) the energy of BE escaping area as a function of radial distance from the primary beam landing position. All those distributions are normalized by the number of primary electrons simulated except for (e) and (f). In the latter two cases, the raw data are shown with the number of BEs and the energy of the BEs in kiloelectronvolts. The users may then apply their own normalization to the data. Once the simulation is completed, the data

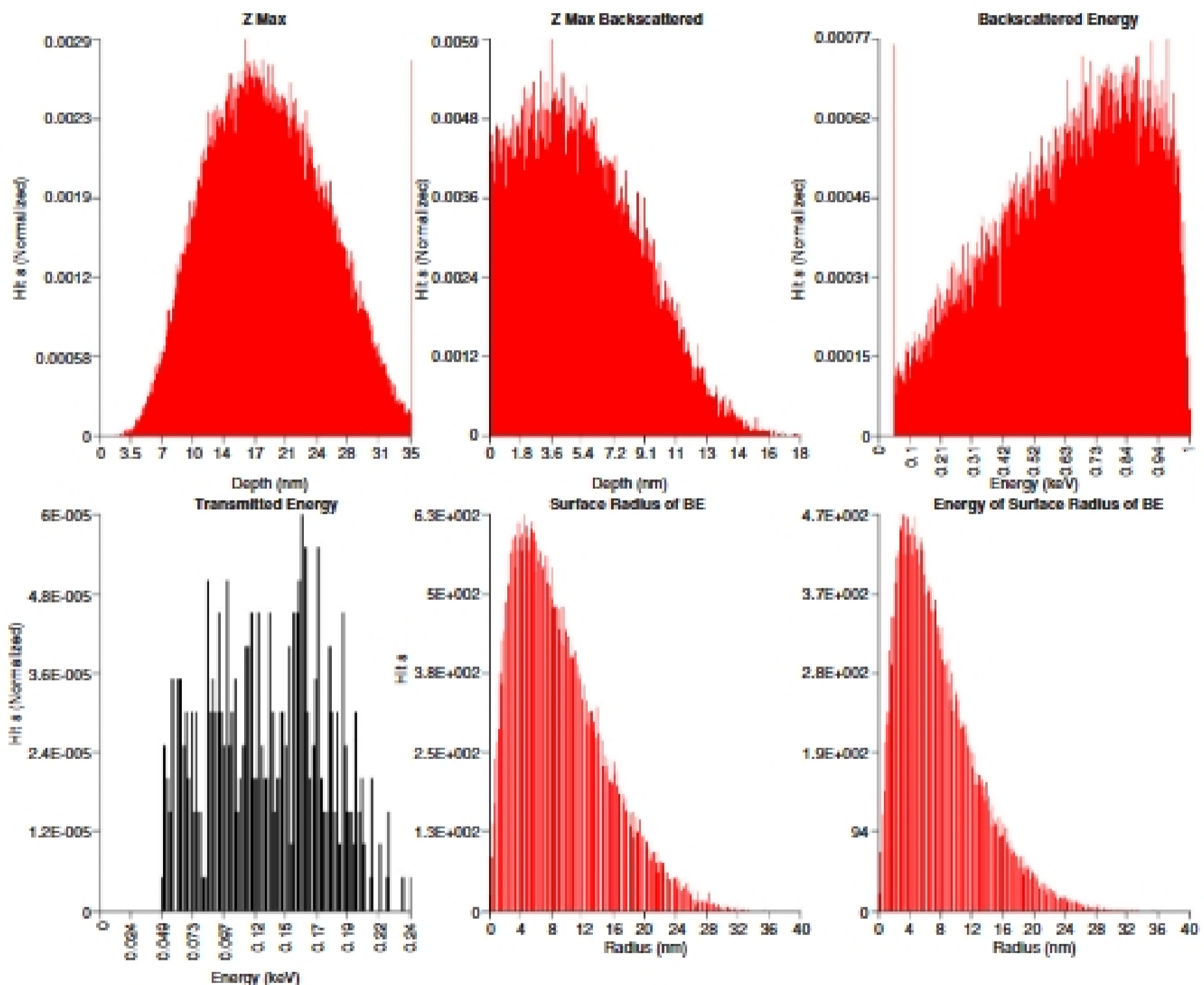


Fig 1. Different distributions of options: (a) maximum penetration depth in the sample of the electron trajectories; (b) maximum penetration depth in the sample of electron trajectories that will escape the sample surface; (c) energy of BEs when escaping the surface of the sample; (d) energy of the transmitted electrons when leaving the bottom of the thin film sample; (e) radial position of BEs calculated from the landing point of the primary beam on the sample; and (f) BE energy as a function of radial escape position calculated from the landing point of the primary beam on the sample. (Sample, thin film (33 nm) of silicon; Accelerating voltage 1 kV, Number of electron trajectories simulated = 200,000).