Metrology for the next generation of semiconductor devices

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The semiconductor industry continues to produce ever smaller devices that are ever more complex in shape and contain ever more types of materials. The ultimate sizes and functionality of these new devices will be affected by fundamental and engineering limits such as heat dissipation, carrier mobility and fault tolerance thresholds. At present, it is unclear which are the best measurement methods needed to evaluate the nanometre-scale features of such devices and how the fundamental limits will affect the required metrology. Here, we review state-of-the-art dimensional metrology methods for integrated circuits, considering the advantages, limitations and potential improvements of the various approaches. We describe how integrated circuit device design and industry requirements will affect lithography options and consequently metrology requirements. We also discuss potentially powerful emerging technologies and highlight measurement problems that at present have no obvious solution.

or over 50 years Moore's law (that the density of transistors will double every two years) has been associated with dramatic decreases in the size (scaling) of components used to fabricate integrated circuits. Scaling has resulted in faster computers and the miniaturization of a wide range of electronic products, but over the next 15 years scaling is expected to reach either its functional limits or a point where cost and reliability issues outweigh the benefits¹⁻³. Within those 15 years, the industry is projected to introduce the smallest and most complex devices yet⁴. For example, by 2024 the gate length of integrated circuits is projected to be 6 nm, and instead of being planar in orientation, the gate will wrap around vertically configured nanowires. The benefits of these devices-including improved current flow and control, low power consumption, and faster switching—are clear⁵ and manufacturing methods are being optimized. What is less obvious is which measurement methods are needed to adequately characterize the nanoscale dimensions of the devices.

As devices shrink in size, and become more three-dimensional (3D) in shape, the relative importance of metrology increases. For example, for some products, more than 50% of the manufacturing steps can involve measurement or characterization. We are also now approaching the point where each atom's position and type within a 3D device needs to be known. And this is in an environment where billions of these devices are required in each chip, and all of them must work to a tight specification. Metrology's role in integrated circuit manufacturing includes exploratory research, technology development and process control⁶. Understanding the metrology needs^{5,7} of a device requires knowledge of key design parameters, including their patterning options⁸ and measurement requirements, as well as available measurement solutions, their capabilities and limits.

In this Review Article, we examine current and proposed device structures and their key metrology requirements. We describe some of the main instruments used, and consider their capabilities, limitations and potential improvements. We also outline some potentially disruptive techniques and trends for metrology, and we identify measurement problems with no obvious solutions. Although the measurands (what is being measured) described below are specific to the integrated circuit industry, owing to the nanoscale size and complexity involved, methods developed for integrated circuit metrology often represent fundamental new capabilities that are later used in other areas.

Integrated circuit device structures

Integrated circuit scaling has been made possible by concurrently reducing device geometrical dimensions, increasing drive current and reducing voltage. This is increasingly difficult to do because of the rising importance of parasitics (for example, coupling capacitance due to feature proximity) and higher manufacturing costs⁹. In addition to geometrical scaling, device structures and designs that allow better drive current scaling¹⁰⁻¹², better connections to the device and better interconnect are needed^{13,14}. The 2017 International Roadmap for Devices and Systems (IRDS)¹⁵ addresses the mainstream device structures that will drive technology development over the next 15 years (Fig. 1a, b).

The fin-based field-effect transistor (FinFET)¹⁵ will remain the mainstream device option until 2021, when gate all around (GAA) devices will need to be introduced to provide enhanced performance at smaller dimensions owing to their better electrostatics control^{9,16}. Lateral GAA (LGAA), which is closer to FinFETs in structure, will be implemented first, followed by vertical GAA (VGAA). It is also projected that from 2021 onwards, 3D assembly integration schemes will support heterogeneous integration as well as memory-on-logic co-integration. Scaling is projected to stall in 2027 (Fig. 1b) because of process and electrical limits. These limits include but are not limited to: worsening resistance- and time-dependent dielectric breakdown in the metals¹⁷; worsening coupling capacitance between gate and drain⁹; worsening short-channel behaviour due to gate length¹⁶; and mobility degradation by reduced device width and mechanical stability of fins and GAA devices¹¹.

In addition to these eventual limitations, advances in chip design create major challenges for future semiconductor patterning, and

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addressing these with novel techniques has created metrology challenges. Patterning challenges arise largely because lithography resolution is continually getting smaller (see select device parameters in Fig. 1b). Also, printed features are small enough that random variations (stochastic effects) in the amount and position of molecules can now create small variations in pattern fidelity that have substantial effects on device performance¹⁸. As such, controlling roughness^{19–24} (or more generally, feature uniformity²⁵) is critical. Also, these stochastic effects²⁶ are large enough relative to the smaller device dimensions that missing patterns or random open and short defects must be thoroughly inspected for.

Furthermore, the trend towards structures that are smaller and more complex in all directions introduces dimensional parameters that need to be controlled and changes how old ones are measured. For example, going from a planar FET device to a FinFET device means that not only does roughness in the width of the gate feature affect performance, but also roughness in the width of the fin. With GAA structures, both the device size and the roughness affect performance and must be measured⁴. Also, going from a lateral GAA to a vertical GAA means that the gate is now a film thickness instead of being estimated by linewidth measurement, thus requiring different analysis techniques. The advent of 3D stacking, and 3D very largescale integration (3DVLSI)14,27,28 will add many steps to integrated circuit production processes, and since these are fully functional tiers, destructive characterization would be prohibitively expensive. This will put a premium on high yield and low defects for each process step. How to do this in a practical and economically viable way is still an open question.

Beyond VGAA, several emerging device candidates have been proposed as replacements for complementary metal–oxide–semiconductor (CMOS) devices. These include transistors that incorporate new materials, such as graphene, carbon nanotubes and transition-metal chalcogenides (for example, molybdenum disulfide; MOS_2) (Fig. 1c,d)^{29,30}. Although most of the dimensional parameters are not yet defined, methods that are applicable to two-dimensional (2D)-materials-based structures are highlighted throughout the Review. Although the structures of most proposed beyond-CMOS structures are not necessarily more complex than those of VGAA structures, this may change as specific technologies advance. Currently, for dimensional parameters, VGAA structures and stacked chips (3DVLSI)³¹ are some of the most complex structures available.

In addition, computing approaches such as neuromorphic computing are driving integrated circuit design and will have challenges for 3D and materials metrology³². Neuromorphic chips aim to mimic the way the brain (or biological systems in general) solves problems. Here, the computing components (neurons) and memory (synapses) are connected in a neural network and can continually change and optimize their response to inputs. An example of this type of chip uses the memristor^{33–35}, which combines both resistive and memory components, and could be implemented in a broad range of materials^{32,34,36,37} using crossbar designs (Fig. 1e). Figure 1f shows a cross-sectional scanning electron microscopy (SEM) image of a 3D stacked cross-bar Si nanowire array memristor implementation³⁸. Figure 1g shows 8 nm \times 8 nm memristors in a crossbar array^{25,32}. Implementations with densities as large as 4.5 terabits per inch (with crossbar of around 2 nm by 2 nm) have also been proposed³⁹. Neuromorphic chips could be integrated into 3DVLSI stacks such as the resistive random access memory (RRAM) shown on the right of Fig. 1a.

Whatever the eventual dimensions for beyond-CMOS structures, the basic measurement questions still hold: what is the measurand, what is the measurement model (instrument, sample, measurement physics, and so on) and when is it valid, how small a feature can one measure with good repeatability, and what are the sources of error?

Metrology challenges for complex device structures

The most difficult metrology challenges involve device structure (shape and layout) complexity, new materials and the statistical limits of controlling sub-5-nm stochastic processes for dimensional, compositional, surface and interfacial measurements where a less than 10% deviation from nominal size could affect device performance⁶.

