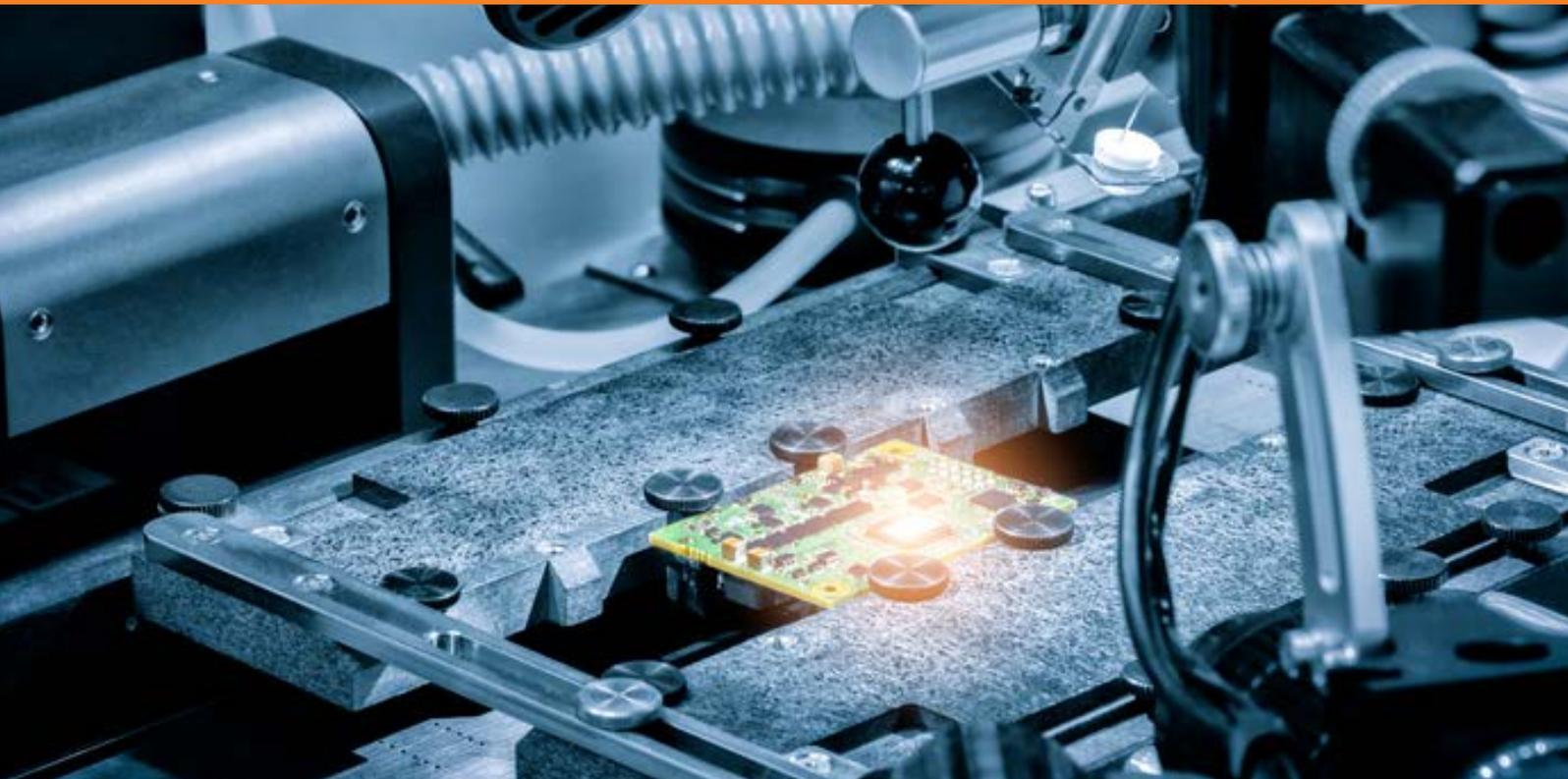# European Metrology Programme for Innovation and Research

Delivering Impact

EURAMET

Improving the speed of determining nanostructure parameters using scatterometry

Advances in technology, such as next-generation silicon chips, pose new measurement challenges. Components are now reducing to the nanometre level and optical methods, needed for quality control, require software to provide sufficient resolution. However, this is computationally expensive and can take days or even weeks, and improvements were required to support European manufacturing in this area.

