FCMN 2026
March 16-19, 2026
Monterey Marriott
Monterey, California USA
International Conference on Frontiers of Characterization and Metrology for Nanoelectronics

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Orbitrap™-SIMS for Accurate Arsenic Quantification in SiGe

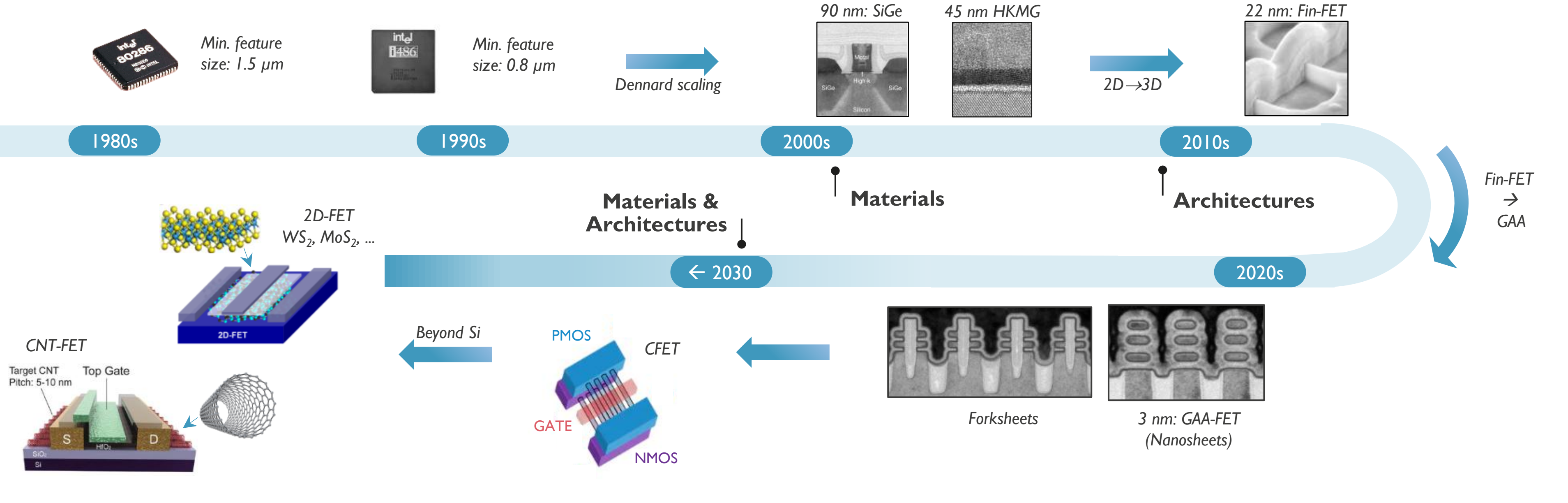
Rita Tilmann, Alexander Pirkl and Alexis Franquet

iONTOF

Outline

- ❑ Introduction and Electronic device evolution & implication on SIMS analysis
  (small volume analysis, Self-Focusing SIMS, Orbitrap^{TM}-SIMS)
- ❑ Mass resolution issue in SIMS for As in SiGe (and Ge)
- ❑ Compare SIMS detector technologies (TOF, Quadrupole, Magnetic Sector (MS), Orbitrap^{TM})
  - Evaluate As detection limit, dynamic range, mass resolution, sputter rate
- ❑ Quantification of As dopant in SiGe (blanket and patterned samples)
- ❑ Summary

Electronic device evolution & implication on SIMS analysis



Microelectronic industry:
R&D to produce smaller, cheaper and more efficient devices

→ **2000s / New, & more and more materials**
- High-k materials for SiO_2 replacement as the gate dielectric
- Replacement of Si as channel material by Ge, SiGe and III/V materials
- Si-based planar stacks to multi-material stacks