Measurements at near-atomic-scale dimensions are sometimes limited by physical property changes owing to decreasing size (quantum confinement, typically starting at <10 nm). An instrument's inherent capability could be restricted by the physical inaccessibility of the measurand, the presence of other materials, the positioning system needed to obtain the required data, and noise. For example, VGAA's orientation results in non-uniform instrument sensitivities at different depths, and smaller confined target volumes, making them harder to measure than LGAA.

Nanoscale roughness (surface, line edge, and so on) is proving challenging to evaluate. This is partly because roughness values are not intrinsic parameters of a surface. For example, two surfaces (or line edges) could have the same roughness value, but differ in texture, frequency components and impact on function. Two surfaces could also have the same apparent final texture, but the underlying frequency components could have been produced at different stages with differing impacts on subsequent processes. Furthermore, although roughness could add to measurement noise, instrument noise (not due to roughness) can also be mistaken for feature roughness, requiring unbiased analysis techniques. Recent work aims to identify evaluation methods based on roughness origin and impact^{23,24,40}, and instrumentation and procedures^{19,24,41}.

High-aspect-ratio structures or devices with multiple layers such as 3DVLSI or 3D stacked Si memristor crossbars (Fig. 1f) would be particularly challenging owing to the required depth of focus, presence of low-contrast materials, and possibility of beam damage, among others. The signal-to-noise ratio (SNR) of localized information (such as single-particle defects) and film thickness from deep and multi-layered structures (including GAA) could be quite low owing to the increased depth. With the advent of lithography techniques such as multi-patterning, smaller feature sizes, number of masks per wafer layer, and increased density, overlay is more important than ever, and will be critical for stacked chips. The overall measurement process (instruments, sampling, data analysis, the metrologist and so on) needs to include an understanding of the properties of the nanoscale materials⁴², of possible sources of error and of the physics of the measurement.

Integrated circuit metrology challenges include but are not limited to measurement of surface and interfacial properties, thickness variation, line edge/width roughness, defects for stacked nanowire, and complex material stacks (layers)^{7,43–45}. Other challenges include measurement of strain⁴⁶, defect density, composition, and material dielectric interfaces for 2D and 3D materials. More broadly, most of the challenges involve measurement of dimensional, compositional and interconnect parameters for 3D structures such as GAA nanowire and 3DVLSI⁴⁷, where each technology level could have different metrology needs. Select dimensional parameters and requirements from the 2017 IRDS metrology roadmap⁴ include the VGAA nanowire diameter (6 nm), its half pitch (7 nm), the nanowire roughness and uniformity (0.3 nm) for the years 2030 to 2033 and its gate length (14 nm) and surface roughness (0.12 nm) for the years 2027 to 2033.

Advanced metrology techniques

Measurements are needed in all aspects of integrated circuit research and development, integration, manufacturing process control and testing. This requires instruments with a wide range of underlying physics^{6,48} including light, electron, X-ray and surface forces, among others, and that span several orders of magnitude in

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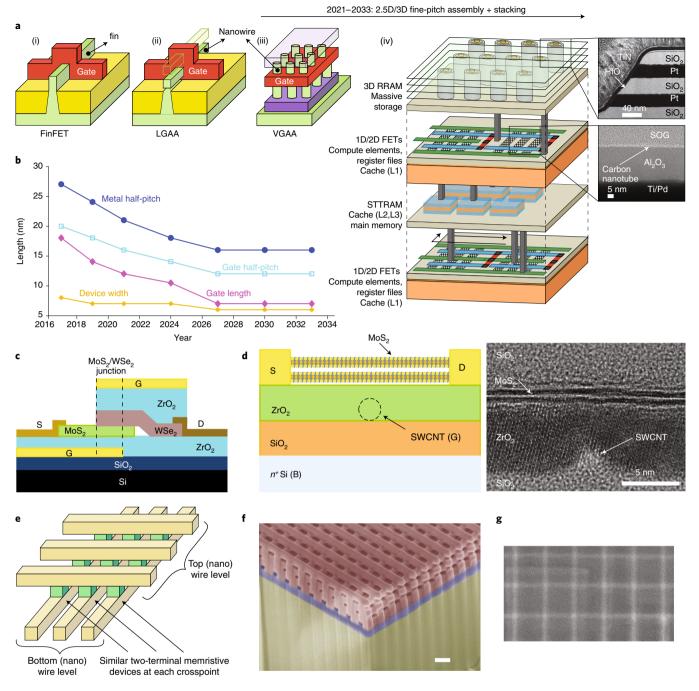


Fig. 1| Proposed advanced integrated circuit devices. a, Evolution of device architectures as forecast by the IRDS. (i) FinFET is projected to be the leading device option until 2021, whereas GAA devices and 3D assembly stacking are projected to commence in 2021. Beyond 2027, 3D device stacking is projected to start with vertical FETs. (ii) For LGAA, the fin is now composed of several nanowires or nanosheets whose size and uniformity would need to be controlled. (iii) For VGAA, the gate is now horizontal (while channel orientation becomes vertical), and requires a measurement of films with multiple stacks. (iv) 3DVLSI have different technologies stacked together, in addition to VGAA metrology issues, and interconnect metrology becomes important. STTRAM, spin-transfer torque magnetic random-access memory. L1, L2 and L3 indicate different layers on the stacked chip. b, Scaling projection of key dimensions such as metal half-pitch, gate (poly) half-pitch, gate length, and device width. c, Schematic diagram of proposed vertical heterostructure tunnel FET using 2D materials (MoS₂ and WSe₂). The gate is a film measurement, so interface properties, film homogeneity and defects are key metrology issues. S, source; D, drain; G, gate. d, Schematic diagram of proposed 1D2D-FET with a MoS₂ channel and single-wall carbon nanotube (SWCNT) gate and a representative TEM cross-sectional image showing a single-wall carbon nanotube gate, ZrO₂ gate dielectric, and bilayer MoS₂ channel. Both the channel material and carbon nanotube would be challenging to measure. e, Schematic diagram of crossbar structures for high-density memristor circuits. f, A cross-sectional SEM image of 3D-stacked Si memristor crossbars of 100 nm x 70 nm, and 200 nm pitch. Scale bar, 200 nm. g, SEM image of 8 nm x 8 nm memristors in a crossbar array. Panel a (i)-(iii) is adapted from ref.⁵ (ECS); panel a (iv) is adapted from ref.¹⁴ (IEEE); panel a (iv) top inset is adapted from ref. 28 (Japan Society of Applied Physics); panel a (iv) bottom inset is adapted from ref. 27 (IEEE); panel c is adapted from ref. 29 (American Chemical Society); panel d is adapted from information in ref. ³⁰ (AAAS); panel e is adapted from ref. ³⁴ (Springer Nature Ltd); panel f is adapted from ref. ³⁸ (Springer Nature Ltd); and panel **g** is adapted from ref. 32 (IEEE).

sensitivity. The parameters being measured include critical dimensions (size and shape), film thickness, surface and interface properties, physical properties, defects and associated parameters that help to illustrate structure–function relationships. The methods described below (and related implementations) are used to address most of the dimensional metrology needs outlined above. They are by no means the only instruments used, but these with their applications are essential to all aspects of integrated circuit fabrication. Table 1 shows a comparison of key metrological quantities for the instruments described below.

SEM. This is one of the most versatile techniques used for in-line integrated circuit measurements, using a finely focused electron beam to scan over the sample. The beam–sample interaction produces secondary and backscattered electrons (and other signals) that are acquired by detectors, to determine feature shape and size (and composition) with sub-nanometre-scale resolution⁴⁹.

Specialized critical dimension SEMs (CD-SEMs) are optimized for integrated circuit manufacturing, and owing to their stringent design requirements, have for the last few decades been central to some key improvements in SEMs⁴⁹. Enhancements such as lowelectron landing energy (typically 300–800 eV), high-efficiency through-lens secondary electron detectors, and fast and accurate sample stages, tailored for repeatable, non-destructive high-speed imaging and measurements of features on semiconductor wafers have made CD-SEMs one of the indispensable instruments of integrated circuit production.

