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Surface chemical analysis — Depth profiling — Non-destructive depth profiling of nanoscale heavy metal oxide thin films on Si substrates with medium energy ion scattering

Analyse chimique des surfaces — Profilage d'épaisseur — Profilage d'épaisseur non destructif de films minces d'oxydes de métaux lourds à l'échelle nanométrique sur des substrats de Si par diffusion d'ions de moyenne énergie

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ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Email: copyright@iso.org
Website: www.iso.org

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Contents

Page

Foreword

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This document was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 4, *Depth profiling*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

Medium energy ion scattering (MEIS) has been considered to be a quantitative surface and interface composition analysis method with single atomic depth resolution since its invention in the early of 1980s. MEIS has been widely used for ultrathin films, especially nm gate oxides analysis to determine its composition, thickness, and the interface. Recently, MEIS has been used for nanoparticle analysis to determine the size and the composition with the core and shell structure information. In addition to the toroidal electrostatic energy analyser used in the early stage, different types of energy analyser such as magnetic energy analyser and time-of-flight (TOF) energy analyser have been used. With the continued scaling down of electronic devices, demands on accurate and reliable depth profiling have reached beyond the limit of sputter depth profiling which provides deteriorated depth profiles due to the sputter damage. Needs have been risen to investigate the consistency between the three types of energy analyser, ion species, and the different energy range of incident ions used for MEIS analysis and to set up a procedure for quantitative MEIS analysis. Two international interlaboratory tests were performed to develop this document which is reported in Annex A.

Surface chemical analysis — Depth profiling — Non-destructive depth profiling of nanoscale heavy metal oxide thin films on Si substrates with medium energy ion scattering

1 Scope

This document specifies a method for the quantitative depth profiling of amorphous heavy metal oxide ultrathin films on Si substrates using medium energy ion scattering (MEIS).

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 18115, *Surface chemical analysis — Vocabulary*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 18115 and the following apply.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at https://www.iso.org/obp
- IEC Electropedia: available at https://www.electropedia.org/

3.1
electronic stopping power
retarding force acting on charged particles, typically alpha and proton particles, due to interaction with electrons, resulting in loss of particle energy

4 Principle and recommendations of MEIS analysis

4.1 Ultrathin films of thickness less than 10 nm can be analysed with MEIS. (100 to 500) keV H^+ or He^+ ions are used for MEIS analysis. Scattered ion energy and angle are measured precisely so that measured MEIS spectra be compared with simulated MEIS spectra. MEIS spectra can be simulated with various programs from free codes such as PowerMeis[1] and SIMNRA[2] in public websites, MEIS expert laboratories, and MEIS manufacturers. Simulation programs calculate scattering cross-sections and electronic stopping powers. Quite often, calculated electronic stopping powers are subject to significant errors so that tabulated electronic stopping power values in the IAEA website[4] are recommended to use.

4.2 If not tabulated, it is recommended to measure electronic stopping power by users for more reliable results. Various types of energy analyzers can be used such as toroidal electrostatic analyser (TEA), magnetic energy analyser (magnetic), and TOF energy analyser. With MEIS analysis procedures specified in this document, less than 10 % uncertainty can be expected for ultrathin films under the guidelines describe in this document. This document is written for amorphous or polycrystalline thin films but not for crystalline thin films. To reduce the uncertainty of MEIS analysis, additional standards for calibration of scattering geometry, ion energy, energy resolution, detector efficiency, sample alignment, are required.

5 MEIS analysis

5.1 Set the ion scattering conditions such as ion energy, scattering angle, incidence angle from the surface normal, ion species, and ion dose for MEIS analysis. The ion dose is recommended to be in the static condition ($<10^{15}/\text{cm}^2$) but the static requirement for MEIS analysis is not strict compared to surface analysis such as XPS and static SIMS.

5.2 For MEIS analysis, specimen should be flat. Slight contamination due to air oxidation and ambient water and hydrocarbon adsorption does not disturb the MEIS analysis badly. However, if the surface contamination layer is thicker than 1 nm it shall be cleaned by appropriate methods such as solvent washing or ion milling.

5.3 Measure a MEIS spectrum of a specimen and generate a MEIS spectrum file with intensity (counts) vs energy (keV) at a specific angle. Specify all the ion scattering conditions such as ion beam energy, ion species, incidence angle from the surface normal, scattering angle, ion dose or ion current with analysis time, beam radius, and the type of energy analyser.

5.4 For MEIS analysis of ultrathin films of approximately 1 nm thickness, a clear plateau does not appear so that it may have poor reproducibility. It is recommended to express MEIS analysis result in surface areal density rather than in thickness or concentration for MEIS analysis of ultrathin films of approximately 1 nm thickness.

5.5 If the primary ion beam current is too high, it can cause multi-hit problems of detector. Under each MEIS analysis condition, it shall be checked whether the data is affected by the multi-hit problem by comparing MEIS results from high ion beam current and low ion beam current available from each MEIS system.

6 MEIS spectra simulation

6.1 MEIS spectra can be simulated with various programs from free codes such as PowerMeis(1) and SIMNRA(2) in public websites and simulation programs from MEIS laboratories and manufacturers as listed in Annex B. Detailed procedures for PowerMeis[1] is also given in Annex B as an example. In this document, general procedures for MEIS spectra simulation are given as a guidance.

Most of MEIS spectra simulation programs are based on Monte Carlo simulation or analytical calculation of binary scatterings and electronic stopping between binary scatterings. Multiple scattering is suggested to be included in all MEIS simulations. Thin films thicker than 5 nm are strongly recommended to be analysed including multiple scattering for the MEIS data obtained by He ions of ion energy lower than 500 keV. SIMNRA[2] provides multiple scattering simulation so that users can choose whether including it or not.

Generally, the integration step, and the slab thickness or atom density in MEIS simulations are 0,1 nm, and 0,1 nm or 1 x10^{15} atoms/cm^2, respectively.

In simulation, line shape, cross-section, electronic stopping power, charge neutralization, and energy straggling shall be selected by users as described below. Electronic stopping power is described in detail in 6.2

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1) http://tars.if.ufrgs.br

2) https://home.mpcdf.mpg.de/~mam/

Generally, simple Gaussian can be used as basic line shape for the first approximation. For MEIS systems with high resolution of δE/E approximately 8x10^{-4} with proton as a projectile, exponentially modified Gaussian is recommended for ultrathin films. However, other options can be chosen, if needed. Line shape parameters for each element, σ_o (additional parameter), is calculated by Casp version 5.2[3)] program for each projectile, projectile energy, and target element. Follow the instructions in Casp version 5.2.

To calculate cross-sections, interatomic potentials can be chosen from Anderson, L'Ecuyer, Moliere potential, or ZBL potential[1]. For MEIS analysis, Moliere potential is widely used. For energy straggling, Chu or Yang can be usually chosen. For charge neutralization, Marion and Young's equation[2] is used for 30 keV to 150 keV H^+ and for 30 keV to 200 keV He^+ and Armstrong's equation for 400 keV to 500 keV He^+. Casp charge-state-fractions algorithm^3 can be used for He with better reliability and for other heavier ions, if available. PowerMeis provides Marion and Young's equation and Casp neutralization. SIMNRA does not include neutralization in simulation.

6.2 Electronic stopping power is automatically calculated by the SRIM 95 or more recent SRIM2013 code, which can be used for non-critical MEIS analysis with inconsistency higher than 10 %. However, electronic stopping power from the SRIM code can have significant errors in the medium energy range. For accurate MEIS analysis with consistency lower than 10 %, it is recommended to use the measured and tabulated electronic stopping power data of elements and compounds from IAEA[4)], as described in Formula (1). If the IAEA database is insufficient or missing, newly measured electronic stopping power data by appropriate methods can be added to the IAEA database to improve the accuracy of the calculated electronic stopping power. The accuracy of electronic stopping power values in the IAEA database is estimated to be less than 8 % as discussed in Annex C.

The electronic stopping power from IAEA database can be obtained by fitting a set of electronic stopping power data in which can be used in Formula (1). The equation that can be used to fit the IAEA database are given in Formula (1). The E is the ion energy, Z is the atomic number of the ion, m is the mass of the ion. The unit of S_t, S_l, and S_h is eV·cm^2/10^{15} atoms, that of E is keV, and that of m is u. For fitting to determine A, B, C, and D, Origin or other appropriate fitting programs can be used.

$$\frac{1}{S_\mathrm{t}(E)^\mathrm{D}}=\frac{1}{S_\mathrm{l}(E)^\mathrm{D}}+\frac{1}{S_\mathrm{h}(E)^\mathrm{D}}$$

$$S_\mathrm{l}(E)=\mathrm{A}\sqrt{E} \tag{1}$$

$$S_\mathrm{h}(E)=\frac{\mathrm{z}^2\mathrm{mB}}{E}\ln\left(\frac{\mathrm{CE}}{\mathrm{m}}+1\right)$$

where

$S_t(E)$	is the total electronic stopping power;
$S_l(E)$	is the electronic stopping power of low energy electrons;
$S_h(E)$	is the electronic stopping power of high energy electrons;
A, B, C, D	are the fitting parameters;
E	is the ion energy;
z	is the atomic number of the ion;
m	is the mass of the ion.

