Publishable Summary for 20IND09 PowerElec
Metrology in manufacturing compound semiconductors for power electronics

Overview

Electrification of transport, smart power distribution, and 5G/6G communications are instrumental in underpinning the European Green Deal and boosting the EU's global competitiveness. Power electronics is crucial to these technologies and European companies are leading the transition from silicon to wide bandgap compound semiconductors. These materials offer huge benefits in terms of performance, but the manufacturing yield and long-term reliability are affected by material defects, which are hard to identify and characterise at the fabrication facility with existing techniques. This project will enable the development of novel metrological methods and instrumentation to support a step-change in productivity of the power electronics industry.

Need

The European Commission's Industrial Strategy seeks to maintain the competitiveness of European industry, whilst pursuing climate neutrality goals and digital transformation. The economic recovery plan following the COVID-19 pandemic re-affirms the need for 'unlocking investment in clean technologies and value chains' including sustainable energy infrastructure and electric vehicles.

Power electronics is currently dominated by silicon devices, which are not able to efficiently handle high electrical power densities, nor to operate efficiently at the high frequencies required for next-generation communications. Wide bandgap (WBG) compound semiconductors offer 'game changing' advantages including the ability to operate at higher power densities, voltages, temperatures, and switching frequencies with low energy losses. Devices using these new materials have reduced energy consumption and can be smaller/lighter than equivalent systems using silicon technology. The European industry is well-placed to lead the transition towards WBG semiconductors (particularly SiC, GaN, and β-Ga_2O_3). However, the performance advantages of these materials are not yet realised due to their intolerance of defects, leading to poor manufacturing yield and disappointing operational reliability. Yield Enhancement is recognised as a Grand Challenge for the semiconductor industry requiring new methods to non-destructively detect and differentiate defects at high speed.

New measurement techniques and data analysis methods are required for quantitative characterisation of WBG semiconductor wafer quality in terms of defect density and species. Metrological traceability and validation of these measurements is required to ensure industry-wide recognition of quality assurance and customer confidence throughout the supply chain.

Effective pull-through of semiconductor technologies requires a 'breadth of collaboration that goes beyond the national level or a single industrial stakeholder'. This effort needs to include National Metrology Institutes (NMIs), research organisations and the semiconductor industry, where the NMIs offer traceability to the SI that is required for mutually recognised quality assurance between commercial organisations.

Objectives

The overall objective of the project is to develop novel measurement techniques for the characterisation of compound semiconductor materials with demonstrable relevance for use in the manufacture of power electronic devices.

The specific objectives of the project are:

1. To develop instruments for the rapid (< 1 minute), accurate and non-destructive detection of nanoscale (< 100 nm) defects in industrially relevant compound semiconductor wafers (≥ 15 cm diameter) and dies. The instruments should be based on optical scatterometric, spectroscopic, compressed sensing or other in-line techniques.
2. To develop highly accurate and traceable methods for the detailed characterisation of defects in industrially relevant compound semiconductors in the 5 nm to 10 μm range. The methods should be based on advanced optical and electrical scanning probe microscopy or other off-line techniques. Multiple methods could be used, but each method should have a spatial resolution better than 50 nm.
3. To develop accurate and traceable methods for quantifying the quality, i.e. defect type and density, of compound semiconductor wafers with uncertainties < 10 %. The results from fast optical spectroscopic analyses should be correlated with those obtained using advanced scanning probe microscopy and both material and processing defects should be considered.
4. To identify key measurands that will ensure the quality of industrially relevant wide-bandgap materials, e.g. GaN and SiC, and other emerging materials e.g. Ga_2O_3. This should include an assessment of the effects of different types of defect on the materials' optoelectronic properties and on the performance of a range of power electronics devices, which use these materials.
5. To facilitate the take up of the technology and measurement infrastructure developed in the project by the measurement supply chain (accredited laboratories, instrumentation manufacturers), standards developing organisations (CEN, ISO) and end users (compound semiconductor industry, power electronics industry).

Progress beyond the state of the art

Objective 1. Instruments and methods for industrially relevant fast and accurate defect detection
Defect inspection and wafer metrology are increasingly important for the WBG semiconductor industry where global shortages of raw wafers have resulted in pressure on material quality and greater awareness of the need to minimise wastage. Multiple techniques are currently in use, with various strengths and weaknesses, but in general there is a trade-off between sensitivity and throughput. This project will overcome this limitation by applying advanced concepts of hybrid metrology, data fusion, and advanced sampling strategies.