CD-SEMs provide top-down images yielding critical integrated circuit dimensional parameters such as linewidth (see (i) in Fig. 2a), edge roughness⁵⁰, and contact holes⁴⁷, and could produce 3D information (see (ii) in Fig. 2a) if the beam is tilted^{49,51,52}. CD-SEMs are capable of measuring FinFET and nanowire devices with 7 nm feature sizes⁴⁷, but could be extended to features of less than 5 nm if measurements are coupled with simulation and modelling to optimize measurements and results interpretation (Fig. 2a–c)^{49,53}. SEMs are also used with other techniques^{47,53,54} (see discussion of hybrid metrology below) to obtain information on parts of a feature that cannot be measured directly. SEM is used for overlay measurements—high-voltage SEM has been proposed as a viable candidate for overlay of buried layers^{47,55}—and contour metrology, where planar two-dimensional profiles are required to verify optical proximity correction^{56,57}.

The top performance of modern SEMs is not limited by the focusing ability of their electron-optical columns⁵⁸, but rather by error sources such as drift, vibration, beam damage, charging and contamination. CD-SEM measurements can be made traceable to the SI (Système International d'Unites or International System of Units) definition of length using calibrated samples, or displacement interferometry, which can also be used to monitor and compensate for sample-stage motions. Although traceability is not always emphasized in integrated circuit metrology, structures such as proposed memristor crossbars³⁹, with an active area of around 2 nm by 2 nm, would require accurate measurement techniques because their sizes determine the available space for computing functions, and overall packing density.

New results from Monte Carlo secondary electron simulations interpolated with measurements from a single image show agreements of less than 1 nm with other techniques^{52,53}. In Fig. 2a, (iii) shows overlaid SEM and transmission electron microscopy (TEM) profiles with a difference of less than 1 nm. Here, the size and shape parameters for libraries of predicted yield versus positions for different feature geometries are adjusted until library values best match the measured image. Such models require a thorough understanding and application of the physics of signal generation and detection, sample properties and error sources, and can be used to optimize measuring conditions and instruments settings (Fig. 2b, c).

Fast imaging⁵⁸⁻⁶¹ with sparse and optimized beam-scanning schemes has been developed to acquire only the information needed. Deep learning algorithms for reducing the noise in SEM images can bring unprecedented improvement both in speed and in imaging performance. A recent example denoises low-dose SEM images by removing the additive white Gaussian noise (from the detector electronics) and the underlying Poisson–Gaussian noise of the image using patch-based algorithms⁶². Another report⁶³ uses non-linear anisotropic diffusion as part of a machine-learning scheme to denoise images for electron tomography.

Recent work shows the use of a single-column SEM with multiple beams and detectors⁶⁴ configured for fast data acquisition from the region of interest (ROI). Here, multiple electron beams from a micro-aperture array (illuminated by a Schottky field source) are focused on the sample, and the secondary electrons from the sample are simultaneously detected by multiple detectors. The system uses up to 91 electron beams and detectors in parallel, and has been applied to semiconductor wafers and masks. Signals from additional detectors could also provide energy and trajectory information of the electrons generated by the beam-sample interaction and 3D maps of the features. Another recent implementation uses multiple beam energies⁶⁵. Since the beam penetration depth depends on the beam energy, the backscattered electrons at each energy level contain different information that is then deconvolved and combined using a blind deconvolution algorithm. A further enhancement of 3D image acquisition would be to extend tilt SEM to multiple angles and combine the images.

Other improvements that could extend the use of CD-SEMs for GAA and beyond include low-damage and very-low-energy operation (coupled with electrons from higher brightness sources), very-low-electron-energy variation, and use of innovative aberration-corrected electron-optical columns⁶⁶, eliminating electron-beam-induced contamination and dose-rate management to minimize sample damage. Low-energy operation would be useful in measuring beam-sensitive low-contrast materials or filaments in nanoionics memristors as was previously done for Ag filaments in an Ag/H₂O/Pt structure⁶⁷ or other types of beyond-CMOS resistive switches and selectors⁶⁸.

CD-SAXS. Critical dimension small-angle X-ray scattering (CD-SAXS)^{69,70} is a variable angle, transmission SAXS⁷¹ measurement where X-rays scattered from a periodic nanostructure are analysed to non-destructively determine the average shape of the nanostructure (Fig. 3a,b). CD-SAXS is essentially single crystal diffraction where the lattice is the period of the structure and the 'atoms' are the repeating nanostructured elements. CD-SAXS is analysed using an inverse, iterative approach where the calculated scattering for a trial shape function is compared to the scattering data. The trial shape is modulated until the calculated scattering matches the scattering data. CD-SAXS requires high-energy X-rays (>17 keV) for transmission through the silicon wafer and low divergence owing to the small scattering angles that must be measured. Since the data are in reciprocal space, the scattering angles get larger and easier to resolve when the length scales get smaller. This makes the technique useful for feature sizes projected for GAA devices. CD-SAXS has been used to characterize a variety of nanostructures including FinFETs, directed self-assembly and multiple patterning structures (Fig. 3c, d)72-75, and can be used to determine parameters such as sidewall angle, linewidth and pitch. Roughness is obtained as the deviation from the average shape and can be separated into lateral and vertical components. The primary limitation for CD-SAXS is the brightness of available compact X-ray sources, which leads to long measurement times⁷².

For next-generation device architectures, the primary factors for CD-SAXS applicability are the scattering contrast and scattering volume. In non-resonant scattering with high-energy X-rays,

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	CD-SEM	Scatterometry	3D AFM	CD-SAXS	TEM
Underlying physics	Electron beam-matter interaction	Light scattering from periodic structures	Surface force-tip interaction	X-ray scattering from electron density spatial variations of about 0.1 nm for average structures, depending on SNR	Electron beam- matter interaction
Resolution (lateral and vertical)	Focusing capability of about 0.3 nm	Model-dependent; about 1 nm, vertical and lateral	<0.01 nm vertical; <1 nm lateral		0.05 nm lateral
Range (field of view)	50 nm to 10 mm	10 μm and larger; dependent on spot size	Tens of nanometres to>500 μm depending on scanner	50-200 μm	Tens of micrometres at low resolution
Advantages (for a hypothetical 5 nm patterned line)	Local and global information; sub-nanometre-level measurement accuracy	Non-scanning (that is, fast); non-destructive; in-line compatibility	Full 3D and limited sample preparation, in-line compatibility; nanometre-level measurement accuracy	Measures ensemble averages for large array; high resolution; larger angles as periodicity gets smaller; Fourier transform calculation is fast	Cross-sectional imaging capability for whole line imaged at atomic resolution; in-line compatibility
Current instrument limitations (for a hypothetical 5 nm patterned line)	Drift; vibration; contamination; beam damage; lack of sub- nanometre beam placement accuracy; information volume must be folded into size or shape determination	Inapplicable to isolated lines; spot size should underfill line arrays	Tip size (dense structures); relatively slow; aspect ratio (such as increased fin height or reduced fin pitch)	Compact X-ray sources limit throughput; scattering interaction is weak; inapplicable to isolated lines	Sample needs to be cross-sectioned (therefore destructive); beam projection artefacts and noise; relatively small high-resolution field of view
Ultimate limitation due to underlying physics	Electron beam wavelength	Non-uniqueness of solutions for inverse light scattering problem	Tip size; difficult to interpret tip-sample interaction in small confined spaces such as contact holes	Interaction volume is small	Electron beam wavelength; beam steering errors
SI length traceability	Calibration samples; displacement interferometry	Calibration results are non-transferable; uncertainty budget challenged owing to geometry approximations	Calibration samples; displacement interferometry	Calibration samples; traceable translation of detector	Lattice information from X-ray diffraction (short traceability path)
Key error sources	Drift; vibration; contamination; electromagnetic fields	Parametric correlation; geometry parametrization; unfitted parameters (for example, pitch)	Tip induced artefacts; tip/ sample interaction interpretation	SNR; shape models that cannot fit the correct solution; uniqueness of solution for noisy data or sample structure is unknown	Lens aberration; sample preparation; beam damage (material dependent)
Potential improvements	Very low electron energy variation; displacement laser interferometry; elimination of electron-beam-induced contamination; dose rate management	Spot size; target area reduction for more in-die placement; hybridization	0	Higher brightness X-ray sources; higher coherence of X-ray source	Electron dose management; improved sample preparation techniques