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3) Available from: http://www/casp-program.org/

4) Available from: https://www-nds.iaea.org/stopping/

From the IAEA data[4], available fitting parameters A, B, C, and D are calculated and tabulated in Annex D for the convenience of the users of this document.

For straggling correction factor, just use 1,0, if the correction factor is not available, which is generally the case.

6.3 In output, energy channel width and angular channel width can be adjusted according to the energy and angular resolution for each MEIS analysis. Energy channel width is generally used as 0,1 keV and angular channel width should be same to the detector angular width when obtaining 1D spectrum.

In beam, atomic number, atomic mass, beam energy, and incidence angle from the surface normal are given. Projectile number can be adjusted to fit the experimentally measured MEIS spectrum of well-defined internal reference.

Analyser type is chosen among electrostatic, TOF, and magnetic. For electrostatic and magnetic analyser type, energy resolution full width half maximum (FWHM) (δE), scattering angle, and angular width ($\Delta\theta$) specified from each MEIS measurements are given. For TOF analyser type, TOF length (L), time resolution (δt), are additionally given according to specific TOF MEIS scattering conditions. Out of plane angle and angular width are used when MEIS scattering data are obtained from out of plane region or large detector. Energy resolution FWHM (δE) or time resolution (δt) can be measured by fitting the leading edge of a MEIS peak from a clean surface peak of heavy metal specimen.

6.4 After all the input parameters for simulation and experimental parameters are given, the structure of a specimen is to be built. Firstly, list up elements used in simulation. Then, construct layered thin film structures with the thickness and composition for each layer. Generally, a substrate layer is included in simulations. If necessary, a surface contamination layer or an interface layer between ultrathin film layers can be introduced to improve the fitting.

6.5 After all the specified and appropriate values are given, start a simulation. If all the input parameters are appropriate, then simulated spectra are given. Adjust the parameter of the projectile number in beam to fit the overall intensity or the intensity of a reference layer for example between measured and simulated MEIS spectra when an internal reference layer is used. Then adjust the thickness and composition of each layer manually and iteratively to get the best agreement between measured and simulated MEIS spectra. A chi-square test can be used to find the best agreement with a properly chosen energy range of spectrum. The low limit of an energy range in χ^2 calculation is recommended to be not lower than 10 keV from the substrate surface peak. In case that a reference layer of known stoichiometry is included in the sample, the height of reference layer can be chosen to generate minimum χ^2 calculation to determine the projectile number and then the composition and the thickness of unknown layers can be determined by changing fitting energy range to the unknown layer peak position to calculate and minimize χ^2. In case of no reference layer, overall χ^2 calculation with an appropriate fitting range can be used to get the best agreement between measured and simulated MEIS spectra.

6.6 MEIS simulation programs generate composition and surface areal density (10^{15} atoms/cm^2) for each layer. Therefore, to convert the areal density to the thickness of each layer, the density of each layer is required. If the density of thin films used in the MEIS analysis is known, use the number. But, generally the number is not known so that the bulk density can be used. In the case of non-stoichiometric compounds or mixtures, the sum rule can be used. According to the sum rule, the density of a non-stoichiometric compound $\rho(A_{x+\delta x}\, B_{y+\delta y})$ can be estimated by the Formula (2).

$$\rho(A_{x+\delta x}\, B_{y+\delta y}) = [(x+\delta x)\mathrm{m}(\mathrm{A}) + (y+\delta y)\mathrm{m}(\mathrm{B})[/\{[x\ \mathrm{m}(\mathrm{A}) + y\ \mathrm{m}(\mathrm{B})]/\rho(\mathrm{A}_x\mathrm{B}_y)\} \qquad (2)$$

where

$\rho(A_{x+\delta x}\, B_{y+\delta y})$ is the density of a non-stoichiometric compound with A constituent of $x+\delta x$ composition and B constituent of $y+\delta y$ composition;

m(A)	is the mass of A constituent;
m(B)	is the mass of B constituent;
$\rho(A_xB_y)$	is the density of a stoichiometric compound with A constituent of x composition and B constituent of y composition.

For mixtures of A and B, the density of the mixture A(x%) and B(y%) can be estimated by the Formula (3).

$$\rho(x\%A{+}y\%B) = [x\,\mathrm{m(A)} + y\,\mathrm{m(B)}]/[x\,\mathrm{m(A)}/\rho(\mathrm{A}) + y\,\mathrm{m(B)}/\rho(\mathrm{B})] \quad (3)$$

In Formulae (2) and (3), the m is the mass of each element or a compound in u.

By dividing the simulated areal atomic density of each layer with the estimated density of each layer, the thickness of each layer can be obtained. The use of bulk density values or the density estimated by the sum rule can generate errors in the depth from MEIS analysis.

7 Reporting MEIS analysis results

7.1 Report all the MEIS analysis conditions such as ion beam energy, ion species, ion current, incidence angle from the surface normal, scattering angle, ion dose, analysis time, beam radius, sample descriptions including surface contamination and surface flatness, sample preparation, MEIS analysis chamber pressure, energy analyser type and specifications, detector type and specifications.

7.2 Details of MEIS spectra simulations shall be specified including simulation program name and all of simulation parameters.

7.3 It is recommended to report MEIS analysis results in the quantity with unit of surface areal density (10^{15} atoms/cm^2), or concentration (atomic fraction) as a function of depth in the unit of areal density (10^{15} atoms/cm^2). Using the bulk density, it can be reported as concentration (atomic fraction) as a function of depth in the unit of thickness (nm), but it shall be clearly stated that the bulk densities are assumed for ultrathin films.

Annex A
(informative)

Interlaboratory test report

A.1 Overview

This annex gives a report of an interlaboratory test on non-destructive depth profiling of nanoscale thin films with medium energy ion scattering.

A.2 Principle

MEIS spectra of HfO_2 thin films with nominal thickness of 1 nm, 3 nm, 5 nm, and 7 nm on a substrate 12 nm SiO_2 on a Si substrate were measured precisely by 12 participants. Three different types of MEIS detector were used such as electrostatic, magnetic, and TOF. Measured MEIS spectra were simulated by each participant laboratories, resulting in the poor consistency of approximately 15 %. They were simulated again by one key laboratory, K-MAC, Korea and sources of poor consistency such as electronic stopping power and neutralization correction were investigated, which improved the consistency of MEIS analysis results less than 8 %.

A.3 Sample description

Samples were prepared at National Nano Fab Center in Daejeon, Korea. Nominally, 1, 3, 5, and 7 nm HfO_2 were deposited by atomic layer deposition method on a 12 nm thermal SiO_2 layer on a 6 inch Si(001) wafer. A 12 nm thermal SiO_2 layer that assists the uniform and flat growth of HfO_2 layer is used as an internal reference in the MEIS analysis. The uniformity of the thickness over a 6 inch wafer was tested by measuring 7 points of the wafer 5 times with ellipsometer. As a result, the standard deviations of thickness were estimated to approximately 0,5 %. The thickness of $HfO_2/SiO_2/Si$ samples was also measured by transmission electron microscopy (TEM). TEM images of $HfO_2/SiO_2/Si$ thin films are shown in Figure A.1 and the average thickness of samples are summarized in Table A.1.

a) 1 nm HfO_2 on a 12 nm thermal SiO_2/Si substrate **b) 3 nm HfO_2 on a 12 nm thermal SiO_2/Si substrate**

c) 5 nm HfO_2 on a 12 nm thermal SiO_2/Si substrate **d) 7 nm HfO_2 on a 12 nm thermal SiO_2/Si substrate**

NOTE The scale bar at the bottom left of the image is 2 nm.