Objective 2. Traceable off-line methods for accurate defect characterisation
Effective classification of defects is reliant on a detailed understanding of their natures and formation mechanisms. Broad categories of defects are well-known but detailed defect characterisation can provide additional information (such as the depth of sub-surface features, and the nanoscale distribution of chemical species at buried interfaces) that is important for process development and control. This project will develop new techniques: near-field optical spectroscopy (IR s-SNOM and TERS/TEPL), and combined cathodoluminescence (CL) and Kelvin probe force microscopy (KPFM) to provide such detailed defect characterisation and discrimination.

Objective 3. Accurate methods for quantifying quality of compound semiconductor wafers
State-of-the-art wafer inspection tools provide defect 'maps' but there are no agreed methods for quantifying the overall quality of a wafer with uncertainties. Documentary standards currently in draft with international standards organisations are beginning to address the need for defect classification but do not extend to quantitative metrics for material quality. This project will apply analytical and numerical modelling to the new wafer-scale optical techniques developed to quantify and validate the sensitivity of these techniques.

Objective 4. Identify key measurands to assess impact of defects on the performance of wide-bandgap materials
End-of-line device performance is of the highest importance to industrial end-users and so this project will evaluate the novel methods developed for defect metrology with the performance of completed devices to identify 'key measurands' of wafer quality for industrial uptake.

Results

Objective 1. Instruments and methods for industrially relevant fast and accurate defect detection
Wafers of high-quality SiC, GaN-on-Si, and GaN-on-SiC have been prepared by industry partners with pre-characterisation data using state-of-the-art inspection tools so that they can be used as reference materials for development and testing of new instruments and methods for defect detection.

Optical metrology techniques are best suited to high-throughput wafer inspection, and several classes of technique are being developed to meet this need:

- Coherent Fourier Scatterometry (CFS) has been applied to SiC and GaN wafer samples containing reference defects and was able to clearly detect them. Furthermore, CFS was able to resolve the structure of these defects as well as to discriminate smaller defects nearby. Work to increase the throughput of the measurement through parallelisation has so far been demonstrated with 3 parallel channels, increasing the measurement speed by the same factor. A suitable image stitching algorithm has been developed to enable this parallelised measurement, and further improvements to the scanning control are being implemented – one of which is expected to offer up to 100× increase in speed.
- Spectroscopic Ellipsometry has been performed on the reference samples for the wavelength range from 192 nm to 25,000 nm. Suitable models have been developed for analysing the data using Effective Medium Analysis (EMA). The results showed that measurements with a large (1.2 mm diameter) beam spot are not suitable for characterisation of individual defects, but are better-suited to measurements of oxide layer thickness and interfacial quality, such as for thermal growth of SiO_2 on SiC, which is a critical process in MOSFET fabrication.
- Mueller Matrix Imaging Ellipsometry (MMIE) has been tested on the reference samples and shows good sensitivity to the relevant material defects in GaN and SiC. Measurements were performed using the range of wavelengths from 400 nm to 800 nm. The use of a polarisation-sensitive camera provides a high throughput for this measurement, whilst also offering detailed characterisation of the defect structures.
- Photoluminescence spectroscopy of WBG materials requires a UV excitation source, and a new instrument has been built incorporating a 325 nm laser with a high-performance spectrometer and a digital multimirror device (DMD) for structuring the excitation light field. This instrument will enable the development of a compressed sensing approach to high-throughput photoluminescence spectroscopy. In parallel, a filter-based method of multispectral photoluminescence imaging has been developed and is undergoing tests. Preliminary results show good sensitivity to the reference defects and will enable substantial increases in measurement speed over traditional spectroscopic methods.

Objective 2. Traceable off-line methods for accurate defect characterisation

The manufacturing partners have provided small samples of SiC, GaN, and β-Ga_2O_3 containing different types of defects for detailed characterisation. These samples are now being used to guide the development of novel techniques for nanoscale-microscope defect measurements.

A novel measurement technique combining cathodoluminescence (CL) with Kelvin Probe Force Microscopy (KPFM) has been demonstrated using a GaN sample, and the results show that the nanoscale dislocations can be resolved. The CL results provide important information about the local charge recombination associated with these defects. Additional capability for temperature-dependent CL, and photoexcited KPFM has also been developed and demonstrated, which provide further sensitivity to charge (de)trapping and surface band-bending phenomena. GaN samples have been shared between partners for comparative KPFM measurements in order to evaluating the quantification of nanoscale work function measurements on these materials.

