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Automated Hyperspectral SIMS Nanoanalytics for Advanced Semiconductor Failure Analysis

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ABSTRACT

As semiconductor devices become increasingly complex and three-dimensional, traditional analytical techniques such as SEM-EDS often struggle to deliver the spatial resolution and chemical sensitivity required for advanced failure analysis. Critical features such as deeply buried interfaces, nanoscale defects, and trace contamination can remain undetected using conventional imaging and microanalysis approaches.

In this work, we present an automated magnetic-sector Secondary Ion Mass Spectrometry (SIMS) platform based on the IONMASTER system, designed for high-resolution semiconductor nanoanalytics. The system combines a vertical focused ion beam (FIB) column equipped with a Liquid Metal Alloy Ion Source (LMAIS), a dedicated magnetic-sector SIMS analyzer, and a laser interferometer-controlled stage, enabling hyperspectral chemical imaging with lateral resolution below 20 nm while maintaining high ion transmission efficiency.

Direct import of GDSII and KLARF data enables automated and highly accurate navigation to regions of interest (ROIs), facilitating the investigation of buried structures and electrically identified failure sites. Application examples demonstrate isotopic imaging, detection of subsurface contamination, and three-dimensional chemical reconstruction of buried device features. These results highlight the potential of high-resolution SIMS to address critical analytical challenges and extend the capabilities of semiconductor failure analysis beyond those achievable with conventional techniques [1].

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Introduction

The continuous scaling and increasing complexity of semiconductor devices require characterization techniques capable of detecting and analyzing nanoscale defects, compositional variations, and process-induced anomalies with exceptional sensitivity and precision. The combination of Focused Ion Beam (FIB) technology and Secondary Ion Mass Spectrometry (SIMS) has emerged as a powerful solution, enabling the correlation of high-resolution structural imaging with highly sensitive elemental and isotopic analysis. This paper presents a novel nanoanalytical platform that combines a Liquid Metal Alloy Ion Source (LMAIS) allowing rapid switching between different ion species [2], with a magnetic-sector SIMS system for parallel mass detection [3]. The instrument supports both high-efficiency milling using heavy ions such as Bi^+ and high-resolution imaging with light ions such as Li^+. In addition, a laser interferometer-controlled stage provides nanometer-scale positioning accuracy and enables automated defect review and navigation workflows. Together, these technologies create a versatile platform for advanced semiconductor characterization and failure analysis (Figure 1).

System Architecture

Integrated SIMS Platform

The analytical platform is centered on a vertically oriented focused ion beam (FIB) column equipped with a Liquid Metal Alloy Ion Source (LMAIS). A Wien filter allows rapid selection and switching between multiple ion species, enabling the optimization of milling, imaging, and analytical conditions for a broad range of materials and applications. Heavy ion species provide efficient sputtering and enhanced secondary ion yields, whereas lighter ions offer superior lateral resolution and increased surface sensitivity for high-resolution imaging.

The system incorporates a magnetic-sector SIMS analyzer that combines the high spatial resolution of the LMAIS with excellent ion transmission efficiency. Full mass spectra are acquired simultaneously at every image pixel, eliminating duty-cycle limitations commonly associated with sequential mass detection approaches. This hyperspectral imaging capability enables retrospective data mining, isotopic discrimination, and multi-element correlation without the need for repeated measurements, significantly improving both analytical flexibility and workflow efficiency (Fig. 1).

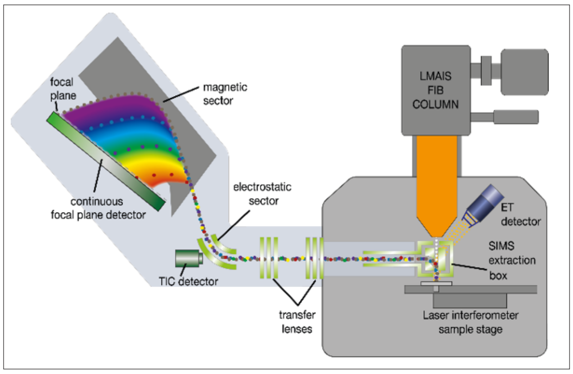

Figure 1: Schematic Setup of the Instrument: Vertical FIB column with LMAIS, high precision laser interferometer stage and SIMS unit with extraction & transfer optic, magnetic sector and continuous focal plate detector

Navigation and Automation via GDSII and KLARF

Accurate localization of failure sites remains one of the most critical challenges in advanced failure analysis, particularly when defects are deeply buried or exhibit minimal contrast in conventional imaging techniques. To address this challenge, the system supports the direct import of GDSII design layouts and KLARF wafer inspection data, enabling automated navigation from electrical test results or inspection-derived defect coordinates directly to the SIMS analysis location.

