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Computer simulation of ion beam analysis of laterally inhomogeneous materials

M. Mayer

Max-Planck-Institut für Plasmaphysik, Boltzmannstr. 2, D-85748 Garching, Germany

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ABSTRACT

The program STRUCTNRA for the simulation of ion beam analysis charged particle spectra from arbitrary two-dimensional distributions of materials is described. The code is validated by comparison to experimental backscattering data from a silicon grating on tantalum at different orientations and incident angles. Simulated spectra for several types of rough thin layers and a chessboard-like arrangement of materials as example for a multi-phase agglomerate material are presented. Ambiguities between back-scattering spectra from two-dimensional and one-dimensional sample structures are discussed.

1. Introduction

Ion beam analysis (IBA) methods such as Rutherford backscattering (RBS), elastic recoil detection analysis (ERDA), nuclear reaction analysis (NRA) and medium energy ion scattering (MEIS) are considered as quantitative methods for depth profiling of elements in the near-surface layer of solids [1]. In a strict sense, however, this is only true for one-dimensional laterally homogeneous materials, i.e. where the material distribution parallel to the surface is homogeneous. In this case concentrations of elements can be described as function of depth by depth profiles. Popular simulation codes for IBA [2] such as SIMNRA [3,4] or NDF [5] describe depth profiles as layered structures in slab geometry assuming atomic mixing of the constituents within each layer.

The success of IBA methods in analyzing one-dimensional sample structures widened the application of IBA methods to analysis of laterally inhomogeneous samples using the same well-developed methods as for one-dimensional samples [6]. Laterally inhomogeneous samples are two- or three-dimensional structures and include all types of rough layers and surfaces; porous materials; or compound multi-phase materials like geological samples, sinter materials, paint, or collections of dust particles. These compound multi-phase materials without layered structure will be called heterogeneous agglomerate materials throughout this paper.

Several models with different levels of generality have been developed for the simulation of IBA spectra from rough substrates or rough layers [7–20] using analytical approximations, straight line models (where incident and exit paths are approximated as straight lines) or Monte-Carlo simulations. Porosity with random distribution of pores can be treated as additional energy spread contribution if the diameter of pores is sufficiently small [21].

The simulation of MEIS spectra from three-dimensional nanostructures at the surface of a substrate has been implemented in the program PowerMeis [22]. The code RBS-MAST [23] allows to simulate RBS spectra from two- or three-dimensional sample structures but neglects all energy spread contributions (energy-loss straggling, multiple scattering, detector resolution, etc.). The Monte-Carlo code CORTEO [24] has been recently extended to use two- or three-dimensional sample structures as input [25].

This paper describes the STRUCTNRA program which allows simulation of two-dimensional sample structures using the well-known SIMNRA program as simulation kernel. The program is validated by comparison to experimental backscattering spectra from a silicon grating structure. Examples for spectra from various rough layers and two-dimensional arrangements of elements are given, and ambiguities between spectra obtained from one- and two-dimensional sample structures are discussed.

2. Computer simulation

2.1. Code structure

The simulation code STRUCTNRA allows the simulation of RBS, ERDA, NRA and MEIS spectra from arbitrary two-dimensional

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structures. The structure can be an image acquired by scanning electron (SEM) or transmission electron microscopy (TEM), or an arbitrary drawing, see Fig. 1. STRUCTNRA allows import of images in 24-bit bitmap (BMP) format. Each color in the image represents a material. A pixel can be empty, or it can contain a material consisting of up to 40 different elements and a mass density. STRUCTNRA uses quadratic pixels with adjustable pixel size Δ, see Fig. 1. Periodic boundary conditions are applied in horizontal direction.

STRUCTNRA uses SIMNRA 6.93 or higher [3,4] as simulation kernel through its COM interfaces. All SIMNRA features are available for simulations: Non-Rutherford and NRA cross-sections, several stopping power data sets, correction factors to Bragg's rule for individual materials, electronic energy loss straggling, finite detector resolution, energy spread by multiple small angle scattering, filter foils in front of the detector, etc. Simulations in back- and forward-scattering and in transmission geometry are possible.

STRUCTNRA assumes trajectories of incident and outgoing particles to be straight, see Fig. 1. Incident trajectories (solid line in Fig. 1) start at quasi-random starting points at the upper edge of the image. Quasi-random starting points are selected due to their more homogeneous coverage of the horizontal direction than a random distribution of starting points. The intersection points between the incident trajectory and the pixel grid are calculated and the path within each pixel is used as layer. This sequence of layers defines the target for incident particles T_{in}, see the dash-dotted lines in Fig. 1 for the layer boundaries of the first 3 layers of T_{in}. The sub-spectrum from each individual pixel (more precisely: from the incident trajectory inside of each pixel) is calculated by constructing a target T_{out} for outgoing particles by starting at the middle point of the path inside the pixel and calculating the intersection points between the outgoing trajectory and the pixel grid, see the dashed line in Fig. 1. This sequence defines the layer structure for the target for outgoing particles T_{out}. T_{in} and T_{out} are connected at the upper edge of the currently calculated pixel: This is realized by an additional shift of T_{out} versus T_{in}. Then the next pixel on the incident trajectory is calculated in the same way by constructing a new target T_{out} (dotted line in Fig. 1). This is repeated until the energy of incident particles decreases below a preset threshold energy typically close to zero.