Figure A.1 — TEM images of HfO_2 on a 12 nm thermal SiO_2/Si substrate

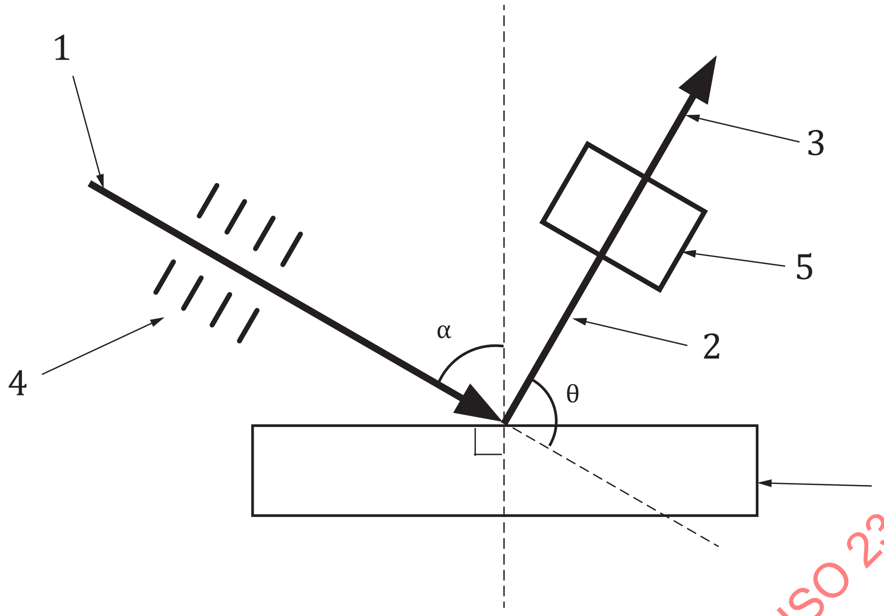
Table A.1 — Thickness of 1 nm, 3 nm, 5 nm and 7 nm HfO_2 measured by TEM

Samples	**Thickness** (nm)	
	Average	**Standard deviation**
1 nm HfO_2	1,72	0,12
3 nm HfO_2	3,29	0,10
5 nm HfO_2	4,86	0,18
7 nm HfO_2	6,39	0,06

A.4 Measurement procedure

A.4.1 Measurement

For MEIS analysis, the energy and the angle of scattered ions are measured to analyse depth profiles of ultrathin films. A MEIS instrument consists of an ion source, an accelerator, an energy analyser, and a detector. A schematic diagram is shown in Figure A.2. Ions generated from an ion source are accelerated to impinge on a sample surface. The energy of projectile ions scattered by target atom nuclei is measured by an energy analyser. The scattering angle is determined by the geometry of an ion source, a sample, and a detector. Electrostatic analyser, and magnetic, TOF are widely used as energy analysers.



Key

1	ion source (H^+ or He^+)
2	scattered particles
3	particles to detector
4	accelerator
5	analyser (electrostatic, magnetic or TOF)
6	sample
α	incident angle
θ	scattering angle

Figure A.2 — Schematic diagram of a MEIS system

Twelve (12) participants in this RRT are UFRGS (Brazil), IBM Watson (US), Western Ontario University (Canada), Kyoto University (Japan), Global Foundry (US), Samsung Advanced Institute of Technology (R. O. Korea), Samsung Electronics (R. O. Korea), SK hynix (R. O. Korea), K-MAC, (R. O. Korea), DGIST (R. O. Korea), KIST (R. O. Korea), and Huddersfield (UK). PowerMeis simulations were performed by W. Min at K-MAC. The experimental conditions of 12 participants are summarized in Table A.2.

Table A.2 — MEIS analysis conditions for each participant

Participants	**Incident ion**	**Incident energy** (keV)	**incident angle** (º)	**scattering angle** (º)	**analyser**
A	H	100	0	120	Electrostatic
B	H	100	54,7	110	Electrostatic
C	H	94	45	135	Electrostatic
D	He	400	31,5	74,1	Magnetic
E	He	400	44,5	83,6	Magnetic
F	He	500	44,2	78,2	Magnetic
G	He	450	54,6	70,5	Magnetic
H	He	400	45	68	Magnetic
I	He	100	45	130	TOF
J	He	80	45	90	TOF

Table A.2 *(continued)*

Participants	Incident ion	Incident energy (keV)	incident angle (°)	scattering angle (°)	analyser
K	He	100	2	120	Electrostatic
L	He	100	54,7	70,5	Electrostatic

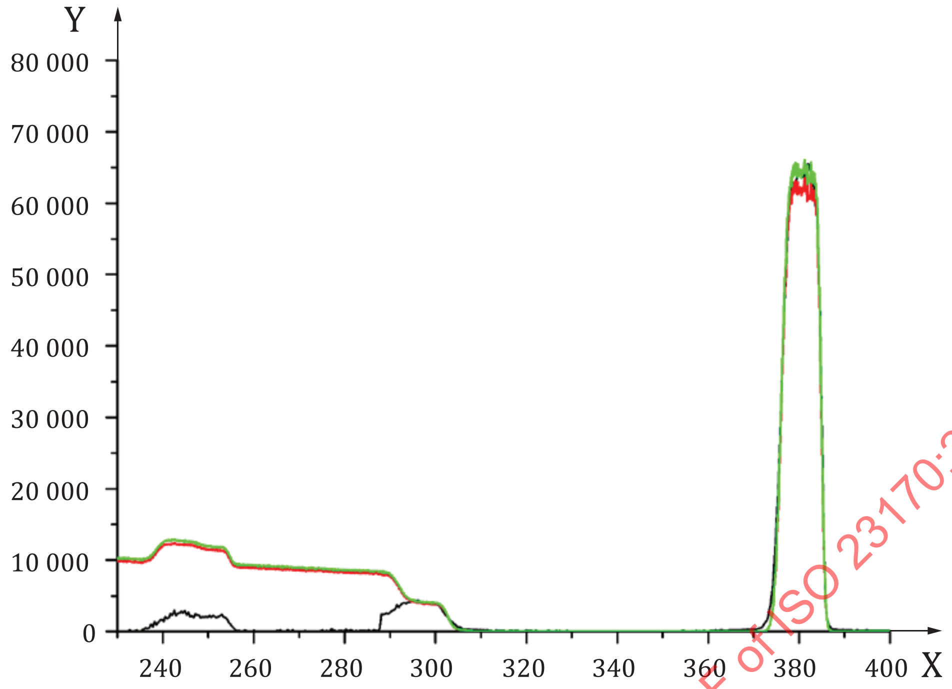
A.4.2 MEIS Spectrum simulation

The PowerMeis program was used as a simulation tool for analysis[3]. It was developed mainly by Mauricio A. Sortica and Gabriel M. Marmitt at the Pedro Grande group of the Universidade Federal do Rio Grande do Sul (UFRGS), Brazil. PowerMeis uses the Monte-Carlo method to simulate a MEIS spectrum by summing individual scattering spectrum from randomly selected scattering points of a sample. The scattered ion energy is calculated by the kinematic factor for each scattering event and by the electronic stopping energy loss according to the ion beam path in the medium. The peak shape of each event is calculated by the straggling according to the beam path for each location and a system resolution.

In this report, the scattering cross-section was calculated by Moliere potential. For the electronic stopping power, both SRIM95 electronic stopping power and the new refitted electronic stopping power were used for comparison, and the Chu model was used for the straggling. Neutralization correction should be applied to the data from electrostatic analyser and magnetic sector. Neutralization of Marion is applied to 100 keV H^+ and He^+[2] and that of Armstrong is applied to 400 keV to 500 keV He^+[4]. Casp program can be used for both cases with better reliability[5]. The density of HfO_2 used in the simulations was 9,68 g/cm^3, and that of SiO_2 was 2,2 g/cm^3 for the thickness calculation.

The stoichiometry of a thermal SiO_2 layer, (Si:O = 1:2) was used as a reference layer. The number of incident particles was determined by the Si height of the thermal SiO_2 layer below the HfO_2 layer in the sample. When determining the number of incident particles by fitting the Si peak height of the SiO_2 layer, background signals between Hf and Si peaks should be subtracted. Background signal is caused by the multiple scattering or the roughness. Given the TEM images of the samples, the background seems to originate from the multiple scattering rather than the roughness. The background signal is almost constant at the energy range between Si and Hf peaks. Since the simulation is based on the single binary scattering, subtracting the multiple scattering contribution to the Si or Hf peak was done before analysis by simulation.

MEIS analysis is performed by changing the model structure of a sample in a simulation to match the experimental Hf peak until the difference between the experimental data and the simulation results minimize. For simplicity, the interfaces between the HfO_2 layer and the SiO_2 layer and that between the SiO_2 layer and the Si substrate were ignored. The thickness of HfO_2 is mainly adjusted to fit the full width half maximum of the Hf peak. In Figure A.3, the solid black line is the experimental data and the red line is a simulation of a fixed HfO_2 composition (Hf:O = 1:2) with a number of incident particles that can fit the SiO_2 height from 293 keV to 300 keV. The Hf peak shows a slight difference between the black and red lines, and the red line is multiplied by a constant, C to the Hf height to generate the green line in a good agreement with the black line so that the composition of Hf increased to 0,33 * C. For all the simulations, the same electronic stopping power for HfO_2 calculated from the SRIM 95 or the refitted electronic stopping power are used as described below.