Table 1 | Comparison of integrated circuit dimensional metrology methods

'In-line' means that it could be used inside a semiconductor manufacturing fabrication ('fab') environment. TEM is increasingly being optimized for use in the fab, see ref.¹⁰³. Scatterometry information is taken from ref.⁹⁵.

the contrast is related to the periodic changes in electron density. Materials with high atomic numbers and high density with empty space between them will scatter strongly, while low atomic number materials and structures with small changes in electron density will scatter weakly. With regard to scattering volume, the primary effects are due to the structure thickness or height. Tall structures such as VGAA and 3DVLSI will scatter strongly. Thin structures such as 2D materials will scatter weakly. For example, although sub-2.5-nm crossbars³⁹ can be measured by CD-SAXS (if the array is \geq 50 µm), the reduced cross-scattering caused by the small sizes would degrade

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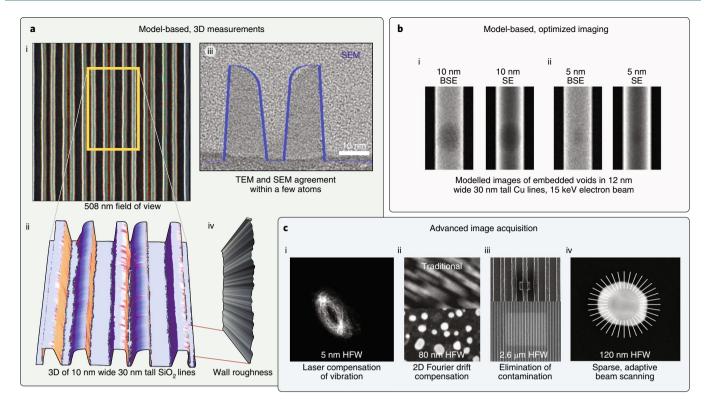


Fig. 2 | Advanced CD-SEM imaging. a, Accurate, model-based 3D measurements of size, shape and roughness of 10 nm FinFET structures. (i) Top down CD-SEM image. (ii) Model-based 3D rendering from multiple angled beam images. (iii) Profile of modelled SEM image overlaid with TEM cross-section showing good agreement; it is also a form of calibration as long as errors are accounted for. (iv) Sidewall roughness of modelled 3D image. **b**, Optimized, model-based determination of best imaging/measurement conditions and signals. Shown are 12 nm lines with 10 nm (i) and 5 nm (ii) embedded voids simulated using a series of instrument settings. The setting(s) that yield the best image are used for actual measurement. BSE, back-scattered electron; SE, secondary electron. **c**, Examples of advanced image acquisition techniques needed to obtain sub-nanometre-resolution images. (i) Laser-interferometry is used to monitor stage vibration and drift for fast image series. (ii) 2D Fourier-transform is used to identify specific image location and align the series to correct vibration and drift effects. Uncompensated image (top) and 2D Fourier drift compensated image (bottom). (iii) Plasma- and laser-based elimination of contamination to ensure ultrahigh cleanliness. (iv) Sparse, adaptive beam scanning strategy. This allows fast image acquisition, minimizing the beam damage by limiting the amount of time the beam is in contact with the sample. HFW, horizontal field width.

the signal. The primary effect of the scattering strength on the measurement is throughput. Weakly scattering samples will require major improvements in compact X-ray source brightness for realistic CD-SAXS characterization times. X-ray sources with tunable energy would allow resonant scattering to highlight the position of specific elements in the nanostructure⁷⁶.

The key advantages of CD-SAXS relevant to next-generation devices are the small X-ray wavelength, the ability to measure optically opaque materials, and the deep penetration that allows nondestructive measurement of complex stacks. These attributes of CD-SAXS make it one of a few methods capable of measuring complicated 3DVLSI stacks without cross-sectioning the film. Many steps in the manufacturing process will have structures where the top layer in a complex stack is optically opaque. Examples include metallization layers and amorphous carbon hard masks, which are frequently used when patterning high-aspect-ratio structures. Another advantage of CD-SAXS is that the result is the average of millions of devices. Imaging techniques such as cross-sectional TEM typically sample too few devices to have the statistical significance needed to extrapolate the results to the billions of devices in the typical integrated circuit. Currently, CD-SAXS is rarely used in the 'fab' owing to the long characterization time, but its use is being intensively researched because of the advantages. Improvements in high-brightness sources (10 to 1,000 times) for CD-SAXS would transform it from a synchrotron and laboratory-based instrument to an in-line tool. CD-SAXS measurements can be made traceable

to the SI length, by using calibration samples, displacement interferometry or length gauges to monitor the translation of the detector. A related method called X-ray ptychography (not covered here) uses coherent X-ray sources, and has been used to create full 3D images of dense processor chips with 14.6 nm resolution⁷⁷ over a range of more than 10 μ m.

Scatterometry. Scatterometry⁷⁸⁻⁸⁰ is a non-imaging optical technique that allows sub-nanometre model-based measurements of overlay effects^{81,82}, geometrical critical dimensions and optical constants (for example, refractive index real and imaginary components n and k) of patterned arrayed structures (Fig. 4a,b). This technique, a specialized variant of ellipsometry, simultaneously captures several deep-subwavelength size variations well below conventional resolution limits through polarization and intensity changes in scattered light (Fig. 4a). Overlay measurements determine displacements between subsequent patterned layers, while optical critical dimension metrology relies upon the parameterization of the nominal geometry (that is, line height h, linewidth w and so on) and each material's complex index of refraction ($\tilde{n} = n + ik$) as inputs for electromagnetic scattering computations. Parametric variation leads to a library of simulated intensity results indexed to these parameters (Fig. 4c). Simulation-to-experiment fitting yields quantitative parametric values, while the parametric uncertainty hinges on both the sensitivity of the measurement to that parameter and on correlations among these parameters. For scatterometry-based

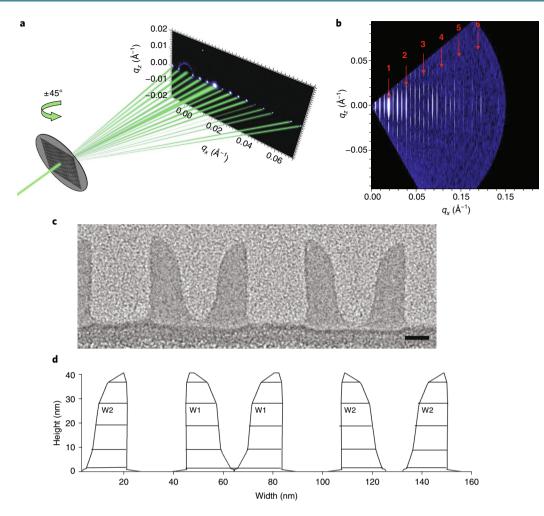


Fig. 3 | CD-SAXS operations and feature shape models. a, Diagram illustrating variable angle transmission SAXS on a periodic nanostructure. **b**, Example of the scattering pattern obtained from a pitch quartering sample. Red arrows mark the peaks from the nominal spacing. Other peaks are superlattice peaks from the pitch quartering. **c**, TEM cross-section of the pitch quartering nanostructure. Scale bar denotes 10 nm. **d**, Six trapezoid stack shape models for cross-sectional view obtained from fitting CD-SAXS data. W1 and W2 denote that the width of the two sets of mirrored pairs is different. The number of parameters in a model is 3N + 5 where *N* is the number of trapezoids in a stack. Defining the edges of the trapezoids with functions instead of allowing them to float reduces the number of parameters but could put constraints on the space sampling of the trapezoid edges and may create correlations between adjacent vertices. Panels **b**, **c** and **d** are adapted from ref.⁷⁴ (International Union of Crystallography).

overlay, displacement between the layers is determined from intensity variations among the diffracted orders from stacked gratings. Although image-based overlay (using specialized optical imaging tools) has traditionally been used in the industry, scatterometrybased overlay^{82,83} is increasingly popular owing to its precision and process compatibility⁴⁷.

