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A virtual instrument for SEM uncertainty analysis

Dominic Gnieser[1,2,a], Carl Georg Frase[1,b], Harald Bosse[1,c], Rainer Tutsch[2,d]

[1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

[2]Technische Universität Braunschweig, Institut für Produktionsmesstechnik (IPROM), Schleinitzstraße 20, 38106 Braunschweig, Germany

[a]Dominic.Gnieser@tu-bs.de, [b]Carl.G.Frase@ptb.de, [c]Harald.Bosse@ptb.de, [d]R.Tutsch@tu-bs.de

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Abstract. To assure the metrological traceability of a measurement, it is required to perform an analysis of the measurement uncertainty specific to the measurement task. An approach to estimate the measurement uncertainty for complex systems is the so-called virtual measuring instrument: The measuring process is simulated taking into account its influencing parameters and a statistical analysis is performed by means of Monte-Carlo calculations.
We present the development of such a virtual measuring instrument for scanning electron microscopy (SEM) which allows to estimate the measurement uncertainty in compliance with GUM for dimensional measuring tasks in nano- and microsystems technology. By application of this virtual instrument, model based corrections of systematic errors are made possible and the cognition of the strength of different perturbing influences can lead to recommendations to optimize measurement instruments and methods. The virtual model programmed in MATLAB is called 'vREM', it includes all essential components of the measuring chain of an SEM as modules: The electron source, the electron-optical lens-system, the scan-generator, the interaction of the electrons within the object, electron detectors, simple analysis procedures and consideration of external disturbances. By adjusting parameters uncertainty contributions can be assigned to the virtual probe, the virtual specimen and the virtual detector signals.

Introduction

To assure the metrological traceability of a measurement, it is required to perform an analysis of the measurement uncertainty specific to the measurement task. An approach to estimate the measurement uncertainty for complex systems is the so-called virtual measuring instrument: The measuring process is simulated taking into account its influencing parameters and a statistical analysis is performed by means of Monte-Carlo calculations.

Such virtual instrument models already exist for some measurement systems used in micro- and nanotechnology [1]. The work presented here is the development of such a virtual measuring instrument for scanning electron microscopy (SEM) which allows to estimate the measurement uncertainty in compliance with GUM for dimensional measuring tasks in nano- and microsystems technology. SEM and dedicated so-called CD-SEM are widely used today in semiconductor industry for control of the dimensional characteristics of lithographic features [2]. The application of virtual instrumentation for SEM and CD-SEM allows model based corrections of systematic errors to be made, and the cognition of the strength of different perturbing influences can lead to recommendations for real measurements.

The virtual model programmed in MATLAB is called 'vREM', it includes all essential components of the measuring chain of an SEM as modules: The electron source, the electron-optical lens-system, the scan-generator, the interaction of the electrons within the object [3], detectors, simple analysis procedures and external disturbances. By adjusting parameters uncertainty contributions can be assigned to the virtual probe, the virtual specimen and the virtual detectors. External factors like temperature, vibrations or disturbing fields have additional effects on

respective components. The functionality and modular structure of vREM is presented in chapter 2, together with some illustrative examples while chapter 3 closes with a summary and conclusion.

2. General structure of the virtual instrument vREM

The virtual instrument called 'vREM' contains all relevant components of the measurement chain of a scanning electron microscope (SEM, or REM in German) as independent modules: The electron source (2.1), the electron-optical lens system (2.2), the raster scan generator (2.3), the probe-sample interaction module (2.4), the detector module (2.5), the external influences module (2.6) and finally the data analysis module (2.7). Within vREM, the assumed values of the input parameters which are adjustable in the different modules together with their assumed variations are taken into account to calculate either individual uncertainty contributions e.g. for the virtual electron probe, the virtual sample or the virtual detector or to combine the different uncertainty contributions for a measurand of interest, like e.g. the width of a nanoscale line feature. External disturbance like temperature variations, vibrations or stray fields could additionally be taken into account. The virtual measuring instrument vREM is based on the Monte- Carlo program MCSem [2] developed at the PTB and implemented in C++, which simulates the signal generation in SEM with a focus on the simulation of the physical interaction between the primary electrons and the material and topography of the sample of interest. An overview of the general structure of vREM is shown in figure 1.