Nanometer-scale positioning accuracy is achieved through a laser interferometer-controlled stage, ensuring precise and repeatable navigation across the entire wafer or sample. By automating region-of-interest (ROI) localization, the system reduces operator intervention, minimizes alignment errors, and enhances both throughput and measurement reproducibility. This capability facilitates the seamless integration of SIMS into established failure analysis, yield learning, and process control workflows, improving the efficiency and reliability of defect characterization.

SIMS Imaging and Application Examples

Hyperspectral Chemical Imaging

Magnetic-sector SIMS enables the simultaneous acquisition of complete mass spectra at every image pixel, generating hyperspectral datasets that reveal elemental and isotopic distributions with lateral resolution better than 20 nm. This approach provides comprehensive chemical information in a single measurement, allowing detailed spatial correlation of multiple species across the sample. The high transmission efficiency of the magnetic-sector analyzer further ensures excellent sensitivity, enabling the reliable detection of trace contaminants, dopants, and light elements even at very low concentrations (Figure 2).

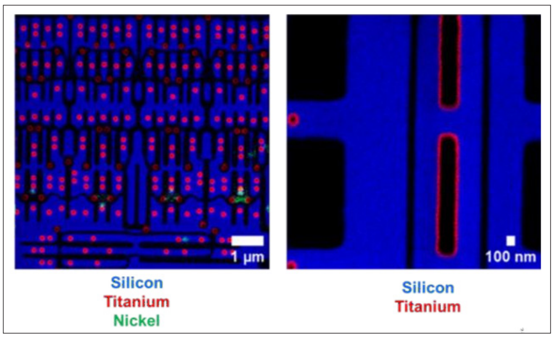

Figure 2: SIMS high-resolution images of a 65 nm CMOS process node logic device in a LGA flip chip package. Under the set measurement parameters (35 keV Bi^+ beam, 5 pA, 0.5 ms/pixel, 512 x 512 pixels) 120 000 full mass spectra are acquired per minute.

Isotopic Mapping in CMOS Stacks

One representative application is the isotopic mapping of advanced CMOS device architectures. High-resolution SIMS imaging reveals isotopic distributions across critical device features, including gate dielectrics, channel regions, and contact structures. This capability provides valuable insight into process-induced compositional variations, dopant behavior, and diffusion mechanisms at the nanoscale. Such information is often beyond the reach of conventional analytical methods such as SEM-EDS and can be difficult to obtain even with advanced TEM-based techniques, making SIMS a powerful complement for comprehensive device characterization.

Detection of Subsurface Contamination

Another important application is the detection and localization of sodium contamination within vias and contact structures. Such residues are typically invisible in secondary electron images and are often challenging to identify using EDS because of their low concentrations and spectral interferences. By contrast, SIMS hyperspectral imaging provides highly sensitive chemical mapping, clearly revealing both the presence and spatial distribution of sodium. This capability enables rapid root-cause analysis of failure mechanisms such as leakage currents, reliability degradation, and undesirable parametric shifts, thereby supporting process optimization and yield improvement (Figures 3 and 4).

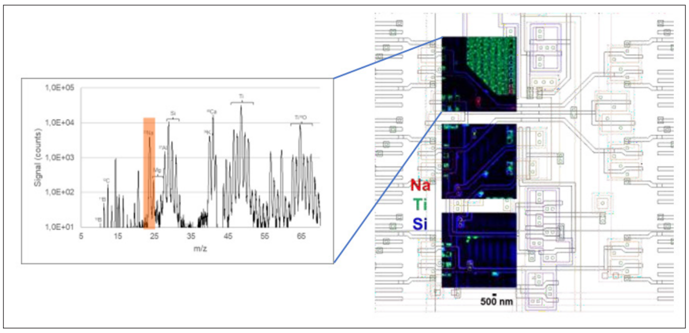

Figure 3: GDSII Design-Based Sample Navigation Enabling Automated Roi Localization and Direct Targeting of Inspection Sites.

Two-dimensional SIMS images are generated from the full mass spectrum acquired at every pixel, ensuring that all detectable ion species are captured during a single measurement. This hyperspectral approach eliminates the risk of overlooking relevant signals and enables a comprehensive characterization of the sample composition. Analysis of the complete mass spectrum clearly identifies sodium (Na) as a contaminant species.

Subsequent chemical mapping of the sodium signal reveals a highly localized and non-uniform distribution, with significant enrichment observed within specific vias. To further investigate this behavior, a virtual line profile was extracted from the hyperspectral dataset during post-processing. The resulting analysis identified vias 6 and 7 as the dominant sources of the detected sodium signal.

These findings highlight vias 6 and 7 as critical regions of interest within the device structure. The elevated sodium concentration suggests localized contamination or a process-induced anomaly associated with these features. Consequently, these vias warrant targeted follow-up investigation and additional characterization to determine the contamination source and evaluate its potential impact on device performance, reliability, and long-term functionality.