Despite inherent ambiguities associated with multi-variable sensitivities, scatterometers are metrology workhorses for determining critical dimension owing to the speed of scattering measurements. As the fitting is an inverse problem without a unique solution (Fig. 4d), sensitivities may not be distinct (for example, Δh and Δw each may alter the scattering similarly). Thus, experimental design is optimized to adequately distinguish among parameters; often, the wavelength λ is scanned from the ultraviolet to the near-infrared (which provides increased sensitivity) for a few fixed angles of incidence. SI traceable scatterometry measurements are difficult owing to the parametric correlations, the number of approximations required⁸⁴, and the subsequent difficulties in establishing a documented uncertainty budget⁸⁵.

Experimental methods used by the industry are evolving to capture the physical characteristics contained within the scattered light more completely. One key technique now applied to scatterometric measurements is Mueller-matrix spectroscopic ellipsometry^{86,87}, performed by augmenting the rotating linear polarizers often found in conventional scatterometry with specific combinations of rotating phase retarders. With this added polarization control and analysis, Mueller-matrix spectroscopic ellipsometry allows the capture of cross-polarization and includes depolarization effects ignored by conventional scatterometry. Feature asymmetries (such as fin bending) and errors in overlay patterning (for example, pitch-walking) have recently been characterized using certain non-symmetric values within the measured 4 × 4 Mueller matrix⁸⁸. Mueller-matrix spectroscopic ellipsometry has also been used to study stress induced dimensional changes in Si and Si/Si_xGe_{1-x}/Si/Si_xGe_{1-x}/Si/Si_xGe_{1-x} nanosheet fin structures⁸⁹, and patterned contact holes⁹⁰ using directed selfassembly. Simulation studies listed 16 parameters and showed reduced parametric correlation for Mueller-matrix spectroscopic ellipsometry for a VGAA parameterization (Fig. 4e)⁹¹. Alternatively, high-magnification optics and angular control have been combined to yield collection of the -1st and 1st diffraction orders from the arrayed features, and used industrially for overlay and optical critical dimension with spot sizes of about 10 µm in diameter⁸¹.

At present, ten or more parameters are modelled, but obtaining adequate measurement resolution (that is, parametric values and

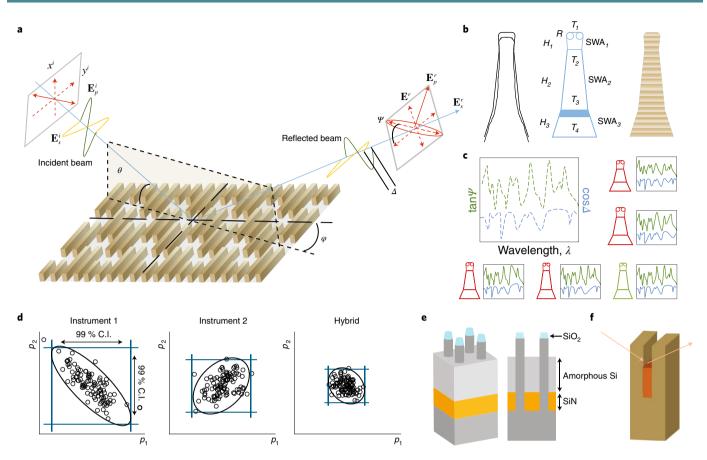


Fig. 4 | Principles of optical scatterometry with future challenges. a, Schematic of light scattering off 3D fin structures. Incident linearly polarized light with amplitude *E* is scattered and collected at angle $-\theta$. Two prominent quantities measured are the rotation of the now-elliptical polarization Ψ and phase lag Δ . The figure is based on information in refs^{86,91}. **b**, Three schematics showing a cross-section of a fin, its geometric parameterization and its segmenting for electromagnetic simulation. This line is represented in parameterization by three trapezoids with heights *H*, widths *T*, and angles SWA, with one trapezoid featuring corner rounding of radius *R*. Variables *T* and SWA correspond to line thickness and its sidewall angle. **c**, Schematic of experimental data and library fitting. Here, tan Ψ and sin Δ are measured as functions of wavelength λ and also determined through simulation for a library of possible parametric values, with the best-fit parametric values corresponding to the green parameterization. **d**, For the parametric uncertainties, increased correlation between parameters p_1 and p_2 of c = -0.81, the 3σ uncertainty (shown by the 99% confidence interval, C.I.) is large. A better-optimized scatterometry Instrument 2 shows less uncertainty for c = 0.35. However, if these two instruments measure the same features and are combined using hybrid metrology, the uncertainty is greatly reduced. Additional information from multiple instruments is probably the necessary requirement for extensibility to future devices, such as VGAA. **e**, Scatterometry model proposed for upcoming VGAA structures featuring 16 parameters to be solved for the 3D structure. A recent publication indicated c > 0.8. **f**, Another example of a scatterometric vertical 3D critical dimension measurement envisioned for an ultrathin material exhibiting a strong anisotropy in its dielectric function ϵ , thus disallowing current, simpler treatments of optical properties as $n\lambda$ and $k(\lambda)$ and r

uncertainties) becomes more difficult with increased structural and materials complexity. As such, approaches to scatterometry target design and methods that more fully utilize the wavelength-dependent optical materials properties $\tilde{n}(\lambda)$ are becoming increasingly important, including tailoring of the optical penetration depth. For monitoring interconnects, cross-grating target approaches that harness surface plasmon polaritons have been proposed for further enhancing the parametric sensitivity to critical dimensions, angles and λ are optimized to nominally limit the measurement depth to that of the parameterized geometry, while well selected infrared λ permits the measurement of buried layers. For 3DVLSI, model-based infrared reflectometry can be considered a type of transmission scatterometry that allows dimensional measurements of high-aspect-ratio features⁹³.

Looking forward, scatterometric metrology of arrays of integrated quantum dots and 2D materials will require not only a measure of periodicity common in lithography but also an even more complete treatment of the optical properties of each material. A prevailing approximation is that the wavelength-dependent dielectric function ϵ (where $\epsilon = \tilde{n}^2$ for nonmagnetic materials) for patterned features may be treated as isotropic. For dimensionally confined systems (Fig. 4f), this assumption may break down (for example, yield poor fits), thus requiring the accurate treatment of the anisotropy in $\epsilon(\lambda)$ as a tensor^{94,95}, and better treatment of this anisotropy is an area of continuing research for Muellermatrix spectroscopic ellipsometry. Dimensional confinement is not limited just to 2D materials but also to features patterned from nominally isotropic materials but with sizes approaching near-atomic scales. Use of the full tensor adds parameters to the fitting, complicating the electromagnetic simulation while also increasing parametric correlations. However, implementing scatterometry as part of a hybrid metrology scheme (explained later) helps reduce parametric uncertainties.

