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Intercomparison of ion beam analysis software for the simulation of backscattering spectra from two-dimensional structures

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ABSTRACT

The codes RBS-MAST, STRUCTNRA, F95-Rough and CORTEO are simulation codes for ion beam analysis spectra from two- or three-dimensional sample structures. The codes were intercompared in a code-code comparison using an idealized grating structure and by comparison to experimental data from a silicon grating on tantalum interlayer. All codes are in excellent agreement at higher incident energies and not too large energy losses. At lower incident energies, grazing angles of incidence and/or larger energy losses plural scattering effects play an increasing role. Simulation codes with plural scattering capabilities offer higher accuracy and better agreement to experimental results in this regime.

1. Introduction

The quantitative application of ion beam analysis (IBA) methods such as Rutherford backscattering (RBS), elastic backscattering (EBS), elastic recoil detection analysis (ERDA), medium energy ion scattering (MEIS) and non-resonant nuclear reaction analysis (NRA) [1] requires the application of computer simulation codes for quantitative evaluation of the measured spectra [2,3]. Available simulation codes for IBA and the implemented physics therein have been reviewed about a decade ago [2]. All codes assume laterally homogeneous samples where the distribution of elements varies only with depth, i.e. perpendicular to the surface, but is invariant in lateral directions, i.e. parallel to the surface. The sample is divided into horizontal slabs with variable thicknesses and compositions, different elements are assumed to be atomically mixed in each slab. Concentrations of elements then can be described as function of depth by concentration depth profiles. An intercomparison of seven different simulation code packages showed very good agreement between the codes for these types of samples [4,5].

In practice, however, often laterally inhomogeneous samples are analyzed using IBA methods. Laterally inhomogeneous samples are all kinds of two- or three-dimensional structures and include all types of rough layers, surfaces and interfaces; nanoparticles, nanopillars or other nanostructures; porous materials; or compound multi-phase materials like geological samples, sinter materials, paint, or collections of dust particles. These laterally inhomogeneous samples constitute new challenges for simulation codes. Several models with different levels of generality have been developed for the simulation of IBA spectra from rough substrates or rough layers [6–20]. A model for porous materials with random distribution of small spherical pores is described in [21]. MEIS spectra from three-dimensional nanostructures at the surface of a substrate can be simulated using the program PowerMeis [22].

The pioneering multi-purpose code for the simulation of RBS spectra from arbitrary two- or three-dimensional sample structures was RBS-MAST [23]. Recently the program STRUCTNRA was developed [24]: It allows simulating IBA spectra from arbitrary two-dimensional sample structures and uses the SIMNRA code [25] as simulation kernel. F95-Rough [26] is a code for the simulation of common RBS spectra including surface roughness as 2D cuts of the measured sample. The Monte-Carlo code CORTEO [27] has been recently extended to use two- or three-dimensional sample structures as input [28].

RBS-MAST [23], STRUCTNRA [24] and F95-Rough [26] are analytical codes [29] approximating incident and exit trajectories as straight lines connected by a single scattering event. RBS-MAST combined with the DEPTH code [30] and STRUCTNRA can additionally take into account the effects of multiple small-angle scattering

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approximately as additional energy spread contribution [30,31]. Lateral deflections are neglected. STRUCTNRA can additionally calculate plural large-angle scattering in the dual scattering approximation [32] using an averaged one-dimensional target structure. CORTEO [27] is a Monte-Carlo code with weight function and takes all effects of plural scattering into account.

This paper is organized as follows: Participating codes and the used input parameters are shortly described in Section 2. Details of the experimental setup are given in Section 3. A code-code comparison for an idealized target structure is presented in Section 4, results of code calculations are compared to experimental data in Section 5.

2. Simulation codes

2.1. RBS-MAST

RBS-MAST is a Monte-Carlo simulation program for calculating RBS spectra taken on 2D or 3D structured samples. The code has been introduced by Z. Hajnal and co-workers for the analysis of porous structures [23] and was developed further by F. Pászti et al. and recently by E. Kótai at the Research Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics in Budapest, Hungary. In RBS-MAST both periodic and randomly distributed structures can be treated. The individual ions are followed both inward and outward as if they would jump in the sample by steps of random length along straight trajectories.

The sample is built up from subsequent layers each constructed from elementary cells. Inside the cells objects of various shape, size and relative positions can be embedded, i.e. spheres, cylinders, bricks, ellipsoids, cones, or wedges of arbitrary atomic composition can be placed. Periodic structures can be treated by applying periodic boundary conditions for the elementary cell, while random structures are modeled by properly shifting and/or tilting the elementary cells when the ion passes through the cell walls.

