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THREE-DIMENSIONAL MODELING OF A TIME-OF-FLIGHT MASS SPECTROMETER: OPTIMIZATION OF SNMS/SIMS TRANSMISSION USING SIMION*

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Introduction.

The software package SIMION 3D© [1] has been used to model the surface analysis by resonance ionization of sputtered atoms (SARISA) SNMS/SIMS instrument, that was developed and built at Argonne National Laboratory [2]. The SARISA instrument (Fig.1), which operates on the time-of-flight principle, has a unique design that uses two hemispherical energy analyzers for energy- and angular-refocusing of sputtered ions and photoionized neutrals. Another feature of the instrument is that the same "front end" ion optics is used for focusing primary ions with normal incidence and for extracting and focusing secondary ions and postionized neutrals. The motivation of this work is to develop a time-of-flight mass spectrometer (TOF MS) with improved useful yield (atoms detected per atoms sputtered) and mass resolution. This is to be accomplished (1) by obtaining accurate quantitative estimates of the instrument transmission and time resolution, (2) by identifying a rational alignment procedure for optimizing these parameters, and (3) by exploring changes in the ion optics design that would lead to these improvements. The techniques and approach used here should be *generally useful to design electrostatic and magnetic mass spectrometers.*

The Model.

Virtual ion optics components (called "instances") were assembled together on a SIMION workbench. Ion trajectories through each component were then calculated under control of the corresponding set of user programs written in the Hewlett Packard calculator based RPN language. Since some of the components of SARISA are identical, the same potential arrays and user programs were used twice to save computer memory. There are 21 "instances" controlled by 18 programs written for 18 unique potential arrays. To correctly define boundaries of electric fields, all the important and complex virtual components were "built" as three dimensional (3D) "instances". Typically, this has been done for areas where cylindrical elements (lenses) were interacting with planar elements (deflectors). The major 3D components are as follows: (1) the "front end" focusing region for primary and secondary ions, which consists of two Einzel lenses separated by planar ion beam deflectors; (2) the

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system of horizontal deflecting plates separated by resistively coated vertical side plates used to bend the primary ion beam onto the secondary ion axis; (3) entrance and exit regions of the specially designed hemispherical energy analyzers with resistive disks, which provide an accurate termination of the electric field lines within the analyzers; and (4) the Colutron™ ion source with its velocity filter, which includes shims plates for shaping the electric field within the filter. The resistive coating used in the energy analyzers and in the bending system was simulated by introducing a number of intermediate electrodes into the corresponding potential arrays. This allowed precise modeling of the resistive coating regions with floating electric potentials. The model part corresponding to the Colutron™ ion source can be used as a separate independent and accurate model of this ion source.

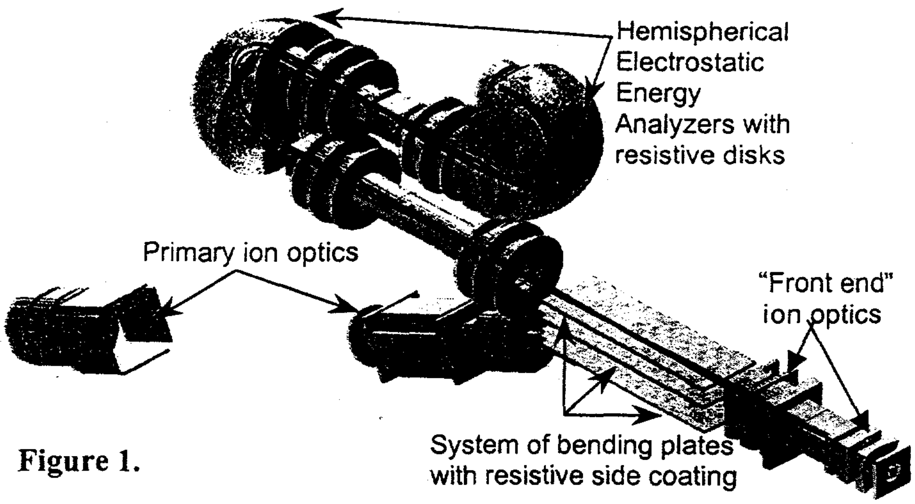

Figure 1.