Challenge

Advanced manufacturing is recognised as a critical technology for the EU's economic security, and, since 2023, the EC's Chips Act has mobilised over 80 billion euros in semiconductor manufacturing and R&D.

Thousands of steps are required to produce silicon wafers and it is important that these are defect free and function as intended. As technology advances chip components are becoming smaller, down to nanometre levels, which poses challenges for in-line inspection techniques, which need to be rapid and non-destructive.

Scatterometry is a suitable optical technique that records light "scattered" from an illuminated sample and the structure is reconstructed by mathematical models. The experimental data is compared to a simulated model, and the process repeats iteratively until the model "fits" the data, allowing parameters such as depth, height and width to be obtained. For accurate results including reliable measurement uncertainties, statistical methods are applied to determine a distribution of the model parameters. This "statistical inverse method" is extremely computationally expensive as it may take hundreds of iterations to get the best "estimation" of the structure - and days or weeks to get the precise sample details. Developing a method to increase the speed of scatterometry reconstruction, whilst retaining accuracy, would be a significant advance for Europe's manufacturing sector.

Solution

During the ATMOC project a range of samples relevant to industry were produced, such as ultra-thin layer systems, complex nanostructures, and novel materials with relevance to next-generation industrial applications.

This included 2D nanosheets and materials with a greater ability to store electrical charge than the silicon dioxide used in conventional computer chips (higher k-materials). The samples were then pre-characterised using methods including ellipsometry, reflectometry, scanning electron and transmission electron microscopy, after which advanced inverse modelling and virtual measurements were applied. The approaches used captured imperfections caused by real world experiments, including fluctuations of the incoming light, sample roughness caused by production techniques, and material degradation over time.

Lastly, several advanced modelling techniques were investigated for time intense numerical modelling algorithms to improve modelling efficiency and data analysis speed, including deep neural networks, polynomial chaos approximations, and tensor compression, and machine learning algorithms.

Impact

JCMwave are experts in developing software for solving problems in areas covering photonics, lithography, computational metrology, photovoltaics, and nanostructures. Due to this, they were asked to join the ATMOC project to help model the nano-samples produced using the "Maxwell equation solver" from their JCMsuite - a powerful and flexible tool for simulating and designing complex nano-optical systems.

During the project the company developed improved numerical methods for the efficient simulation of nanostructures from scattered light and Machine Learning software. The latter predicts the probability of a good agreement between simulation and measurement thereby guiding the search for the best fit. It reduces the time for reconstructing geometries from days to a few hours – along with providing measurement uncertainty. JCMwave have now integrated these developments into their JCMsuite, acknowledging the access to complex nano-samples in the project, and the knowledge gained from comparing the various methods for solving inverse problems, was instrumental in this.

Through the ATMOC project improved methods now exist for characterising advanced semiconductors and materials. In the long-term this will help companies develop new materials with tailored properties boosting European competitiveness in this important area.

Advancing the technologies for new or improved materials in European manufacturing

The ATMOC project:

- identified, manufactured and characterised key nano optical test and reference samples to support the development of next generation photolithography including ultra-thin layer systems of various thicknesses, diverse nanostructures, and multiple fabrication procedures.

- derived uncertainty budgets for reflectometry, Mueller ellipsometry and scatterometry, which were characterised and calibrated, advancing the development of traceable measurements involving inverse modelling.

- developed different inverse model approaches and uncertainty estimations, including determination of uncertainties, interlayer roughness modelling, surrogates and other machine learning techniques.

- optimised the performance of algorithms for inverse modelling methods, including Bayesian and polynomial chaos surrogates for computationally intensive processes.

- produced a database for optical constants required by industry for a new generation of computer chips based on novel materials, including uncertainties, detailed measurement descriptions, and modelling information.

This work will strengthen European know-how in innovative technologies, paving the way for such things as computer chips based on advanced materials, optical coatings and lithography masks.

www.euramet.org/project-20IND04

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