Key

X energy in keV

Y scattered ion intensity in counts

Figure A.3 — Example of MEIS analysis to determine the thickness and the concentration of a HfO_2 /SiO_2/Si ultrathin film

A.4.3 SRIM electronic stopping power

The Hf concentration and the thickness of the HfO_2 layer are obtained in the RRT using the SRIM95 electronic stopping power calculated automatically by the PowerMeis simulation program. Scattering cross-sections from Moliere potential[6] and Chu straggling[7] were used. Results are summarized in Table A.3. The average value of the 7 nm sample data are 32,3 % in Hf concentration, 6,52 nm in thickness, and $1{,}74 \times 10^{16}$ atoms/cm^2 in the amount. The standard deviation of the 7 nm sample data are 1,7 % in concentration, 1,00 nm in thickness, and $2{,}31 \times 10^{15}$ atoms/cm^2 in quantity or the surface areal density of Hf. The relative standard deviations are 5,3 % for concentration, 15 % for thickness, and 13,3 % for the amount of Hf, which are too high to be a routine practical analysis method.

Table A.3 — Analysis results by using SRIM95 electronic stopping, Moliere potential, and Chu straggling[a]

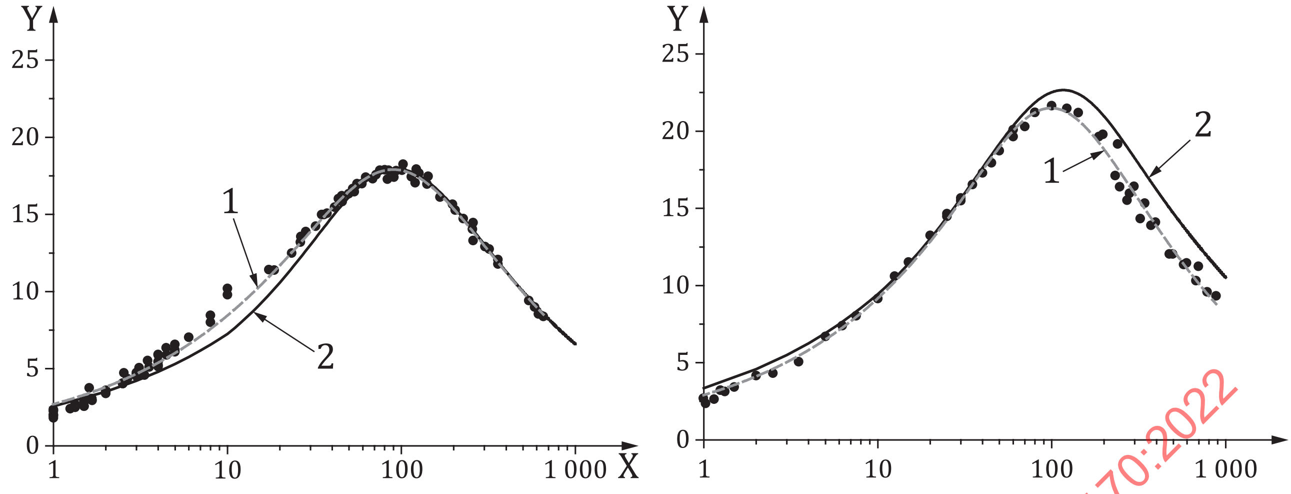
	Concentration of Hf				**Thickness** (nm)				**Quantity of Hf** ($1x10^{15}$ atoms/cm^2)			
Partici-pants	1 nm	3 nm	5 nm	7 nm	1 nm	3 nm	5 nm	7 nm	1 nm	3 nm	5 nm	7 nm
A	0,133	0,297	0,29	0,318	1,60	2,60	4,0	5,9	1,77	6,41	9,64	15,61
B		0,29	0,29	0,31		2,50	4,50	6,38		6,02	10,84	16,61
C	0,21	0,303	0,30	0,303	1,07	2,55	4,20	5,95	1,87	6,43	10,47	15,00
D	0,23	0,343	0,343	0,352	0,88	2,45	3,95	5,85	1,71	6,99	11,27	17,09
E	0,205	0,322	0,35	0,347	1,10	2,50	4,18	5,90	1,87	6,68	12,16	16,69
F	0,273	0,328	0,323	0,35	0,78	2,41	3,78	5,45	1,77	6,57	10,16	15,85
G	0,26	0,306	0,324	0,327	0,78	2,55	4,15	5,75	1,69	6,50	11,18	15,61
H	0,205	0,307	0,31	0,317	0,92	2,27	3,80	5,55	1,57	5,78	9,79	14,60
I	0,295	0,305	0,305	0,307	0,95	3,10	5,30	7,55	2,33	7,86	13,43	19,26
J	0,237	0,303	0,31	0,31	1,25	3,40	5,60	8,20	2,46	8,57	14,42	21,58
K	0,2	0,31	0,312	0,327	1,12	3,60	5,20	7,75	1,86	9,27	13,47	21,03
L	0,213	0,267	0,305	0,298	1,20	3,20	5,50	8,05	2,13	7,09	13,94	19,95
Average	0,224	0,307	0,314	0,323	1,06	2,76	4,51	6,52	1,89	7,00	11,53	17,43
Standard deviation	0,041 (18 %)	0,018 (5,9 %)	0,018 (5,7 %)	0,017 (5,3 %)	0,23 (22 %)	0,42 (15 %)	0,66 (15 %)	1,00 (15 %)	0,27 14 %)	1,00 (14,3 %)	1,64 (14,2 %)	2,31 (13,3 %)

[a] For the results by magnetic sector and electrostatic analyser, neutralization of Marion is used for 100 keV H^+ and He^+, and that of Armstrong for 400 keV to 500 keV He^+.

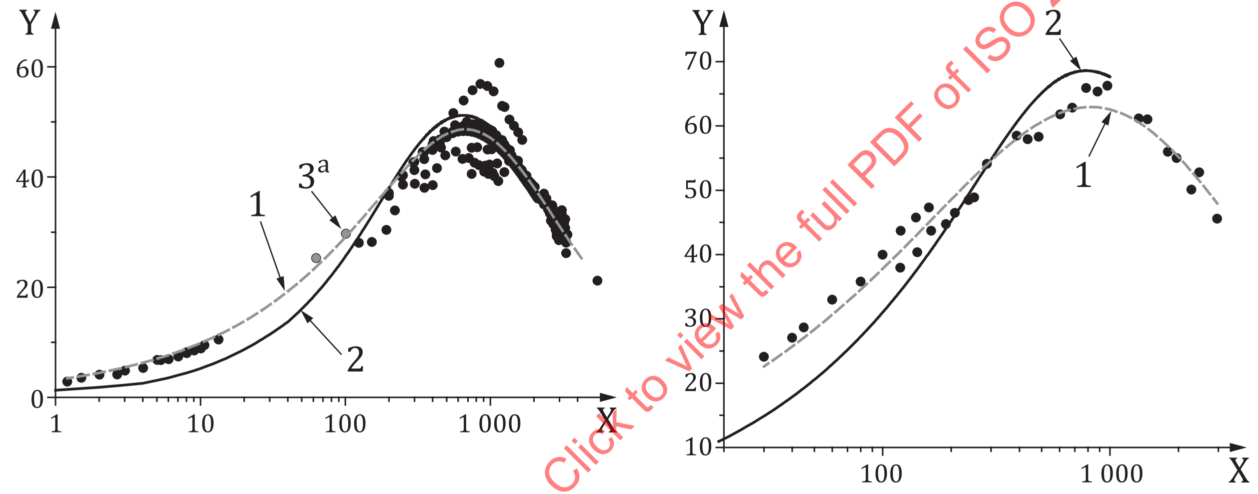
A.4.4 Newly fitted electronic stopping power

Among the factors affecting the MEIS analysis results, the scattering cross-section and the electronic stopping power have high influence. The models for the cross-sections of Hf and Si are reliable and are in good agreement with the measurement data[8]. On the other hand, electronic stopping power values of HfO_2 and SiO_2 from SRIM95 do not fit well with the measurement data set of black lines in Figure A.4. In fact, there is no data available in the range of 15 keV to 100 keV for He^+ on SiO_2 in the IAEA database. To eliminate the ambiguity, the electronic stopping powers of 62,3 keV He^+ and 100 keV He^+ on SiO_2 were measured and added to the public electronic stopping power data set of He^+ on SiO_2 from IAEA to obtain a new fitted electronic stopping curve. Two newly measured electronic stopping power values were added, which were obtained by measuring the height of the MEIS spectrum using 100 keV He^+ with two different incidence angles and the same scattering angle[9].