To investigate the influence each component has on the final transmission of the SARISA instrument, 3D computer displays of ion trajectories were constructed. These simulations have identified several changes in operating conditions that improved instrument transmission. A set of user programs is used (1) to control voltages applied to all the virtual electrodes, (2) to control appearance ("birth") of ions with predetermined initial coordinates, velocities and angles of motion within any of 21 "instances" and (3) to monitor ions parameters during their flight through the ion optical system. An algorithm has been developed that allows a means of estimating the instruments transmission. This algorithm allows small sets of ions (up to 27) with definable initial parameters to be created internally by SIMION in real time. Due to limitations of the build-in RPN compiler of SIMION, large sets of ions (200 and more) are imported from ASCII files generated externally. In this case, the ion generating part of the user programs is skipped and only subroutines that monitor ion parameters and set voltages on virtual ion optics electrodes are used. These two modes of operation provide substantial flexibility when using the computer model as discussed below.

1. The *alignment mode* is used for quickly identifying the optimal alignments of the instrument for ions with initial kinetic energies equal to the most probable energy. In this mode, the ion generating routine calculates (a) the emission of secondary ions homogeneously distributed within a controllable solid angle from a circular spot with a controllable position and diameter ("SIMS regime") or (b) the appearance of postionized sputtered neutrals homogeneously distributed within a volume of controllable size located at a controllable distance from the controllable emission spot mentioned above ("SNMS regime"). For neutrals, angles of the initial ion motion are calculated from the relationship between locations and sizes of the emission spot and the cylindrical ionization volume. Octagons are used to simulate circles of the emission spot and the ionization cylinder.

2. The *transmission mode* makes use of externally generated files containing initial parameters for the ions. The algorithm for calculating initial parameters is the same as used internally by SIMION. However, in this mode, it is possible to generate large sets of ions (>30) with varying initial energies, coordinates, angles of motion, times of birth etc. Any appropriate external software can be used for this purpose. A larger number of ions and a wide variety of initial parameters are used in the *transmission mode* to more accurately calculate the transmission. Despite the fact that it is not difficult to generate sets of thousands of ions representing all the possible angles and energies, sets of hundreds of ions seem to be sufficient for good accuracy.

In both operating modes, SIMION monitors the parameters of ions as they fly through SARISA. These parameters are read by the set of user programs to calculate transmission and time resolution. Voltages for SARISA that are optimized in the *alignment mode* are then used in the *transmission mode* to obtain more precise quantitative estimates of transmission and time resolution. Two definitions for the transmission of the instrument are used: (1) the *ordinary transmission* is the ratio of the number of detected ions to the number of emitted ions, and (2) the *weighted transmission* is the ratio of the sum of weighting factors of detected ions to the sum of weighting factors of emitted ions. *By introducing weighting factors, the angular and energy distributions of emitted particles can be taken into account.* After the last ion has been generated, the programs calculate minimal and maximal times of flight for the set of ions. Those times are used to estimate the time resolution of the system as the ratio between the average time of flight and the difference between maximal and minimal times of flight. The average time of flight of ions is defined as a ratio between the sum of products of times of flight of detected ions to their weighting factors and the sum of the weighting factors of detected ions.

Results and discussion.

Estimates of the transmission of the SARISA instrument, operated in the SIMS regime with the extraction voltage of secondary ions of 1 kV, were obtained by performing the following computer "experiments". A total of 49 emission spots each with a diameter of 0.3 mm were equally spaced within a square (6 mm×6 mm) on the target. From each spot 241 secondary ions are emitted with energies of 5 eV and 20 eV. Emission angles (φ) for the ions were selected over the range 0° to 180° in steps of 1.5°. This caused the ions to be equally spaced over the emission hemisphere.. Results of the computer experiments to estimate transmission are shown in Figs. 2 and 3. Figure 2 shows ordinary and weighted transmission maps for secondary ions The used non-linear grayscale is selected to emphasize areas with the transmission higher than 0.7. The weighting factor used to calculate the transmission was $\cos^n \varphi$, where n = 1. As seen in Fig. 2, the weighted transmission is higher than the ordinary transmission because ions emitted with oblique angles do not substantially contribute to the detected signal. From the