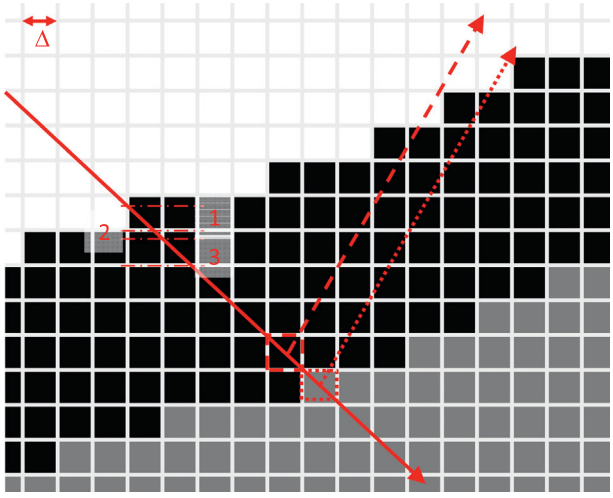

Fig. 1. Schematic representation of the calculational scheme of STRUCTNRA. Different colors indicate different materials. White pixels are assumed to be void, gray and black pixels can contain different materials. Δ: pixel size. Solid line: one trajectory of incident particles; dashed line: trajectory of outgoing particles from the dashed pixel; dotted line: trajectory of outgoing particles from the dotted pixel; dash-dotted lines: boundaries of layers 1, 2, and 3 of the target for incident particles T_{in}.

Multiple small-angle scattering is taken into account as energy spread, lateral spread is neglected. Dual large-angle scattering [26] is approximated in slab geometry, with the composition of each slab as average composition of all pixels in a row.

The necessary pixel size depends on incident particle species, energy, and materials of the pixels. Typical pixel sizes are in the range from a few nm to a few ten nm. Too large pixels can result in distortions of simulated spectra, too small pixels increase the computing time. The number of necessary incident trajectories depends on the complexity of the structure, typically between hundred and a few thousand trajectories are necessary. Typically a few thousand to a few millions of SIMNRA spectra have to be calculated. The computing time is proportional to the number of incident trajectories, the computing time for each trajectory is between $\propto m$ and $\propto m^2$ (with m the number of traversed pixels in vertical direction).

STRUCTNRA uses 2-dimensional sample structures, i.e. the sample shown in Fig. 1 is assumed to extend infinitely perpendicular to the paper plane. The plane of the sample cross-section is identical to the plane spawned by incident and exit beams. Note that at some geometries (for example Cornell geometry at oblique incidence) the cross-section of this plane with the sample may be non-parallel to the surface normal.

The spectrum of a random 3-dimensional sample, such as a rough surface without preferential lateral orientation or a porous layer without texture, is identical to the spectrum calculated from the 2-dimensional section of the sample with the plane spawned by incident and exit beams. The spectrum of a regular 3-dimensional object or structure (for example a spherical or cylindrical structure at the surface, see [22, Fig. 2] for illustration; or a 3-dimensional heterostructure) can be calculated as linear superpositions of spectra of 2-dimensional sample sections at different z-positions, where the z-axis is perpendicular to the paper plane in Fig. 1.

2.2. Comparison to experimental data

For code validation experimental RBS data were measured from a two-dimensional silicon grating on tantalum with 1500 keV incident ^{4}He ions at a scattering angle of 165°. The measurements were performed in parallel geometry where the detection plane, i.e. the plane formed by incident and exit beams, is parallel to the grating structure (see Fig. 2(a)), and in perpendicular geometry at different incident angles with the detection plane perpendicular to the grating structure (see Fig. 2(b)). A focused ion beam (FIB) cross-section of the grating structure is shown in Fig. 2(c). Based on the quantitative evaluation of several FIB cross-sections and by fitting RBS spectra measured at 1000 keV (not shown here) and 1500 keV at normal incidence, 45° and 60° incident angles an idealized grating structure was derived and is shown in Fig. 2 (d). This sample structure was used for all subsequent simulations. As can be seen from the FIB cross-section the side walls are not perfectly perpendicular but are slightly inclined. This inclination is difficult to measure quantitatively from the FIB images, but can be determined from the RBS spectra in parallel orientation as already described in [20]. Comparing Si layer thicknesses derived from FIB cross-sections and from RBS data yields the atomic density of the Si layer, which was natural density within the uncertainty of this measurement.

RBS spectra in parallel orientation at normal incidence and in perpendicular orientation at normal incidence, 45° and 60° incident angles are shown in Fig. 3 together with the corresponding simulations using the target structure from Fig. 2(d). The signal