A new fitted electronic stopping power was calculated by refitting a set of electronic stopping power data. The equation used to fit the data are shown in Formula (1) and the fitting results are shown in Table A.4. The E is the ion energy, Z is the atomic number of the ion, m is the mass of the ion. The unit of S_t, S_l, and S_h is eV·cm^2/10^{15} atoms, that of E is keV, and that of m is u.



a) H⁺ on SiO$_2$ **b) H⁺ on HfO$_2$**



c) He⁺ on SiO$_2$ **d) He⁺ on HfO$_2$**

Key

X energy (keV)

Y electronic stopping power [10^{-15}eVcm^2/atom]

● stopping data set

1 fitted electronic stopping power from the IAEA experimental data (scattered dot)

2 SRIM 95

3 added experimental results (KMAC)

[a] Newly measured additional electronic stopping values.

Figure A.4 — SRIM95 and new fitted electronic stopping power

Table A.4 — Fitting results of electronic stopping power

	A [$\mathrm{eV}^{-0,5}\cdot\mathrm{cm}^2/10^{16.5}$ atoms]		**B** [$\mathrm{eV}^2\cdot\mathrm{cm}^2/\mathrm{u}\cdot10^{12}$ atoms]		**C** [u/keV]		**D**	
	Value	**Std. Err**	**Value**	**Std. Err**	**Value**	**Std. Err**	**Value**	**Std. Err**
H on SiO_2	2,70	$3{,}73 \times 10^{-2}$	$2{,}47 \times 10^3$	$2{,}76 \times 10^2$	$1{,}29 \times 10^{-2}$	$2{,}95 \times 10^{-3}$	2,74	$3{,}86 \times 10^{-1}$
H on HfO_2	2,91	$4{,}56 \times 10^{-2}$	$3{,}17 \times 10^3$	$2{,}73 \times 10^2$	$1{,}12 \times 10^{-2}$	$2{,}09 \times 10^{-3}$	3,27	$4{,}80 \times 10^{-1}$
He on SiO_2	3,16	0,04	$2{,}11 \times 10^3$	$8{,}02 \times 10^2$	$2{,}62 \times 10^{-2}$	$3{,}94 \times 10^{-2}$	1,29	$4{,}19 \times 10^{-1}$
He on HfO_2	4,48	3,35	$4{,}89 \times 10^3$	$3{,}57 \times 10^4$	$9{,}72 \times 10^{-2}$	$2{,}56 \times 10^{-1}$	1,15	9,94

The PowerMeis program introduced a correction factor for electronic stopping power to use a new fitted electronic stopping power. Newly fitted electronic stopping power values are applied by multiplying the correction factor for each layer to the value from SRIM95 already installed in the PowerMeis program. The electronic stopping power depends on the projectile ion energy, the projectile ion species, and the composition of a sample so that it varies before and after the collision event. Therefore, the correction factor is determined by taking into consideration for the incident and scattered ion beam path, the electronic stopping power from SRIM95, and the new fitted electronic stopping power for E_0 and KE_0. The correction factor for the unit layer was obtained by Formula (A.1). K is the kinematic factor for the scattering angle, α is the incident angle, β is the exit angle, and E_0 is the initial energy of the ion. Since the sample for this interlaboratory test is thin enough and there is no grazing angle experiment, the ion beam energy change during the ion beam path is not very significant except for scattering events. Therefore, it is assumed that the electronic stopping power does not change significantly from the value of E_0 during the intake path and the value of KE_0 in the outgoing path.

$$S_s = K\frac{S_s(E_0)}{\cos\pm} + \frac{S_s(KE_0)}{\cos^2}$$

$$S_N = K\frac{S_N(E_0)}{\cos\pm} + \frac{S_N(KE_0)}{\cos^2} \qquad \text{(A.1)}$$

$$C_1 = \frac{S_N}{S_S}$$

where

C_1 is the correction factor;

S_s is the electronic stopping power calculated by SRIM;

S_N is the newly fitted electronic stopping power.

The MEIS analyses were performed again with the newly fitted electronic stopping power as shown in Table A.5. The average value of the 7 nm HfO_2 layer is 31,5 % in the Hf concentration, 6,25 nm in the thickness, and $1{,}63 \times 10^{16}$ atoms/cm^2 in the amount of Hf. The standard deviation of the 7 nm sample is 2,3 % for the concentration, 0,28 nm for the thickness, and $1{,}15 \times 10^{15}$ atoms/cm^2 for the amount of Hf. The relative standard deviation is 7,3 % for concentration, 4,5 % for thickness, 7,0 % for Hf quantity, which showed a significant improvement compared to the former one in Table A.3. The improvement of the consistency by using the new refitted electronic stopping power is quite clear, which demonstrates that the use of accurate electronic stopping powers is critical for quantitative and reliable MEIS analysis. It should be mentioned that the relative standard deviation of the concentration of Hf for 1 nm HfO_2 is still poor compared to HfO_2 layers thicker than 3 nm in contrast to those of the thickness and the quantity of Hf. For 1 nm HfO_2 layer, the plateau of the Hf peak did not appear clearly so that the reliability of MEIS analysis of ultrathin films thinner than 1 nm is not enough. It is recommended to express MEIS analysis result in surface areal density rather than in thickness or concentration for ultrathin films of approximately 1 nm thickness.

Table A.5 — Analysis results with newly fitted electronic stopping power

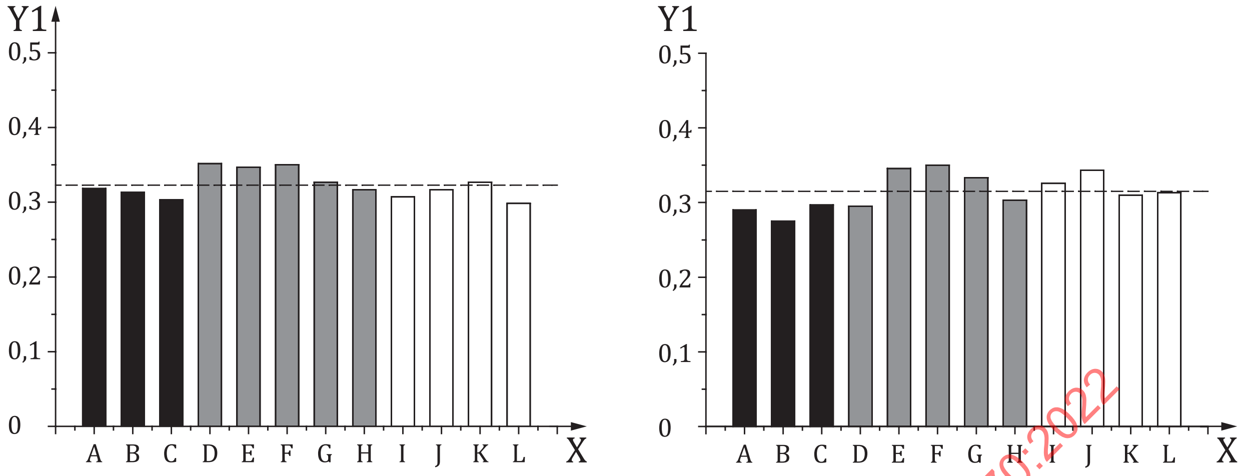
	Concentration of Hf				**Thickness** (nm)				**Quantity of Hf** ($1\text{x}10^{15}$ atoms/cm^2)			
Partici-pants	1 nm	3 nm	5 nm	7 nm	1 nm	3 nm	5 nm	7 nm	1 nm	3 nm	5 nm	7 nm
A	0,127	0,263	0,267	0,29	1,69	2,93	4,38	6,30	1,78	6,41	9,70	15,18
B		0,26	0,268	0,275		2,65	4,78	6,88		5,87	10,66	15,67
C	0,205	0,29	0,278	0,297	1,10	2,70	4,48	6,35	1,87	6,51	10,36	15,65
D	0,217	0,323	0,288	0,295	0,92	2,55	4,10	6,05	1,66	6,85	9,82	14,83
E	0,21	0,317	0,343	0,346	1,15	2,60	4,35	6,18	2,01	6,84	12,41	17,75
F	0,264	0,317	0,326	0,35	0,85	2,58	4,02	5,85	1,86	6,79	10,89	17,01
G	0,243	0,312	0,323	0,333	0,90	2,72	4,42	6,12	1,82	7,04	11,87	16,69
H	0,203	0,316	0,313	0,303	0,96	2,31	3,95	5,80	1,62	6,07	10,28	14,62
I	0,215	0,32	0,323	0,325	1,03	2,55	4,30	6,17	1,84	6,78	11,55	16,70
J	0,247	0,333	0,33	0,343	1,03	2,64	4,38	6,50	2,11	7,31	12,01	18,54
K	0,213	0,305	0,322	0,31	0,96	2,87	4,20	6,27	1,70	7,27	11,23	16,15
L	0,220	0,273	0,287	0,313	0,98	2,60	4,50	6,55	1,79	5,90	10,72	17,05
Average	0,214	0,303	0,306	0,315	1,06	2,64	4,32	6,25	1,83	6,64	10,96	16,34
Standard deviation	0,033 (15 %)	0,023 (7,6 %)	0,025 (8,2 %)	0,023 (7,3 %)	0,02 (2 %)	0,15 (5,7 %)	0,22 (5,1 %)	0,28 (4,5 %)	0,14 (7,7 %)	0,47 (7,1 %)	0,83 (7,6 %)	1,15 (7,0 %)

NOTE 1 Moliere potential[6], and Chu straggling[7] were applied.