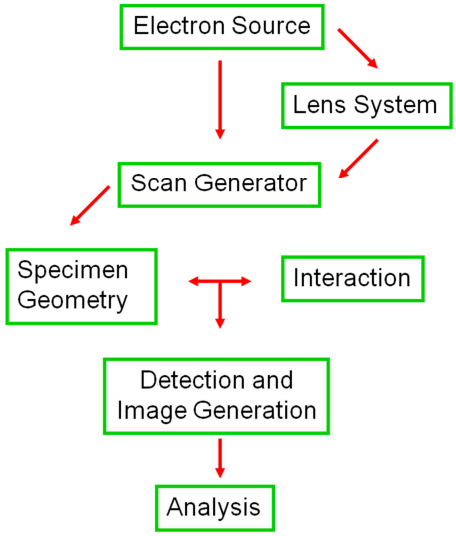

Fig. 1 Modular structure of the program vREM

For the estimation of measurement uncertainties for a specific measurement task with vREM several parameters of the virtual SEM are to be varied in addition to the already time-consuming Monte-Carlo-simulations of the probe sample interaction itself. We decided to use MATLAB as the programming environment for vREM, which already provides optimized calculation routines for different tasks, and which also allows parallel execution of program code if properly programmed. In addition MATLAB offers an easy generation of graphical user interfaces (GUI) for input of setting parameters for the virtual instrument, optimized for the later use of vREM also by less experienced users. From the main GUI of vREM (and main module), the individual modules 2.1-2.7 described in more detail below are accessible. The selectable parameters within the modules are already pre-defined with default values (value and variation ranges for each selectable parameter), but can be modified individually via the GUI interfaces. During a complete simulation of the vREM virtual instrument a selectable number of repeat runs are performed and the input parameters are varied in each run according to the specified variation ranges of the input parameters using statistical Monte Carlo techniques.

2.1 Electron source module

In the electron source module different types of electron emitters can be implemented by using different parameters for electron emitters. These parameters are:

The virtual cathode diameter describes the diameter of the first crossover point of the cathode, which is demagnified and imaged by the electron-optical lens system onto the sample surface. This parameter is about 20-50 µm for thermal electron emitters, while Schottky emitters and fieldemission (FE) cathodes could generate virtual diameters of below 10 nm.

For emission from the cathode material the electrons need to overcome the work function. The cathode temperature alone as for the thermal emitter or in combination with external electrical fields as for the Schottky emitter provides the necessary energy for the electrons to be emitted from the cathode material. For thermal emitters the necessary cathode temperature is between 1500 K and 3000K in dependence of the cathode material (for work function between 2.7 eV und 4.5 eV). For Schottky emitters the effective work function is reduced by the impact of a high voltage field and thus lower cathode temperatures already allow electron emission. Schottky emitters often are operated in the range 1000 K – 1500 K.

The cathode temperature and the work function of a material can be used to calculate the electron beam density of the electron emitter (Richardson law). The variation of the temperature and of the extraction electric field of the cathode determines the energy variation of the primary electrons (here simplified without taking into account the electron-electron interaction (Boersch-effect)). Further parameters for the simulation of the cathode are the assumed primary energy the electrons are accelerated to and the fluctuations of the corresponding accelerating voltage U/U. From the electron beam current density, the primary energy and the temperature, the maximum brightness of the emitter can be calculated, from which the aperture angle of the beam current at the sample can be derived. The implemented formulae for description of the emission characteristics of the different types of electron cathodes were taken from standard SEM textbooks, like e.g. [4].

2.2 Electron-optical lens system module

This module serves to take into account the most important aberrations of the electron-optical lens system of a SEM in a simple way, again following text book knowledge for electron-optical systems [4].

The diameter of the electron beam spot in the plane of least confusion d_S which is due to the *spherical aberration* can be described by the spherical aberration coefficient C_S and the aperture angle α: $d_S = 0{,}5\ C_S \cdot \alpha^3$. Please note that for the weak magnetic lenses often used in SEM the spherical aberration coefficient C_S is also dependent on the focal length f of the lens ($C_S \sim f^3$).