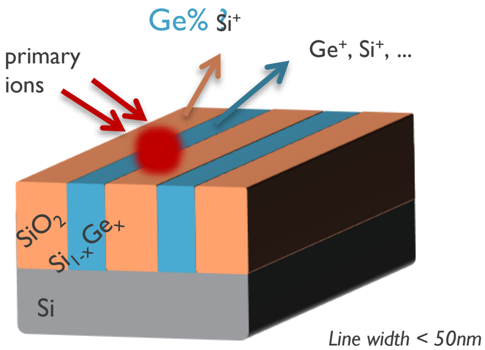
→ **2010s / New (& more complicated) device concepts**
- 2D → 3D
- Fin-FET → GAA (nanosheets, forksheets, ...)
- nm scale features and co-integration of different materials within the same device structure

→ **2030s / New architectures & materials**
- CFET with PMOS and NMOS
- 2D FET and CNT-FET

SIMS on very small structures

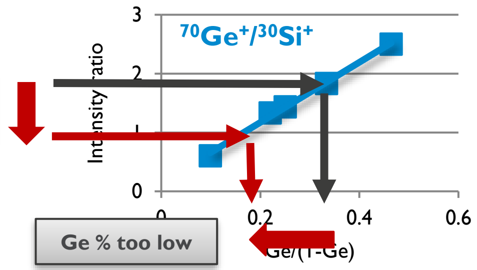
Blanket samples → Patterned samples

Standard SIMS



- Secondary ions (Ge and Si signals) originate from the impact point of the ion beam.
- Quantification is based on Ge/Si intensity.
- Si-signal from surrounding SiO_2 layer will influence quantification.

Si will be too large
Ge/Si too low

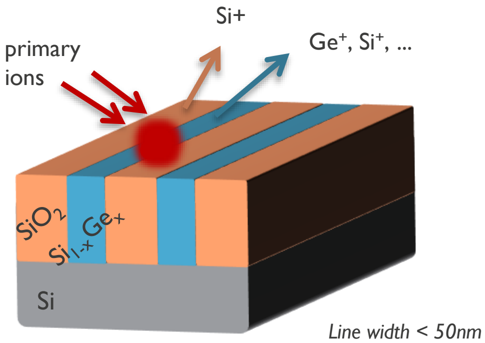


Ge % too low

SIMS on very small structures

Blanket samples → Patterned samples

Standard SIMS



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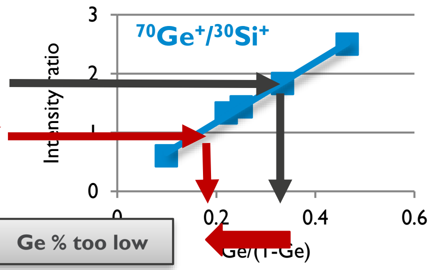
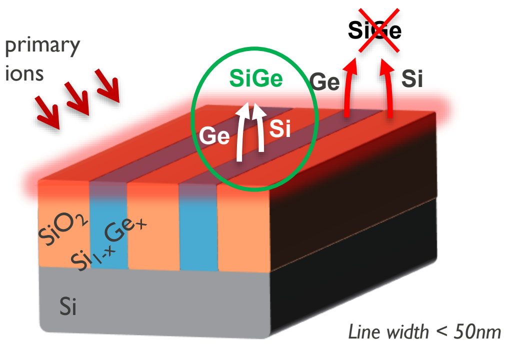


Ge % too low

Self Focusing SIMS
(SF-SIMS) = Array of structures analyzed



- Time and space correlations to form a cluster imply that the constituents originate from the same ion impact, i.e. same point of origin **= self focus**

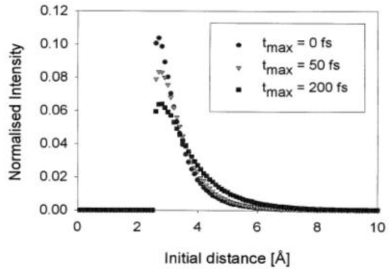
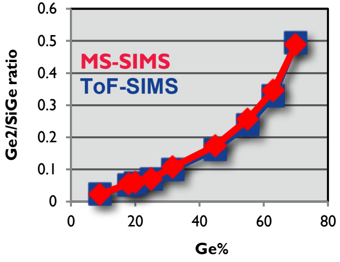


Figure 6. Initial distance between the dimer particles at the sample surface, calculated for three values of t_{max}: t_{max} = 0, 50, and 200 fs.