NOTE 2 For the magnetic sector and electrostatic analyser results, Marion neutralization[2] was applied for 100 keV H$^+$ and He$^+$, and Armstrong's neutralization[4] was applied for 400 keV to 500 keV He$^+$.

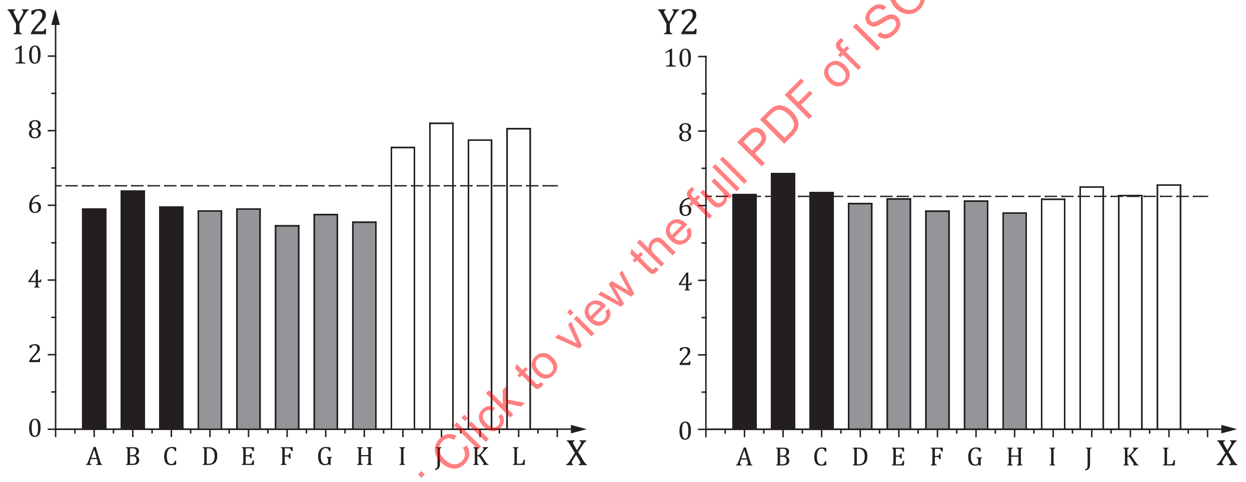
A.4.5 Comparison

Shown in Figure A.5 are the concentration, the thickness, and the amount of Hf for the 7 nm HfO$_2$ sample analysed by SRIM95 electronic stopping power and a new fitted electronic stopping power for comparison. As shown in Figure A.5, the concentration determined by using SRIM95 electronic stopping power show relatively good agreement. However, the thickness and the amount of Hf show poor agreement. MEIS analysis results by using 80 keV to 100 keV He$^+$ are higher than those by 100 keV H$^+$ or 400 keV to 500 keV He$^+$ regardless of the analyser type. On the other hand, the use of newly fitted electronic stopping powers significantly reduces the standard deviation of the thickness and the quantity of Hf, while the standard deviation of the concentration increases slightly. This demonstrates that accurate electronic stopping power is critical for quantitative MEIS analysis. Electronic stopping power from SRIM95 can be the starting point but if experimentally determined values are available from the IAEA home page, it is strongly recommended to use the electronic stopping power from the IAEA. If electronic stopping powers are not available or not sufficient from the IAEA home page, they may be measured by each user for more reliable MEIS analysis.



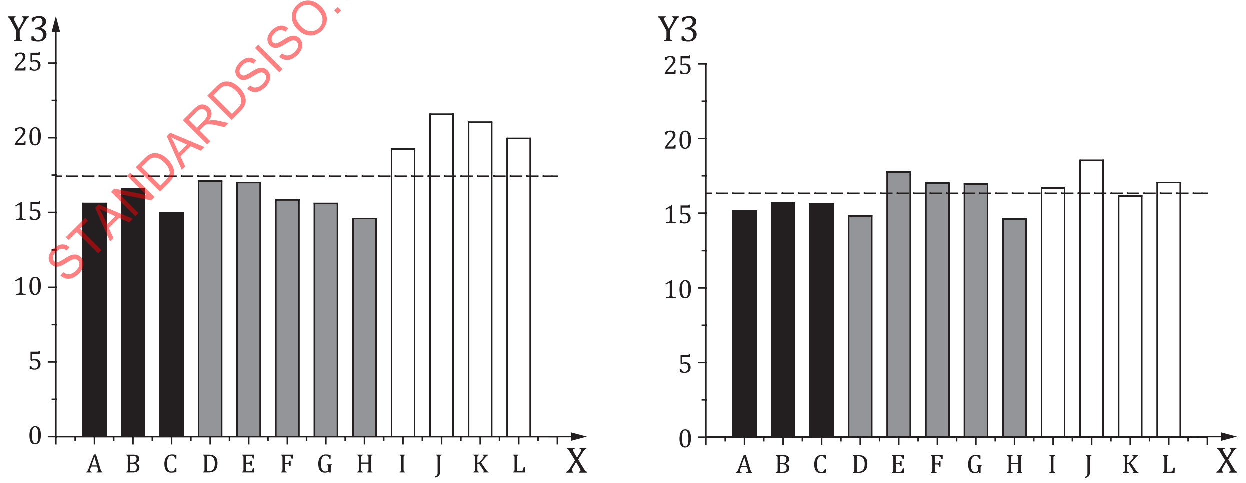
a) Concentration result of 7 nm HfO_2 sample by using SRIM 95

b) Concentration result of 7 nm HfO_2 sample by using newly fitted electronic stopping power



c) Thickness of 7 nm HfO_2 sample by using SRIM 95

d) Thickness of 7 nm HfO_2 sample by using newly fitted electronic stopping power



e) Quantity of Hf of 7 nm HfO_2 sample by using SRIM 95

f) Quantity of Hf of 7 nm HfO_2 sample by using newly fitted electronic stopping power

Key

X	participants
Y1	concentration of Hf
Y2	thickness of HfO_2(nm)
Y3	quantity of Hf ($1x10^{15}$ atoms/cm^2)
■	100 keV He^+
▒	300 keV to 500 keV He^+
□	80 keV to 100 keV He^+
------	average

Figure A.5 — Concentration, thickness, and quantity of Hf results of 7 nm HfO_2 sample by using SRIM95 and newly fitted electronic stopping power

A.4.6 Measurement of electronic stopping power

This report includes the newly measured 62,3 keV He+ and 100 keV He^+ electronic stopping powers for SiO_2[9]. Since there were no data for 15 keV to 100 keV He^+ in SiO_2, measurements were required to increase the accuracy of the electronic stopping power in the range of approximately 100 keV. This value was added to the IAEA electronic stopping power data of He^+ on SiO_2 to obtain a newly fitted electronic stopping curve.