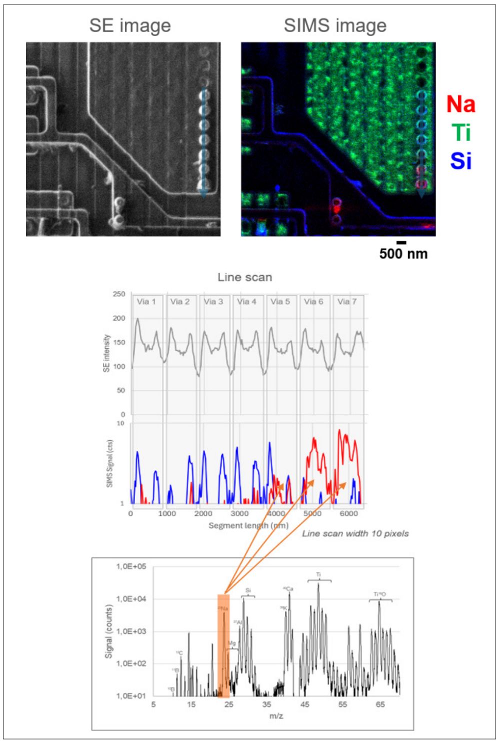

Figure 4: Virtual SIMS line Scans Over the Vias Reveal Buried Sodium Contamination in Vias 5, 6 and 7. The Vias are Identified as Critical Points

3D Reconstruction of the Buried Contamination in the Critical Points

By alternating sputtering and SIMS imaging cycles, three-dimensional chemical reconstructions of the vias, subsurface structures and contamination sites are generated. This volumetric information supports comprehensive failure analysis, revealing the true spatial relationship between defects, interfaces, and material variations.

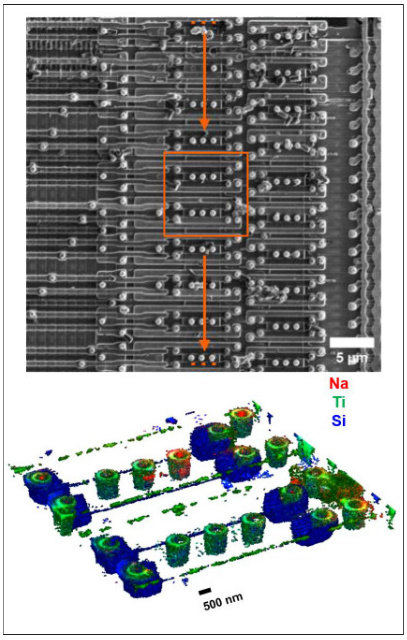

Figure 5: Vias are identified in the design file and analyzed automatically in 3D, revealing the buried alkali contamination

Impact on Failure Analysis and Semiconductor Metrology

The presented automated SIMS platform overcomes several key limitations of conventional failure analysis techniques and provides significant advantages for advanced semiconductor characterization:

- **Ultra-High Spatial Resolution:** Lateral resolution below 20 nm enables the investigation of defects, interfaces, and compositional variations at length scales relevant to leading-edge semiconductor technologies.
- **Exceptional Analytical Sensitivity:** The high secondary ion yield and efficient ion collection enable the detection of trace elements, dopants, and isotopes at concentrations that are often beyond the capabilities of EDS-based techniques.
- **Precise Defect Localization:** Automated navigation based on GDSII layouts and KLARF defect data allows accurate targeting of buried structures and low-contrast failure sites, improving the reliability of defect characterization.
- **Enhanced Workflow Productivity:** Automated alignment, navigation, and analysis significantly reduce operator involvement, increasing throughput while improving measurement repeatability and data consistency.

By combining high spatial resolution, excellent chemical sensitivity, precise navigation, and workflow automation, the system positions SIMS as a highly effective solution for routine failure analysis, defect review, yield enhancement, and advanced semiconductor process characterization

Conclusions

Automated magnetic-sector SIMS nanoanalytics combines exceptional spatial resolution, outstanding chemical sensitivity, and highly accurate sample navigation, making it ideally suited for the challenges of modern semiconductor failure analysis. The integration of GDSII- and KLARF-based navigation with hyperspectral SIMS imaging enables the reliable localization and characterization of buried defects, trace contamination, isotopic distributions, and complex material interactions that are difficult or impossible to access using conventional analytical techniques.

The presented application examples demonstrate that automated SIMS significantly extends the capabilities of established failure analysis workflows. By providing comprehensive chemical and isotopic information at the nanoscale, it enables the identification of failure mechanisms that would otherwise remain undetected. As semiconductor devices continue to scale in complexity, automated SIMS inspection provides a powerful solution for closing critical analytical gaps, supporting both root-cause failure investigations and advanced process monitoring in leading-edge semiconductor manufacturing.

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