The beam spot size due to *chromatic aberration* d_c is determined by the corresponding aberration coefficient C_C, the aperture angle α and a combination of the variation of the acceleration voltage, the ratio of this energy variation to the primary energy and the variation of the lens currents dealt with in this electron-optical lens module:

$d_C = C_C \cdot \Delta f/f \cdot \alpha$, with $\Delta f/f = [(\Delta U/U)^2 + (2\ \Delta I/I)^2 + (\Delta E/E)^2]^{1/2}$

Please note that by the introduction of compound electrostatic and magnetic objective lenses in the early 1990s, the spherical and the chromatic aberrations could be reduced by approximately a factor of 10 in comparison to purely magnetic weak lenses, which drastically improved the imaging capabilities especially for low energy SEM. For example in [5] aberration coefficients of 3.7 mm for the spherical and 1.8 mm for the chromatic aberration constant at a beam energy of 500 eV and a working distance of 4 mm were reported.

The effect of *astigmatism* is proportional to the distance Δf_A between the sagittal und the meridional focus lines and the aperture angle: $d_A = \Delta f_A \cdot \alpha$.

The beam broadening due to *electron diffraction* can be described by Fraunhofer diffraction and is proportional to the de Broglie wavelength λ of the electron (dependent on its energy), and inversely proportional to the aperture angle. The sinc-function has a halfwidth of $d_B = 0.61\ \lambda/\alpha$.

The resulting beam broadening of the primary electron probe at the sample d_p can be expressed as the geometric sum of the individual aberration beam diameters and the demagnified image of the

virtual cathode beam diameter d_0: $d_p = [d_0^2 + ds^2 + d_C^2 + d_B^2]^{1/2}$. (Please note that in the current version of vREM the demagification factor by the electron-optical lens system is not yet a freely to choose parameter, but is a fixed parameter in the program code). For every primary electron simulated within vREM, its distribution onto the different aberration beam spots is statistically varied by means of the Monte Carlo method. The aperture angle α is calculated from the arc tangent of the ratio of the radius of the main aperture to the working distance. If the main aperture is located above the objective lens, the radius of the exit pupil (the image of the main aperture by the objective lens) has to be chosen as parameter.

In figure 2 simulated data for the mean radius of the resulting beam spot for different working distances (and associated different aperture angles) are shown (applied simulation parameters are for a conventional SEM with weak magnetic lenses: virtual cathode diameter: 30 µm; primary energy: 10 keV; main aperture radius 10 µm; C_S: 50 mm; C_C: 4.5 mm; Astigmatic focus distance Δf_A: 0 µm).

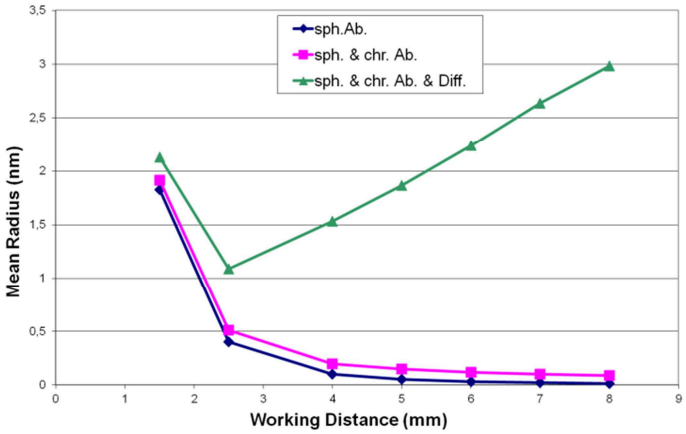

Fig. 2 Influence of different aberrations on the calculated beam spot size in dependence of the working distance

The lowest curve (diamond symbols) illustrates the effect of the spherical aberration alone (here assumed without the additional focus dependence of C_s), the mean curve (square symbols) contains effects from spherical and chromatic aberrations while the upper curve (triangle symbols) in addition also takes into account the diffraction broadening (not as sinc- or Gaussian function, but as uniform distribution). One recognizes that the chromatic contribution is of minor importance for the 10 keV primary energy used for this simulation. For larger working distances (and corresponding smaller aperture angles) the diffraction contribution becomes stronger while for small working distances (larger aperture angles) the spherical aberration has the strongest impact. Please note that for the triangle symbols in this example we deliberately decreased the aperture radius by a factor of 10 to exaggerate the effect of diffraction broadening.

2.3 Raster scan generator module

For the functionality of the raster scan generator an own module was implemented, separated from the electron-optical lens system module. The required parameters describe the area, which is to be scanned by the primary electrons, defined by x- and y-start coordinates (described in the sample coordinate system), in which the electron beam should hit on the sample at the beginning of the scanning process, the size of the scan area (fast and slow scan direction) in pixels and defined pixel size. In addition a value for the scan rotation is needed to describe any intended deviation in orientation of the scan direction from the principle axis of the raster scan coils.