Two near-field optical spectroscopy techniques have also been developed within this project: tip-enhanced optical spectroscopy (TEOS) and infrared scattering-scanning near-field optical microscopy (IR s-SNOM). These techniques offer ground-breaking super-resolution characterisation of samples that will give unprecedented insight into the structure of nanoscale defects. Results from the last period demonstrate super-resolution sensitivity to doping density and material polytypes (which are both important parameters for assessing material quality) as well as defects in GaN, SiC, and β-Ga_2O_3 samples.

Objective 3. Accurate methods for quantifying quality of compound semiconductor wafers

The use of advanced sampling strategies for high-sensitivity, high-throughput wafer metrology requires a novel metrological approach for quantifying the material parameters measured. Work so far has identified 3 advanced sampling strategies for consideration: compressed sensing for optical spectroscopy in the spatial domain, compressed sensing for optical spectroscopy in the spectral domain, and advanced sampling for scanning probe microscopy. These methods have been evaluated in terms of the instrumentation requirements for implementation and through modelling to quantify the expected benefits.

Modelling of spatial-domain compressed sampling of optical spectroscopic imaging using a sample hyperspectral datacube for a polytype inclusion defect in SiC has demonstrated the feasibility of this approach. New software tools have been developed for handling and visualising hyperspectral data. Simulation results show that accurate reconstruction of data can be achieved with undersampling down to 20% of the full dataset corresponding with a ×5 increase in measurement speed. The reconstruction is highly sensitive to measurement noise, but with appropriate hardware, further speed increases could be achieved.

Numerical simulations using Finite Element Modelling (FEM) and Finite Difference Time Domain (FDTD) approaches have been created for near-field optical spectroscopy and far-field scatterometry/ellipsometry measurements. These simulations correspond with measurement techniques being developed in Objectives 1 and 2. This project is using these simulations to relate off-line, detailed characterisation results with fast, wafer-scale metrology to enable high-throughput quantification of material quality. In the last period, the applicability of these simulations has been explored to evaluate their applicability to a range of different shapes and sizes of nanoscale defects. This has given estimates of the detection limits for particle defects, and interfacial layer defects.

Objective 4. Identify key measurands to assess impact of defects on the performance of wide-bandgap materials

Industrial and metrological partners within the project have discussed the industrially relevant range of test conditions and accuracy required for reliability testing of SiC MOSFET devices. Guided by the industry need for reduced device testing times, the project has chosen to develop capability for Accelerated Life-Time High-Temperature Reverse Bias (ALT-HTRB) testing, where devices are subjected to higher reverse biases and temperatures than their specified rating to induce rapid failure. This measurement capability will be implemented and applied to completed devices in order to relate the end-of-line device performance to key measurands of material quality.

Oxidation of SiC to create a high-quality SiC/SiO_2 interface is key to achieving high-performance devices, and low-pressure chemical vapour deposition (LPCVD) has been optimised, using different plasma pre-treatments to create a set of samples for comparison within this project. The electronic properties of these samples have been measured to compare trap state density with process parameters and the results obtained using the novel characterisation tools developed in this project (see Objective 2) to identify the most suitable material measurands for ensuring high end-of-line performance. Electrical characteristics of β-Ga_2O_3 samples have also been measured for comparison with material defect studies described above. In the next part of this project, device performance testing will be extended to GaN and SiC devices.

Impact

Close interaction with industry stakeholders through a programme of two-way knowledge transfer, training, dissemination, and exploitation is key to delivering impact through this project. The focus for the first half of the project has been to establish effective communication with stakeholders and build the profile of the PowerElec project within the compound semiconductor manufacturing community. In the second half of the project the focus has been on dissemination of research outcomes and knowledge transfer. To this aim, the project has hosted special sessions in the international SMSI 2023 and SPIE Optical Metrology conferences, as well as jointly hosting a PhD summer school on SiC and GaN power electronics with the YESvGaN and TRANSFORM projects. 25 presentations have been delivered in national and international conferences. 8 peer-reviewed papers have been published in journals and a training workshop on MOCVD growth for WBG semiconductors for power applications was delivered.