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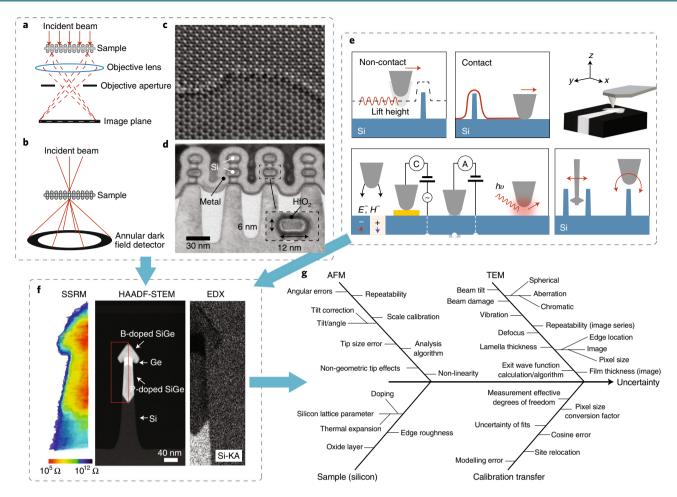


Fig. 5 | Combined TEM and AFM measurements. a, b, Simplified schematic diagram of high-resolution TEM (**a**) and high-angle-annular-dark-field scanning (HAADF)-TEM (**b**). **c**, Exit wave phase image of double-layer graphene reconstructed using a series of HRTEM through-focal lattice images. **d**, TEM images of GAA silicon nanosheets. At this length scale whole devices can be imaged, though not with atomic resolution. **e**, Schematic representations of the basic principles of operation for AFM modes. A nanosized tip is used to sense the surface by non-contact or contact tip-sample interaction. Long-range forces including electric and magnetic fields can be measured by studying the frequency changes in an oscillating tip, while local electrical properties such as capacitance or resistance are measured when the tip is in direct contact with the biased sample. In addition, near-field optics techniques are used to explore chemical mapping and optical properties with nanometre precision. Since the advent of fins, the conventional sensing scheme of AFM has been modified by dedicated tip geometry (that is, T-shaped apex) and tilting scan heads for advanced process monitoring of fins (for example, sidewall and edge roughness). *E*, electric field; *H*, magnetic field; C, capacitance meter; A, ammeter. **f**, Site-specific structural, chemical and electrical information obtained by combination of TEM and scanning spreading resistance microscopy (SSRM) on raised source/drain regions of a SiGe-based FinFET (in the red rectangle). EDX, energy dispersive X-ray spectroscopy; Si-KA, silicon K electron shell and alpha X-ray line. **g**, A fishbone diagram showing possible calibration errors when TEM is used to calibrate other instruments or when measurements from two instruments are combined. Possible error sources include influencing factors from TEM, the sample, CD-AFM, and the calibration process itself. The uncertainty values of artefacts calibrated with TEM could be as low as 0.8 nm. Panel **c** adapted from ref. ⁹⁹ (Elsevier);

TEM. Two modes of TEM⁹⁶ (Fig. 5a,b) are mainly used for integrated circuit metrology, high-resolution TEM and high-angleannular-dark-field scanning TEM. High-resolution TEM images are formed by interference patterns from diffracted and transmitted electrons from a coherent incident beam illuminating the entire ROI. The apparent fringes do not necessarily correspond to the actual atomic columns. High-angle-annular-dark-field scanning TEM imaging uses a focused electron probe scanned point by point across the ROI. The scattered electrons come from a single atom or atomic column, and are detected by an annular ring detector where the observed intensity is either proportional to the Rutherford crosssection (about Z^2) or monotonic contrast in Z (this is more common). The resolution of state-of-the-art instruments is about⁹⁷ 0.05 nm, and is useful for current and future integrated circuit device measurement needs for 3D and 2D materials98 including atomic and device structures (Fig. 5c,d)99,100, strain46, interface analysis44 and

film thickness¹⁰¹. Whole GAA device cross-sections can be imaged at lower resolution, and specific locations at higher resolution.

However, images of 'atomic locations' do not necessarily mean true atomic resolution. Reliable atomic resolution could be obtained by probe/sample deconvolution, or reconstruction of the exit-plane wavefunction, which contains phase information corresponding to positions of the projected atomic locations. Resolution is influenced by lens spherical aberration and sample thickness, among others (see Fig. 5g for select dimensional error sources). The SI traceability of TEM comes from atomic lattice measurements (through X-ray diffraction) and is one of the few techniques where the rigorous steps necessary for obtaining the best resolution the method has to offer virtually ensures that the measurements could be made SI length traceable¹⁰².

Recently, the use of an automated focused ion beam combined with scanning TEM has been developed to extract site- specific

ultrathin samples for reference metrology in an implementation referred to as CD-TEM¹⁰³, and are also used for TEM tomography, allowing 3D measurements. Work is under way to enable the use of the same type of automated focused ion beam capabilities to fabricate on-demand functionalized critical dimension atomic force microscopy (CD-AFM) tips, and evaluate them in the TEM. The TEM information adds length traceability, but could also be used to model and correct tip-induced geometric distortions. TEM tomography images combined with molecular simulations have been used to provide insight into the origin of defects in block copolymer materials used for directed self-assembly¹⁰⁴, leading to better designs of directed self-assembly templates.

Some of the most difficult samples to image with TEM are beamsensitive low-contrast materials (such as carbon nanotubes, graphene and MoS₂) proposed for beyond-CMOS architectures (Fig. 1c,d). TEM ptychography (coherent diffractive imaging)¹⁰⁵ methods are under development to allow acquisition of high-resolution images from low-contrast materials. One technique acquires simultaneous scanning TEM and quantitative phase-contrast images by locating a ptychographic camera at the high-angle annular detector (Fig. 5b) and recording the non-aberration-corrected signals (needed for phase imaging). The signal is processed to obtain the phase image and then corrected for aberrations. Another new approach uses pixel array detectors with a large dynamic range and full field ptychographic techniques to recover the phase information¹⁰⁶. The z-contrast images are complemented by the phase images, allowing practical imaging of 2D materials at high resolution. Other applications that will benefit from such beam-sensitive implementations include in situ memristor characterization⁶⁷, where TEM has been used to study the influence of geometry, and thickness variation in interfacial layers¹⁰⁷, among other parameters.

Compressed sensing was recently demonstrated for scanning TEM¹⁰⁸, where the relevant information could be reconstructed from a subset of the acquired data. Here, the beam was blanked intermittently using a pseudorandom generator as it scanned the sample, limiting the dwell time and possible damage. Such techniques could be combined with TEM ptychography and used for low-contrast materials. A consideration would be to ensure that the reconstructed information is enough for metrology applications. The main limitation of the TEM is that it is destructive; most samples need to be cross-sectioned and thinned down to well below 100 nm. This precludes certain applications.

AFM. The basic principles of AFMs involve positioning a small tip (<10 nm radius) to interact with the surface, where it can sense a wide range of forces while scanning the sample. For topography measurements, sub-nanometre resolution (<1 nm lateral and <0.1 nm vertical) is routine, and true atomic resolution is achievable under suitable conditions¹⁰⁹. The variety of forces detected during the tipsample interaction, including attractive and repulsive, induced by electrostatic, magnetic and chemical coupling has resulted in modes that are optimized for specific physical properties (Fig. 5e). With the tip in near-contact, applications include direct probing of electric fields (electrostatic force microscopy), work function differences (kelvin probe force microscopy)¹¹⁰, and magnetic fields (magnetic force microscopy). Lateral resolution of about 10 nm to 20 nm has been demonstrated for these techniques. Important for nanoelectronics is the direct probing of carrier profiles; these could be obtained by sensing capacitance or spreading resistance changes at the tip-sample junction. These techniques have a lateral resolution ranging from 1 nm to 10 nm, high dopant gradient resolution (about 3 nm per decade) and dynamic range¹¹¹ of 10¹⁵ to 10²¹ atoms per cm³. However, shallower junctions and lateral dopant diffusion in 3D devices calls for a full 3D analysis attempted by different concepts but still challenging¹¹¹. All AFM modes can be applied to integrated circuit measurements; here we focus on dimensional applications.