Moreover, so-called ‘dead pixels’ were introduced, i.e. additional pixels outside of the scan area, which are probed by the electron beam, but which should not be registered and further analyzed by the measurement system. The pixel rate describes the local velocity of the electron beam scanning over a pixel of the scan area. Two further parameters are defined in vREM for handling of scan nonlinearities (as determined e.g. in [6]), due to the reluctance of magnetic scanning coils (described by a function of the type: $A\,(1 - \exp(-t / T))$.

A significant difference to the treatment of beam scanning in MCSem is that the electrons impinging on the sample are no longer allocated to the 'intended' pixel coordinate, but that each electron now has been given a time index – calculated from beam current, pixel rate and number of pixels to be scanned (including 'dead pixels'), which is allocated to a corresponding image pixel in the detector module by means of recording or sampling time intervals.

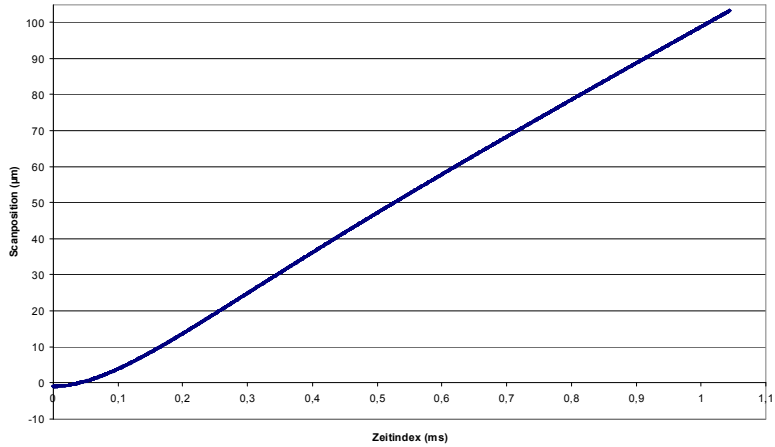

Fig. 3 Nonlinearity of the scan position in dependence of the time index, pixel size of 100 nm in a 1024 pixel line plus each 10 'dead pixel' at the start and at the end of the line

In figure 3 the dependence of the fast scan position on the time index was simulated with vREM for one scan line. One can observe the intended delay at the beginning of the scan process. The first ten pixels (those with negative position values) are declared as 'dead pixels' to mask the strong non-linearity in this scan region and to exclude it from further evaluation.

As output of this module, each primary electron is described using the parameters and distributions determined in the prior modules (including the random numbers) by a set of state variables, consisting of position coordinates (x, y, z), direction angles (θ, φ), its primary energy and time index.

2.4 Probe-sample interaction module

The interaction of the electrons with the material of the solid state sample and the module for the specimen geometry, that provides the interaction part with data of the materials dependent on the position of the electron, has been translated from the C++ program MCSem to MATLAB code and was integrated into the vREM structure, thereby transferring the C++ simulation sequence based upon loops as best as possible into MATLAB parallel statements based on matrices and vectors to achieve as fast as possible calculation speed.

Using the 3D-geometry module it is possible to assemble arbitrary structures out of an assembly of basic geometric primitives like cuboids, ellipsoids, cylinders, layers or triangular prisms, each of these basic geometries consisting of a single material. This material can be chosen to be a sole element or a composite of multiple elements (or vacuum). The interaction module simulates the movement of the electrons inside the solid state sample. The elastic scattering of the primary electrons is calculated by using tabulated Mott scattering cross-sections, computed by a modified version of the program PWADIR by Salvat and Mayol [7]. The inelastic scattering is modeled by Bethe's continuous slowing down approximation (CSDA) [8] with a modification of Joy and Luo [9]. Secondary electrons (SE) generation and transport is handled by a simple exponential, parametric model, using two material dependent parameters: a mean SE excitation energy and a mean free path. The time index assigned to the generated secondary electrons is identical to the index their creating primary electron possesses.

In figure 4 an output window of MATLAB is shown with the paths of 100 primary electrons of 10 keV primary energy in a SiO_2-layer, simulated by vREM.