Impact on industrial and other user communities

This project is developing new defect metrology techniques for use in the WBG semiconductor power electronics industry, which will be validated against state-of-the-art methods in both industrial and laboratory settings. The associated knowhow and supporting metrological framework will be immediately available to European stakeholders through new measurement services, new IP and licensing. The planned activities to support early update will accelerate optimisation and commercialisation of these techniques for deployment on commercial wafer fabrication facilities, where they will provide improved sensitivity and throughput of wafer inspection. This will enable SiC and GaN manufacturers to add value to their products through higher levels of quality assurance, increased manufacturing yield, and shorter time to market. This project will also benefit manufacturers and users of MOCVD (Metal-Organic Chemical Vapour Deposition) tools through insights into defect physics, which are critical for the successful scale up of β-Ga_2O_3 bulk epitaxial growth.

The impact described above will be supported and enabled by a programme of engagement activities to strengthen relationships between NMIs, academia and industry:

- An Industry Stakeholder Workshop was hosted in Cardiff, UK with 26 attendees from industry, academia, and metrology institutes. This workshop enabled project partners to understand detailed industrial requirements for semiconductor metrology, as well as presenting novel metrological methods to potential industry users. This has led to 2 new collaborations.
- A database has been created to track and manage stakeholder engagement throughout the project.
- IP exploitation planning is ongoing, with two new instruments currently being considered for IP protection.
- Case studies will be developed within the project to demonstrate the new metrological techniques developed, including evaluation by the industry partners based on their reference samples.
- A new facility for accelerated device reliability testing is being developed within the project and will form a basis for an enduring commercial capability made available to industry.
- One of the project partners has become recognised as a Competence Centre by the European Centre for Power Electronics, and links with other trade organisations and technical consortia are being exploited to disseminate project results to a wider network of industrial stakeholders.
- The project partnered with other European industrial projects on wide bandgap semiconductors (YESvGaN and TRANSFORM) to host a summer school on SiC and GaN power electronics, which has strengthened interactions with stakeholders.

Impact on the metrology and scientific communities

This project will develop and demonstrate capability (including novel instrumentation and measurement methods) and expertise across European NMIs in metrology for WBG semiconductor manufacture, which represents a significant evolution from the established focus on silicon technology.

The technical outcomes from this project regarding semiconductor defect metrology and manufacturing process development will open new routes for epitaxial growth of semiconductors, defect engineering and device optimisation with significant impact in numerous areas of solid-state physics, materials science and engineering. In addition, this project will encourage uptake of compressed sensing and hybrid metrology which are universal measurement paradigms with enormous potential for enhancing the speed and accuracy of measurements across all disciplines but are not well-known within the metrology community.

To ensure wide impact in the scientific and metrology communities, this project has planned an effective collaboration and dissemination strategy, using both traditional and bespoke targeted dissemination and training activities:

- 25 presentations have been delivered at national and international conferences.
- 8 peer-reviewed papers have already been published, with 4 more having been submitted and a further 3in draft/review.
- A training workshop on MOCVD growth for WBG semiconductors for power applications was delivered.
- A special session was hosted at SPIE Optical Metrology 2023 within the Modelling Aspects in Optical Metrology IX conference, which focused on the use of compressed sensing in metrology.
- A special session was hosted at the SMSI 2023 conference, and a further session at a large European research conference (ALTECH, E-MRS Spring 2024) is being planned, which will help to disseminate results from the PowerElec project to a wider academic and industrial audience.
- Software tools (Gwyscan) to support advanced sampling and compressive sensing methods scanning probe microscopy have been made available for the open-source Gwyddion software for scanning probe microscopy.
- An e-learning course for training in Metrology for Compound Semiconductors is currently in preparation with content being contributed by the project partners.

Impact on relevant standards

This project will provide a long-lasting impact on international standardisation activities related to defect inspection in WBG semiconductors and the associated metrology tools developed in this project.

The outcomes of this project will provide metrological support for the proposed formation of a new sub-committee on Optical Spectroscopic Analysis based on ISO TC 201 WG5 which has strong support from the semiconductor industry. Results from this project on wafer inspection will also be presented to other relevant ISO and IEC standards committees, and their national mirror committees. Project partners have already contributed to 4 documentary standards and participated in several national and international standards committees.

Technical results from this project demonstrate the need to develop standardised methods for Kelvin probe force microscopy of wide bandgap materials and an ongoing pilot study, will provide the evidence base required to initiate a pre-normative VAMAS (Versailles Agreement on Advanced Materials and Standards) interlaboratory study on the reproducibility of KPFM measurements applied to WBG semiconductor materials and also build new relationships between NMIs and industry-specific semiconductor standards organisations. Representing European interests in the development of new international standards will help maintain the global competitiveness of European industry.