AFMs optimized for critical dimensions (3D-AFM)¹¹²⁻¹¹⁵ are used for nanowires and related dimensional parameters with uncertainties^{116,117} of less than 1 nm. 3D-AFM, which uses twoaxes cantilever vibration or tilting of the scanning head, eliminates certain tip-shape distortions¹¹⁸, but the larger tips or the clearance needed for rotating heads limit trench sizes that could be measured. In topography mode, AFM is less sensitive to differences in materials and as such could be used for low-contrast materials such as those shown in Fig. 1d or in probing memristor nanodevices⁶⁷, where it has been used to study the shape-dependent performance of ribbed and planar TiO₂ structures¹¹⁹. AFMs can be made directly traceable to the SI length using displacement interferometry, or with calibrated samples¹²⁰⁻¹²². See Fig. 5g for selected error sources. A method of extracting contours for optical proximity correction verification from CD-AFM images was recently demonstrated¹²³. Since CD-AFM images contain reference sidewall data in the scan direction only, the techniques include profile extraction from orthogonal scan directions, filtering and composite contour formation. The output could be used to directly verify optical proximity correction features or to calibrate CD-SEM optical proximity correction profiles.

For patterned features, the proximity of two sidewalls can make it difficult to interpret surface forces and limits the size of the tip that could be used. Recent work using distributed force models to interpret tip-sample interactions show that 3D-AFM sidewall measurement uncertainty could be reduced¹²⁴ to less than 1 nm. Studies with focused-ion-beam fabricated ball-capped and bent carbon nanotube tips indicate that complex feature geometries could be imaged by using tips that are optimized for specific shapes¹²⁵. Tip-wear¹²⁶, size and shape characterization¹²⁷ remain active areas of research because they affect the apparent size and shape of measured features. Activities include developing wear-resistant tips¹¹⁶, wear monitoring techniques¹²⁸, and developing a fundamental understanding of nanoscale wear mechanisms such as by systematically studying different external tip loading conditions and sliding distances, among other parameters¹²⁹. Other activities include new tip characterization methods for CD-AFM using Si/SiO₂ heterostructures, reconstruction methods using dexel representation¹³⁰ and blind reconstruction¹³¹. Improved tip/cantilever technologies have been shown to increase positional stability (to <0.03 nm)¹³² and reduce drift, which is important for applications with subnanometre tolerances.

Among scanning instruments, atomic force microscopes are relatively slow, and although used in most areas of nanotechnology research, for fast-paced measurements required in integrated circuit production, AFM is limited to niche applications or where faster options are unsuitable. Promising new research includes non-raster scanning using contours of the feature to obtain 3D information. A recent example uses constant angular velocity spiral scanning in the centre and transitions to constant linear velocity toward the edge of the scan¹³³, reducing image acquisition time. Other proposed non-raster scanning strategies include rotational¹¹², spiral scanning134,135 and two-dimensional Lissajous136. High-speed AFM combines small cantilevers (with low spring constants and high resonant frequencies), fast scanners and detectors, and vibration control to image samples at 10 to 20 frames per second (essentially video-rate speed)137. Although high-speed AFM has been mostly applied to biological samples, it could be useful for integrated circuit applications where the general patterns are known, and the scan can be optimized accordingly.

Hybrid or combined metrology

No single instrument has the full capabilities (such as resolution, speed, low levels of uncertainty) needed to characterize the whole set of parameters of complex devices, so the integration of multiple tools is required. As such, hybrid or combined metrology is one of

the most important measurement strategies that could be used to extend the applicability of current instruments. Statistical and combinatorial methods have been used to allow complementary analysis techniques to be applied to the same area, utilizing the best measurement attributes of each technique¹³⁸.

Although multiple instruments are routinely used to obtain information (for example, correlative microscopy), statistical hybrid metrology methods for model-based measurements reduce parametric uncertainties for all parameters, not just those provided by a second instrument. For example, in scatterometry-based linewidth measurements, regression models include several parameters where values and uncertainties from instruments better suited for such measurements (for example, CD-AFM for sidewall angle and line edge roughness), can be incorporated, thus constraining the set of potential fitting solutions (Fig. 4d)¹³⁹. Improvements of as much as 4 nm for top width after optical critical dimension hybridization with AFM are common¹³⁸. Other combinations include CD-SAXS and SEM^{53,140}; SEM and optical critical dimension^{140,141}, AFM and SEM¹²³; AFM and TEM (Fig. 5f)¹⁴²; high-angle-annular-dark-field scanning TEM and atom probe tomography¹⁴³; optical critical dimension, X-ray fluorescence and electrical characterization¹⁴⁴; and electrical, AFM and optical metrology methods¹⁴⁵.

A key issue that will increasingly affect all aspects of integrated circuit device measurements is traceability^{145,146}. Given that properties and functionality at the nanoscale are governed by absolute size, traceability of nanoscale dimensional measurements is crucial to the success of nanomanufacturing, and indispensable for valid comparisons of the results of various measurement techniques. This is necessitated by smaller feature sizes and the hybrid metrology implementations mentioned above. We note that traceability does not necessarily ensure high precision or accuracy and indicates only that the results can be traced through an unbroken chain of measurements to a standard or reference. Measurement precision and stability as currently used by the industry are still more important than absolute accuracy or traceability for most applications. Traceability is not a priority if either the instrument or process is unstable. If the measurement tolerance is large enough and the resolution of the instrument is good enough, then measurement precision and instrument fleet matching can be adequate.

However, traceability to a reference¹¹⁵ becomes important when comparing different instruments, combining their results, or comparing results of measurements made at different facilities¹⁴⁷. Also, in some cases, the size and performance dependence of the measurand could preclude methods that are not traceable. For example, the channel thickness and placement of gate electrode for the proposed 1-nm gate length MoS₂ transistor shown in Fig. 1d affects performance. When comparing the performance of such transistors, subnanometre deviations could produce very different results, and instrument traceability (with its associated rigorous analysis of error sources) is one of the few ways to help identify and eliminate errors at this length scale. The same goes for the device areas of around 2 nm by 2 nm proposed for the memristors³⁹, where sub-nanometre differences could represent a considerable change in overall area, and hence device density and performance.

A related issue to consider when using different instruments for the same parameter is methods divergence¹⁴⁸, which is when different techniques produce different results for the same nominal measurand owing to differences in error sources, dimensionality/ content definition¹⁴⁹, probe–sample interaction, and measurand definition. Two techniques could each have a measurement precision of less 0.1 nm, but deviate by more than 3 nm, indicating that each instrument's response to the same parameter is different. Examples include an offset of 2.7 nm between the middle critical dimension as measured by CD-AFM and extreme ultraviolet scatterometry¹⁵⁰ and a difference of 0.8 nm in critical dimension for nominally 13 nm lines as measured by CD-SAXS and model-based library SEM⁵³. In these cases, traceability to a reference (and carefully identifying the error sources) could help reduce deviations¹⁴⁰, and clarify whether these are fundamental differences in the measurement physics. In addition, standardized parameter definitions and sample registration methods need to be implemented to ensure agreement at the nanoscale. At reduced dimensions, understanding these factors will be fundamental to rectifying apparent discrepancies.

Emerging and potentially disruptive technologies

In addition to hybrid or combined metrology, the following technologies have the potential of fundamentally changing the way integrated circuit metrology is done, owing to the nature of the problems they address and their broad applicability.