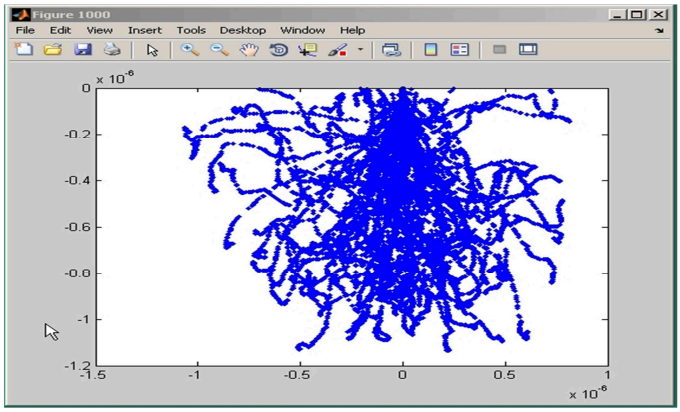

Fig. 4 Primary electron paths simulated by vREM

2.5 Detector module

In the detector module up to now the electrons leaving the specimen, emitting into a solid angle - selectable by a parameter - and with an energy within a defined range (except for the SE) are just rudimentarily assigned to a pixel based on their time-index. In the future already existing detector-efficiency tables will be used, variations of the efficiencies (e.g. caused by fluctuations in the cascade effects of the dynodes) will be included, the detector-signals will be digitized as well as noise and amplification factors of the electronics will be handled. The signals will be converted via contrast and brightness parameters into intensity values per pixel. It is planned to be able to use averaging techniques e.g. for multiple scan-rows.

2.6 External influences module

A main source of disturbances by external influences are vibrations, coupled into the SEM. Figure 5 (left) exemplarily shows a measurement with a high pixel rate of an edge structure of a lithographic silicon line feature, which illustrates this problem. In vREM a possibility has been realized to simulate a vibration between the sample of interest and the impinging primary electron beam. For this, the frequency and the amplitude in x- and y-direction (in sample coordinate system) can be chosen and used for investigations. Figure 5 (right) shows such the impact of such a simulated vibration on the simulated material edge contrast of an ideal feature.

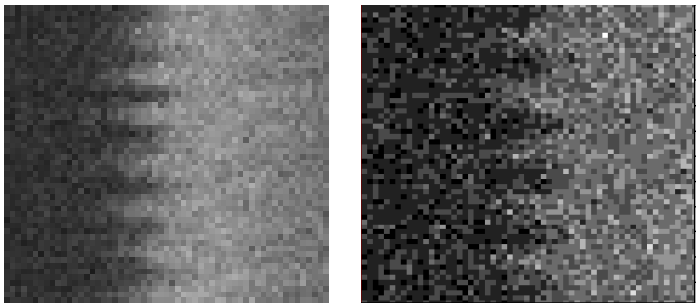

Fig. 5 Left: SEM image of an edge structure (measured by the electron-optical metrology system of the PTB), disturbed by external vibrations. Right: Simulation of an external vibration and the resulting material edge contrast on a flat sample, determined by means of vREM.

In addition to the vibration effects described above, also the influence of varying external magnetic and electric fields on the primary electrons as well as on the generated secondary electrons are planned to be investigated with the help of vREM (not implemented yet in the current version).

2.7 Data analysis module

This program module contains some simple evaluation algorithms for analysis of measurands on features of interest on samples simulated with vREM. The variation of the input parameters in the aforementioned program modules can then be used to determine the measurement uncertainties for

the different measurands of interest on the assumed sample. The observation of the influence of the evaluation on the determination of the measurand as well as investigations concerning the robustness of an algorithm are further application possibilities of this program module.

3. Summary and outlook

The virtual instrument vREM has been developed and implemented in MATLAB to serve as a tool for the investigation of the most relevant uncertainty contributions for measurements with scanning electron microscopy (SEM) and the determination of measurement uncertainties of measurands defined for features of interest on samples to be characterized with SEM. The main components of the modular program structure of vREM, i.e. the electron source, the electron-optical lens-system, the scan-generator, the interaction of the electrons within the object, the detectors, some simple analysis procedures and a module for consideration of external disturbances were motivated and described in adequate detail. Some examples of output parameters of individual program modules were presented and discussed.

Further work will concentrate on necessary refinements of implementation of functionality for the different modules as well as making use of the developed vREM virtual instrument implementation for systematic investigations of the achievable measurement uncertainty for different types of samples of interest (1D -, 2D- and 3D features) for different kinds of SEM.

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