Two newly measured electronic stopping power values were obtained by measuring the height of the MEIS spectrum using 100 keV He^+ with two different incidence angles at the same scattering angle. The spectral height at energy KE_0 of the MEIS measurement is given by Formula (A.2). It is affected by the stopping power as well as the incident angle, the cross-section at the scattering angle, the number of incident particles and the detector efficiency. K is the kinematic factor, S_1 is the stopping power of E_0 in the intake path, S_2 is the stopping power of KE_0 in the exit path, α is the incident angle, and β is the exit angle. C is the concentration of the element, A is a constant, Q is the number of incident ions, ΔE_{ch} is the channel width of the energy spectrum, σ is the scattering cross-section, and Ω is the solid angle of the detector. Formula (A.2) has two unknown values (S_1 and S_2), which can be solved if there are two expressions. At this time, it is assumed that the scattering cross-section is correct. The experimental geometry is presented in Figure A.6. α_1 and α_2 is the incident angles, β_1 and β_2 is the exit angles, Y_1 and Y_2 is yield for each experiment as given in Formulae (A.3) and (A.4), respectively, θ is the scattering angle.

$$\mathrm{Y}\left(\mathrm{KE}_{0,\alpha,\beta}\right)=\frac{\mathrm{Ac}}{\mathrm{KS}_1+S_2\left(\frac{\cos\alpha}{\cos\beta}\right)} \tag{A.2}$$

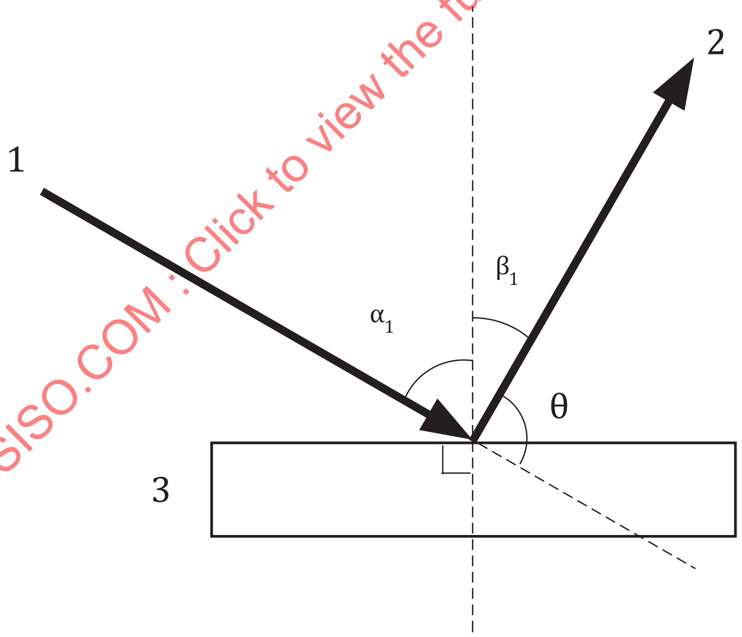
$$\mathrm{Ac}=\mathrm{Cc}\cdot\mathrm{Q}\cdot\Delta\mathrm{E}_{\mathrm{ch}}\cdot\int_{\mathrm{D}}\frac{d\sigma_{\mathrm{e}}}{d\Omega}d\Omega$$

$$Y_1\left(\mathrm{KE}_{0,\,\alpha 1,\beta 1}\right)=\frac{\mathrm{A}}{\mathrm{KS}_1+S_2\left(\frac{\cos\alpha_1}{\cos\beta_1}\right)} \tag{A.3}$$

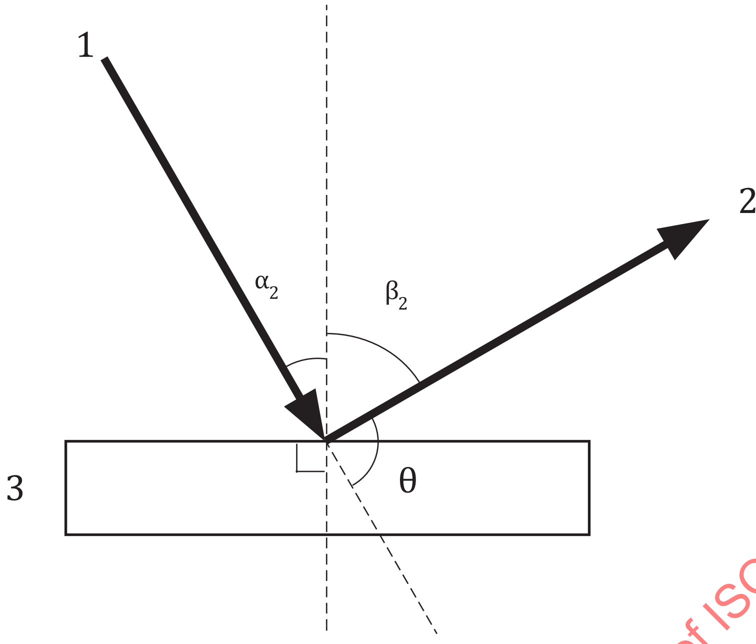
$$Y_2\left(\mathrm{KE}_{0,\,\alpha 2,\beta 2}\right)=\frac{\mathrm{A}}{\mathrm{KS}_1+S_2\left(\frac{\cos\alpha_2}{\cos\beta_2}\right)} \tag{A.4}$$

where

K	is the kinematic factor;
S_1	is the stopping power of E_0 in the intake path;
S_2	is the stopping power of KE_0 in the exit path;
$\alpha, \alpha_1, \alpha_2$	is the incident angle;
β, β_1, β_2	is the exit angle;
C	is the concentration of the element;
Q	is the number of incident ions;
ΔE_{ch}	is the channel width of the energy spectrum;
σ	is the scattering cross-section;
Ω	is the solid angle of the detector;
θ	is the scattering angle.



a)



b)

Key

1	incident ions
2	scattered particles to detector
3	sample
α_1 , α_2	incident angle
β_1 , β_2	exit angle
θ	scattering angle

Figure A.6 — Experimental geometry of newly measured electronic stopping power

This method requires carefully controlled measurement of the spectrum height, the number of incident particles, the detector efficiency. The incident ion count is controlled by faraday cup monitoring and the detector efficiency is adjusted by Ag with a sufficient electronic stopping power database. The measurement is performed by TOF-MEIS in K-MAC and there is no neutralization by using a TOF analyser. In addition, multiple scattering amounts are included in the calculation.

A.5 Summary of the interlaboratory test results

An interlaboratory test was conducted to investigate the consistency of the amount and the concentration of Hf, and the thickness of HfO_2 from MEIS analysis for nominally 1 nm, 3 nm, 5 nm, and 7 nm HfO_2 samples. Twelve participants obtained MEIS data under their own analysis conditions and the data was analysed at K-MAC with Moliere potential[6] and Chu straggling[7]. For analysis of data from the magnetic sector and electrostatic analyser, Marion and Young's neutralization[2] for 100 keV H^+ and He^+, and Armstrong's neutralization[4] for 400 keV He^+ to 500 keV He^+ were used. For electronic stopping power, MEIS analysis results using electronic stopping power from SRIM95 and the corrected electronic stopping power by the data of IAEA site are compared. The comparison demonstrated that the corrected electronic stopping power provides more consistent results with relative standard deviations of (2 to 8,2) % than those from SRIM95 with relative standard deviations of 5,3 % to 15 % for the concentration and the amount of Hf, and the thickness of HfO_2 layer. The interlaboratory test showed that using correct electronic stopping power is critical for quantitative MEIS analysis.

Annex B
(informative)

List of MEIS spectra simulation program sources and a procedure of MEIS spectra simulation using PowerMeis

B.1 List of MEIS laboratories using their own spectra simulation programs

Institute	Reference	Instrument type
Rutgers University, USA	See Reference [10]	TEA
UFRGS, Brazil	See Reference [11]	TEA
Kyoto University, Japan	See Reference [12]	HRRBS
Western University, Canada	See Reference [13]	TEA
University of Huddersfield, UK	See Reference [14]	TEA
Uppsala University	See Reference [15]	TOF
K-MAC, Korea	See Reference [16]	TOF

B.2 MEIS spectra simulation procedure using PowerMeis

B.2.1 MEIS spectra can be simulated with PowerMeis[1]. When PowerMeis simulation is on, it asks several input data for simulation as follows.

In algorithm, number of interactions, integration step, voxel size are 10^6, 1 Angstrom, and 1 Angstrom, respectively. For integration method, default MC is chosen generally.

In calculation, for line shape, cross-section, energy stopping power, and energy straggling, generally chosen are exponentially modified Gaussian, Corrected, SRIM, and Chu. For charge neutralization, Marion's equation is used for 100 keV H^+ and He^+ and Armstrong's for 400 keV to 500 keV He^+. Casp charge-state-fractions algorithm can be used for He with better reliability and for other heavier ions Exponentially modified Gaussian is better for ultrathin films. Corrected cross-sections are calculated by Moliere potential. If measured electronic stopping power data from IAEA database[3] is available, it is recommended to use the electronic stopping power from the IAEA database for more reliable results. To use the IAEA tabulated electronic stopping power value, calculate a correction factor as given in B.2.2 and input the correction factor *dE/dx* ratio in compounds for the structure of a specimen. If the IAEA database is insufficient or missing, newly measured electronic stopping power data by appropriate methods can be added to the IAEA database to improve the accuracy of the calculated electronic stopping power. The reliability of the IAEA database is described in Annex C.

In output, histogram mode, energy channel width (dE), angular channel width (dθ), minimum energy (E_{min}), and maximum energy (E_{max}), are simple, 0,1 keV, 20°, and appropriate minimum energy and maximum energy for each MEIS analysis. Energy channel width and angular channel width can be adjusted according to the energy and angular resolution for each MEIS analysis. Angular channel width should be larger than the detector angular width.