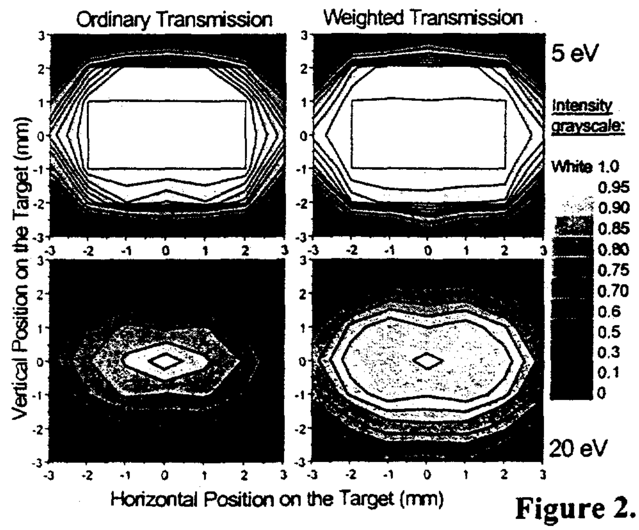

Figure 2.

maps shown in Fig.2, ion optics elements that limit the transmission of SARISA can be identified. The low transmission areas of the map are formed by shadowing of the flying ions by specific elements that can be identified by analyzing ion trajectories. Examining the high transmission rectangular area for 5 eV in Fig. 2, leads to the conclusion that the high transmission area in the vertical dimension (±1 mm) is limited by the bending plates (14 mm high), and the high transmission area in the horizontal dimension (±2 mm) is controlled by the Einzel lenses (inner diameter 24 mm) in front of the entrance to the first hemispherical energy analyzer. The same conclusions can be derived by examining the 20 eV data. Further, the asymmetry of the transmission in the vertical direction for 5 eV can be traced to the hole in the bending plates used to introduce the primary ion beam. Thus, full-scale 3D modeling of the ion optics allowed tracing features that could not be identified by using two-dimensional approaches.

Figure 3 shows the weighted transmission for the two ion energies as 3D plots. A linear grayscale linked to the Z axis is used to indicate the corresponding transmission. The XY plane of Fig. 3 corresponds to the target surface mapped in Fig. 2. Note that the transmission of the instrument is lower than unity (typically, 0.8-0.85) for 20 eV ions even if they are emitted from the center of the target, since fast ions moving at oblique angles do not reach the detector. In general, the simulation proves the high transmission of the SARISA instrument assumed in Ref. [3]. The weighted transmission is equal to unity for secondary ions with energies less than 10 eV, which covers the range of the most probable energies for the majority of secondary ions.

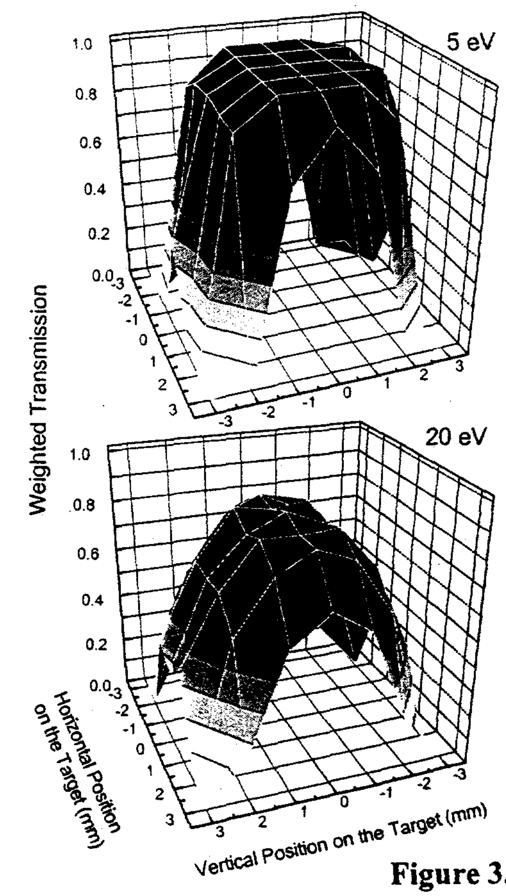

Figure 3.

Conclusions.

A computer program that models secondary ion and postionized neutral trajectories through the SARISA instrument has been developed. The program has been tested by determining the transmission of secondary ions for two different ion energies. Results indicate that the model accurately reflects the transmission of the SARISA instrument. The developed algorithm for creating ions and monitoring their parameters is generic and can be used for examining other SIMS/SNMS instruments and ion sources.

References.

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