Advanced data analytics. Advanced data analytics refer to methods used for big data handling, inference, prediction and decision making, and include machine learning and deep learning¹⁵¹ among others. Owing to fully automated measurements throughout the integrated circuit manufacturing process, large amounts of data that could be mined for insight are already being collected. For example, high-resolution SEM and interferometric optical microscopy can easily produce gigabits of data in a single set of measurements¹⁵². Although metrology has always been computationally intensive, what is different about the new methods and makes them potentially disruptive are their autonomous or semi-autonomous implementation and applicability to different aspects of integrated circuit such as material discovery¹⁵³, development, manufacturing and testing. An approach that is gaining wide application is machine learning, which uses computational techniques to learn information directly from data without the use of physical models. This is proving to be useful in situations where the system is not well understood or has too many variables with unknown correlations. Different types of machine-learning models can use known input and output data to develop predictions of similar input data (supervised) or could use just input data to find hidden patterns, structure, or correlations (unsupervised). For metrology, this could be extremely helpful for parameters that cannot be directly measured, but could be correlated with measurable quantities. In cases where physical systems modelling is computationally intensive (or some relationships are not fully understood), machine learning can be used to develop data-driven models that are faster and can discern previously unidentified connections between process parameters and decrease time to solution. Results from machine learning can also help reduce physical modelling variables.

Machine learning and other advanced data analytics techniques are already being applied to a wide range of metrology issues and can be used for specific measurands or for factory-wide applications. For example, deep learning techniques have been applied to image recognition, automatic categorization and labelling of images. SEM data were classified into categories to form a labelled training set that could be used to recognize and classify features such as 1D nanowires, 2D films, and 3D patterned surfaces among others¹⁵⁴, leading not only to faster analysis of individual images but also to correlations within the data. In another example, a neural network was trained with resist shrinkage and CD-AFM data and Bayesian probabilistic weight determination was used to estimate critical dimensions for extreme-ultraviolet resist trenches¹⁵⁵. The results showed lower measurement uncertainties when compared with other methods, and highlights how machine learning could be used to optimize a hybrid metrology setup. Cognitive learning (a type of machine learning) has also been used to speed up complex characterization and analysis of integrated circuit features, such as object detection, classification and automated measurements¹⁵⁶. In another example, pre-exposure metrology data from ultraviolet level sensor of a lithography system was used to predict clamped wafer shape, and then hierarchical clustering with dendrograms provided insight

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on overlay^{157,158}. Other interesting uses include autonomous probe tip monitoring and reconditioning, where a neural network was trained (by a small set of images) to identify isolated dangling bonds at the end of a tip and to apply electrical pulses to sharpen the tip¹⁵⁹; using machine learning to develop sampling strategies for optical critical dimension and X-ray fluorescence for electrical test prediction; and pattern analysis and prediction for automated design layout¹⁶⁰. We note that machine learning and related techniques could be implemented as part of established automated process control¹⁶¹ and virtual metrology¹⁶² techniques currently used in the industry, and the information linked to factory-wide data. Virtual metrology refers to "...the technology of prediction of post process metrology variables (either measurable or nonmeasurable) using process and wafer state information that could include upstream metrology and/ or sensor data" and would benefit from these techniques¹⁶³.

More broadly, Kalinin et al. have proposed a framework for using data analytics to advance the scientific discovery process¹⁶⁴. They illustrate how advances in acquisition techniques and data analytics could be used to capture, transfer and compare multimode microscopy data to a wide body of work stored in 'multimodel response libraries', thus reducing the time between data acquisition and when it becomes useful 'community-wide knowledge'. This is an interesting concept, and although much broader in scope (with some intellectual property issues to consider), it could be particularly useful for metrology. Information on instrument response to different samples, operating conditions and applications from a wide range of users could be used to improve instrument capability, and would complement automated process control, hybrid and virtual metrology.

Sub-wavelength imaging techniques. These techniques allow imaging beyond classical diffraction limits and can be particularly useful if configured to characterize nanodevice parameters not covered by the examples above. Promising techniques include plasmonic assisted optical focusing¹⁶⁵ which can focus light to subwavelength size and can detect optical losses, chemical properties, and defects in hard-to-reach areas of device structure. Evanescent waves¹⁶⁶ could be leveraged to use near-field nonresonant effects to produce nanoscale-resolution (<25 nm) frequency-independent imaging from the visible to the terahertz regimes. A technique that could be borrowed from biological imaging is super-resolution microscopy. Here, different measurands are imaged by localizing and activating different parts of the sample¹⁶⁷, measuring them separately and then combining them to achieve a resolution that one image could not have produced. These methods are not optimized for integrated circuit applications and in some cases the resolutions are relatively large, but their capabilities make them promising candidates for further investigation, and if successful could have an impact on integrated circuit metrology.

Open measurement questions

Although progress has been made in improving instrument capabilities, challenges (and opportunities) remain. Noise is the most pervasive, and comes from a variety of sources (including vibration, shot noise, probe/sample interaction, the detector and stray electromagnetic fields). Even if an instrument has the capability to discern 1 nm differences, noise at just below that level could make some measurements unfeasible or dramatically increase the uncertainty. More specifically, for VGAA, key patterned features such as 6 nm holes need to be measured at the bottom and the top to check for dimensional variation in the hole. At a different length scale, the advent of stacked chips means that measurement of (tens of micometres long) through-silicon vias¹⁶⁸ would be critical. For 3DVLSI structures, the presence of different technologies at each layer could make it difficult for techniques (even those with sufficient depth of focus) to simultaneously capture multiple parameters owing to differences in material contrast.

Unfortunately, no single method has the range or resolution to make these measurements adequately. Better defect detection capabilities are needed. Optical instruments at present wavelengths are not adequate for single-particle defect inspection, and higher resolution instruments do not have the range and throughput needed⁵⁴. Although electron beam techniques are widely used, assessing beam damage for thin structures is difficult, limiting the type and thickness of samples that can be measured.

Conclusions

The 1994 National Technology Roadmap for Semiconductors¹⁶⁹ projected a minimum feature size of 0.35 µm for 1995. By comparison, the smallest device width projected by the IRDS for the years 2027–2033 is 6 nm (Fig. 1b). As device sizes shrank, and new lithography techniques and materials were introduced, the underlying device architecture stayed the same. That changed with the introduction of FinFETs, and is about to change again with GAA, 3DVLSI and eventually to a yet-to-be-defined beyond-CMOS architecture in what was recently referred to as the era of hyper-scaling¹⁷⁰.

We have reviewed the main integrated circuit dimensional metrology instruments that would be used for these devices, their capabilities, limitations and potential for improvement. These techniques already have key roles in integrated circuit dimensional measurements or, in the case of CD-SAXS, have the potential to do so. The combination of small feature sizes, functionally important nonplanar parameters, and increased significance of stochastic effects means that no single instrument would be able to meet the demands of some of the measurands. Hence, improved instruments, hybrid metrology, increased use of modelling and simulation, or adaptations from other fields are needed. Overall, current instrument limitations are mostly driven by engineering issues, rather than the underlying physics (Table 1). This does not make the limitations any less daunting, but indicates that there is room for improvement.

Looking forward, advanced data analytics could help ensure that only the data needed for critical decisions are collected, thereby reducing the overall cost. The use of techniques such as machine learning and measurement physics modelling in combination with process information would not only solve metrology problems, but could help develop measurement techniques for these end-of-roadmap devices. It is also possible that technological advances could obviate the need for some measurements. Defect tolerant systems for neuromorphic chips is an area of active research^{171,172}, and could be applied more broadly. In such systems, the chips can learn to work around certain deficiencies (dimensional variations, for example) and reallocate resources to optimize performance. Such implementations would not remove the need for all measurements but could help in specific scenarios where measurements are prohibitively expensive.

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Author contributions

All authors contributed to project planning, discussions and manuscript writing at all stages.

Competing interests

The authors declare no competing interests

Additional information

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