The program first calculates a raw spectrum that takes into consideration only the geometric effects caused by the 3D structure of the sample. To add the classical energy spread contributions, the resulted spectrum can be convolved with a response function with given full width at half maximum (FWHM). In this work a Gaussian-type response function was used, its FWHM was calculated as a function of depth with the DEPTH code [30] using an averaged one-dimensional target structure. In the DEPTH code the energy resolution of the detector and Chu + Yang electronic energy loss straggling [33] were used. Optionally, the effect of multiple scattering was also taken into account as additional energy spread contribution [30]. In all RBS-MAST simulations presented here Rutherford cross-sections with Andersen screening [34] and SRIM-2003 stopping powers [35] were used.

Note, RBS-MAST previously has been applied in the 3D structure analysis of porous materials [23], non-continuous layers [36], fish otoliths [37], nanoparticles, and surfaces patterned by nanosphere lithography [38–40].

2.2. SIMNRA/STRUCTNRA

The STRUCTNRA program is described in detail in [24]. It allows the simulation of RBS, ERDA, NRA and MEIS spectra from arbitrary two-dimensional sample structures. The sample is defined by an image with quadratic pixels of adjustable size. This image can be an artificial drawing of the sample cross-section or a scanning or transmission electron microscopy image. Each color represents a material or can be empty. Strictly speaking the image is the intersection of the plane spawned by incident and exit beams with the sample and is not necessarily perpendicular to the sample surface. Periodic boundary conditions are applied in horizontal direction. The starting points of incident trajectories are distributed quasi-randomly. SIMNRA 6.98 [25,41] was used as simulation kernel. For the presented simulations Rutherford cross-sections with Andersen screening [34] were used. SRIM-2008 stopping powers [35] and Chu + Yang electronic energy loss straggling [33] were used. STRUCTNRA assumes trajectories of incident and outgoing particles to be straight. Multiple small-angle scattering is taken into account approximately as additional energy spread [30,31], lateral spread is neglected. Dual large-angle scattering [32] is approximated in slab geometry, with the composition of each slab as average composition of all material pixels in one row. Simulations with perpendicular orientation of the grating, see Section 4, were performed using STRUCTNRA. Simulations with parallel orientation of the grating were performed using the general roughness algorithm of SIMNRA [20,41].

2.3. F95-Rough

The basic idea of the F95-Rough code is to generate a large number of particular RBS spectra for the ion beam impinging the sample surface at different, randomly chosen entrance points and scattered under identical conditions. The sum of all particular spectra simulates the real spectrum from the rough sample. The calculation is performed using 2D profiles provided as a perpendicular cut of the sample surface/interface. For the sake of simplicity the surface/interface profile is represented by a polyline consisting of points and line segments between consecutive points. The trajectories of the incident and emerging ions are approximated by straight lines and the slowdown process is separated from the scattering events. Multiple and plural scattering are not taken into account. The length of the ion trajectory, measured from the first particle entrance point, is incremented by a small, constant step (can be liberally chosen) and the penetrating ion energy is changed accordingly using the appropriate stopping powers particularly valid for the investigated local ion position. For this purpose SRIM stopping powers [35] and Bohr straggling [42] are used. At each incremental step during the simulation the current ion coordinates are tested if they are positioned in the sample surface or in the underlying substrate in order to decide what physical parameters as cross sections, kinematic factors and related parameters should be used for the simulation. At each incident ion position virtual scattering into the direction to the detector is considered with the probability proportional to the appropriate Rutherford cross section with L'Écuyer screening [43]. The ingoing ion is removed from the simulation as the ion reaches the sample back side or the ion energy falls below some the predefined value. The outgoing trajectory of the scattered ion is treated in the same manner.

In such a way for each ion trajectory a full RBS spectrum is obtained, respecting ion entrance point coordinates and the local appropriate sample properties. Each ion generates the RBS spectrum by the procedure described above and is stored in a virtual multichannel analyzer. The calculation is repeated many times with randomly generated ion entrance points spread over a representative sample area to obtain sufficient statistics covering as much as possible the surface morphological artifacts distribution. At last, the final RBS spectrum is summed over all ions and is convoluted with a Gaussian function containing the assumed detector resolution with energy spread estimated with the code DEPTH [30] for the mean layer thickness. To take into account the fine features of the sample surface properly, typically several hundred ion trajectories have to be generated. The simulation of about 500 trajectories using 2 MeV He^+ ions as projectiles requires approximately 600 s on a standard PC computer.