In beam, projectile is generally ion but molecule can be chosen, when molecular ions are used. Particles x sr is generally 10^{12} but it can be adjusted to fit the experimentally measured MEIS spectra. Atomic number, atomic mass, beam energy, and incidence angle from the surface normal are from specific ion scattering conditions.

In detector, detector type is chosen among electrostatic, time of flight, and magnetic. For electrostatic and magnetic detector type, energy resolution FWHM (δE), scattering angle (θ), and angular width (Δθ) specified from each MEIS analysis are given. For TOF detector type, TOF length (L) in m, time resolution (δt), out of plane angle (α) and out of plane angular width (δα) are additionally given according to specific TOF MEIS scattering conditions. Out of plane angle and angular width are used when TOF MEIS scattering data from out of plane region in a large solid angle detector are used. Energy resolution FWHM (δE) or time resolution (δt) can be measured by fitting the leading edge of a MEIS peak from a clean surface.

In graph, 1D can be chosen generally for spectrum type. Measured MEIS spectra in txt file with intensity vs energy is uploaded by pressing upload experimental.

After all the input parameters for simulation and experimental parameters are given, the structure of a specimen is to be built. First, press elements to list up elements used in simulation. Line shape parameters for each element, σ_0 (additional parameter) can be set zero in the first approximation. For MEIS systems with high resolution of δE/E approximately 8×10^{-4} with proton as a projectile, the line shape parameters are recommended to calculated by Casp 5.2. Line shape parameters for each element, σ_0 (additional parameter), is calculated by Casp 5.2 program[3] for each projectile, projectile energy, and target element. Follow the instructions in Casp 5.2. Use the calculated line shape parameter as the additional parameter for each element for the structure of a specimen.

Then press compounds to make a list of compounds used in simulation. Give density to convert the number density to the depth scale. If the density of thin films used in the MEIS analysis is known, use the number. But, generally the number is not known so that just use the bulk density. In the case of non-stoichiometric compounds or mixtures, just use the sum rule. According to the sum rule, the density of a non-stoichiometric compound $\rho(A_{x+\delta x} B_{y+\delta y})$ can be estimated by the Formula (B.1).

$$\rho(A_{x+\delta x} B_{y+\delta y}) = \{(x+\delta x)\ m(A) + (y+\delta y)\ m(B)\}/[\{x\ m(A) + y\ m(B)\}/\rho(A_xB_y)] \tag{B.1}$$

where m is the mass of each element or a compound in u

For mixtures of A and B, the density of the mixture A(x%) and B(y%) can be estimated by the Formula (B.2).

$$\rho(x\%A+y\%B) = \{x\ m(A) + y\ m(B)\}/\{x\ m(A)/\rho(A) + y\ m(B)/\rho(B)\} \tag{B.2}$$

where m is the mass of each element or a compound in u.

The use of bulk density values or the density estimated by the sum rule, which is incorporated in PowerMeis can generate errors in the depth from MEIS analysis. For straggling correction factor, that is, dw^2/dx ratio, just use 1.0, if the correction factor is not available, which is generally the case.

Press layers to construct layered thin film structures. Give the thickness in Angstrom and compound name for each layer. The first layer is the substrate layer, not the surface layer. If necessary, a surface contamination layer or an interface layer between ultrathin film layers can be introduced to improve the fitting.

B.2.2 Electronic stopping power is automatically calculated by the SRIM code, which can be used for non-critical MEIS analysis with inconsistency higher than 10 %. However, electronic stopping power from the SRIM code can have significant errors in the medium energy range. For accurate MEIS analysis with consistency lower than 10 %, it is recommended to use the measured and tabulated electronic stopping power data of elements and compounds from IAEA[3], as described in Formulae (1) and (A.1). The accuracy of electronic stopping power values in the IAEA database is estimated to be less than 8 % as discussed in Annex C.

The electronic stopping power from IAEA database can be obtained by fitting a set of electronic stopping power data. The equation used to fit the data are shown in Formula (1).

From the IAEA data, available fitting parameters A, B, C, and D are calculated and tabulated in Annex D for the convenience of users.

The correction factor is determined by taking into consideration the input / output beam path and electronic stopping power of SRIM and the new electronic stopping power for E_0 and KE_0. The correction factor for the unit layer was obtained by Formula (A.1). K is the kinematic factor for the scattering angle, α is the incident angle, β is the exit angle, and E_0 is the initial energy of the ion. The correction factors from Formula (A.1) can be used in inelastic energy loss correction dE/dx ratio in compounds. $d\omega^2/dx$ ratio is 1.0 for no straggling correction.

B.2.3 After all the specified and appropriate values are given, press start. Adjust the parameter of projectile number (Particles *Sr) in beam to fit the intensity of a reference layer for example between measured and simulated MEIS spectra when the internal reference layer is used as the (Particles *Sr) calculation. Then adjust the thickness and composition of each layer manually and iteratively to get the best agreement between measured and simulated MEIS spectra. χ^2 calculation can be used to find the best agreement with a properly chosen energy range of spectrum. The low limit of an energy range in χ^2 calculation is recommended to be not lower than 10 keV from the substrate surface peak. In case that a reference layer of known stoichiometry is included in the sample, the height of reference layer can be chosen to generate the minimum χ^2 calculation to determine the projectile number. And then the composition and the thickness of unknown layers can be determined by changing the fitting energy range to the unknown layer peak position to calculate and minimize χ^2. In case of no reference layer, overall χ^2 calculation with an appropriate fitting range can be used to get the best agreement between measured and simulated MEIS spectra.

Annex C
(informative)

Reliability of the IAEA electronic stopping power data

C.1 General

The interlaboratory test report in Annex A demonstrated that using correct electronic stopping power is critical for quantitative MEIS analysis. The IAEA nuclear data services are recommended for a reliable source of electronic stopping power data. Addressed here is the reliability of the IAEA electronic stopping power data based on the statistical analysis of the mean normalized difference and its standard deviation taken from the IAEA nuclear data services[3] for the medium energy range. For a certain range of Z_1, for a certain range of target atomic numbers Z_2, and for every data point in a certain range of specific energy E/A_1 (where Z_1 is the projectile's atomic number, E its energy and A_1 its mass number), the normalized difference δ is calculated by the Formula (C.1):

$$\delta = 100 \times \left(S_{exp}^{p} - S_{tbl}^{p} \right) / \left(S_{exp}^{p} \right) \tag{C.1}$$

Here, S^p is calculated by the Formula (C.2) is the mass stopping power, ρ is the density,

$$S^{p} = S / P \tag{C.2}$$

S, -dE/dx is the linear stopping power, and *x* is the path length. In every range of specific energy, determined are the mean normalized difference $\Delta = \langle \delta \rangle$ and its standard deviation σ is calculated by the Formula (C.3):

$$\sigma = \sqrt{\left\langle \delta^{2} \right\rangle - \langle \delta \rangle^{2}} \tag{C.3}$$

Here, < > signifies an unweighted average, S_{exp} is an experimental stopping power value taken from our collection, and S_{tbl} the corresponding value from a particular stopping power table or program. A small /Δ/ usually signifies good agreement between table and data, and the standard deviation σ is related to the accuracy of the experimental data. If /Δ/ is small, as it is frequently found, σ may be taken as a measure of the accuracy of the table, as determined from experiment. For details, visit the homepage.

C.2 Statistical Analysis for protons and alphas in elements

Results for ZBL 85 and SRIM2003 program are mentioned here, because they are the most widely used in MEIS analysis simulation. For 0,01 MeV to 0,1 MeV energy range, mean normalized differences Δ ± σ (in %) for H ions in 17 solid elements for ZBL 85 and SRIM2003 are −1,2 ± 12 and 0,6 ± 11, respectively. Mean normalized differences Δ ± *σ* (in %) for He ions in 16 elemental solids for ZBL 85 and SRIM2003 are - 2,6 ± 5,7 and −0,1 ± 3,2, respectively. For 0,1 MeV to 1 MeV energy range, mean normalized differences Δ ± σ (in %) for H ions in 17 solid elements for ZBL 85 and SRIM2003 are −3,0 ± 7,8 and −0,9 ± 6,8, respectively. Mean normalized differences Δ ± σ (in %) for He ions in 16 elemental solids for ZBL 85 and SRIM2003 are 0,7 ± 5,8 and 0,5 ± 5,4, respectively. The number of solid elements for H ions is 17 and that for He ions is 16.

As summary, the reliability of the electronic stopping power of H^+ ions and He^+ ions calculated by PowerMeis for elemental solids are less than 12 % and 6 %, respectively.