Longer-term economic, social and environmental impacts

Since the start of this project, increased recognition of the importance of semiconductor technology has resulted in massive investment in semiconductor manufacturing around the world. The €43bn EU CHIPS act demonstrates a European intention to double its share of global semiconductor manufacture. Power electronics is a rapidly growing part of the semiconductor market, and this project will enable European manufacturers of power electronic devices to maintain and increase their global competitiveness through improved production efficiency, and enhanced quality assurance of products leading to potential growth in market share.

By improving the efficiency of the power electronics supply chain and through increased confidence in the performance of WBG semiconductor devices, this project aims to enable the acceleration of transport electrification. This will reduce the cost of electric vehicles as well as increasing their range through more efficient energy conversion. Electrification of transport is consistently recognised as a key route towards achieving the European Commission’s ‘Green Deal’, reducing lifetime emissions by 17-30 % compared with traditional vehicles.

This project will also contribute to tackling climate change through lowering cost and increasing uptake of WBG semiconductors in power generation and smart-grids, such as SiC inverters and GaN power supplies, where they can reduce electrical energy losses by 50 % compared with silicon power electronics.

Electrification of transport and 5G communications are both areas where this project will accelerate progress leading to higher performance and lower cost products with wide-spread societal impact. Increased mobility of populations and improved information connectivity will improve quality of life and help to reduce regional disparities based on infrastructural inequality.

List of publications

"Assessment of Subsampling Schemes for Compressive Nano-FTIR Imaging", S. Metzner, B. Kästner, M. Marschall, G. Wübbeler, S. Wundrack, A. Bakin, A. Hoehl, E. Rühl, C. Elster, *IEEE Trans. Instrum. Meas.*, 71, 4506208, **(2022)**. doi: 10.1109/TIM.2022.3204072.

“Hybrid optical measurement technique for detection of defects in epitaxially grown 4H-SiC layers”, E. Ermilova, M. Weise, A. Hertwig, *EPJ Web Conf.*, 266, 10001, **(2022)**. doi: 10.1051/epjconf/202226610001.

“Kelvin Probe Force Microscopy under Variable Illumination: A Novel Technique To Unveil Charge Carrier Dynamics in GaN”, P. González-Izquierdo, N. Rochat, M. Charles, T. Sochacki, Ł. Borowik, *J. Phys. Chem. C,* 127, 26, 12727, **(2023)**. doi: 10.1021/acs.jpcc.3c01887

“Electrical Characterization of the SiO_2/4H-SiC Interface”, C. Nanjappan, G. Pfusterschmied, U. Schmid, *SMSI 2023 Proc.*, D5.3, **(2023)**. doi: 10.5162/SMSI2023/D5.3

"Optical and Tactile Measurements on SiC Sample Defects" J. Grundmann, B. Bodemann, E. Ermilova, A. Hertwig, P. Klapetek, S. Pereira, J. Rafighdoost, *SMSI 2023 Proc.*, D5.2, **(2023)**. doi: 10.5162/SMSI2023/D5.2

"Compressed nano-FTIR Hyperspectral Imaging for Characterizing Defects in Semiconductors", B. Kästner, C. Elster, A. Hoehl, M. Marschall, D. Siebenkotten, G. Wübbeler, E. Rühl, S. Wood, *SMSI 2023 Proc.*, D5.1, **(2023)**. doi: 10.5162/SMSI2023/D5.1

"Compressed Sensing Spectral Photoluminescence Imaging of Wide Bandgap Semiconductor Materials for Power Electronics Applications", S. Wood, J. Blakesley, G. Koutsourakis, A. Thompson, *SMSI 2023 Proc.*, D5.0, **(2023)**. doi: 10.5162/SMSI2023/D5.0

"Compressed Sensing Time Resolved Photoluminescence Imaging for Semiconductor Characterisation", A. Baltusis, G. Koutsourakis, S. Wood, S. Sweeney, *SMSI 2023 Proc.*, D5.4, **(2023)**. doi: 10.5162/SMSI2023/D5.4

This list is also available here: https://www.euramet.org/repository/research-publications-repository-link

Project start date and duration:	01 June 2021, 36 Months	
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Internal Funded Partners: 1. NPL, United Kingdom 2. BAM, Germany 3. BEV-PTP, Austria 4. CMI, Czechia 5. PTB, Germany 6. TUBITAK, Turkey	External Funded Partners: 7. AIXTRON, Germany 8. CEA, France 9. CSC, United Kingdom 10. FVB, Germany 11. TU Delft, Netherlands 12. TU WIEN, Austria	Unfunded Partners: 13.Infineon, Austria
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