Calibration curve (various standards):
Ge_2/SiGe intensity ratio

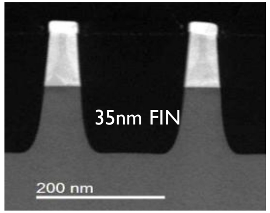


J. Vlekken, W.Vandervorst et al., Journ Amer Soc.Mass Spect. (1999), 10, 246–253
A. Franquet, W. Vandervorst et al., Appl Surf Sci 365 (2016) 143–152
A. Franquet, W. Vandervorst et al., J. Vac. Sci. Technol. B 34(3) (2016) 03H127-1
A. Franquet et al. Vacuum doi 10.1016/j.vacuum.2022.111182

SF-SIMS examples

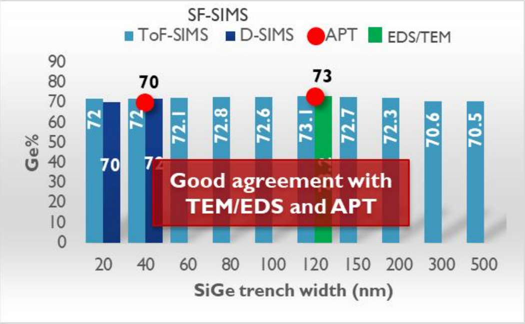
Bulk composition

SiGe

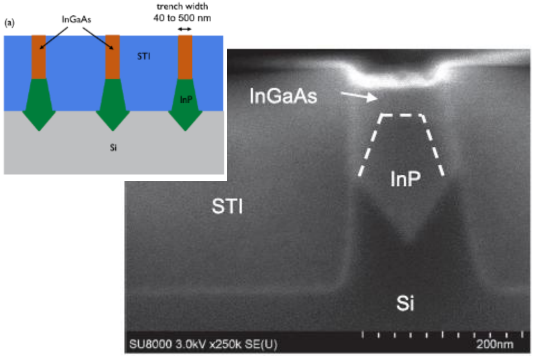


Various SiGe fin widths (20-500nm)
nominal value: 70 at.% Ge

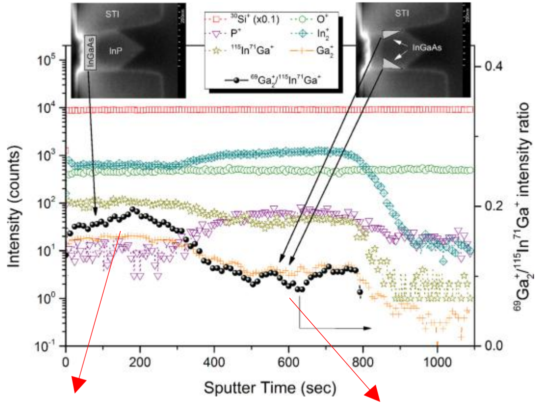
SF clusters $Ge_2^-/SiGe^-$



InGaAs



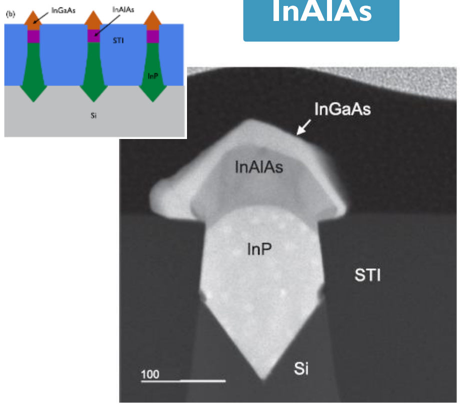
SF clusters $Ga_2^+/InGa^+$



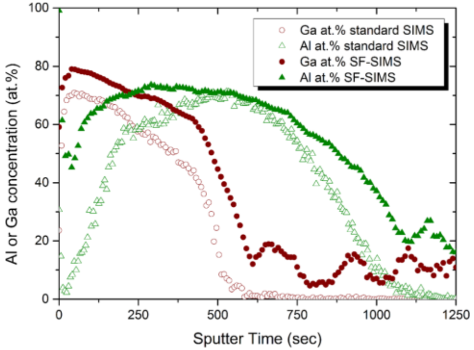
~54 at.% In

~68 at.% In

InGaAs InAlAs



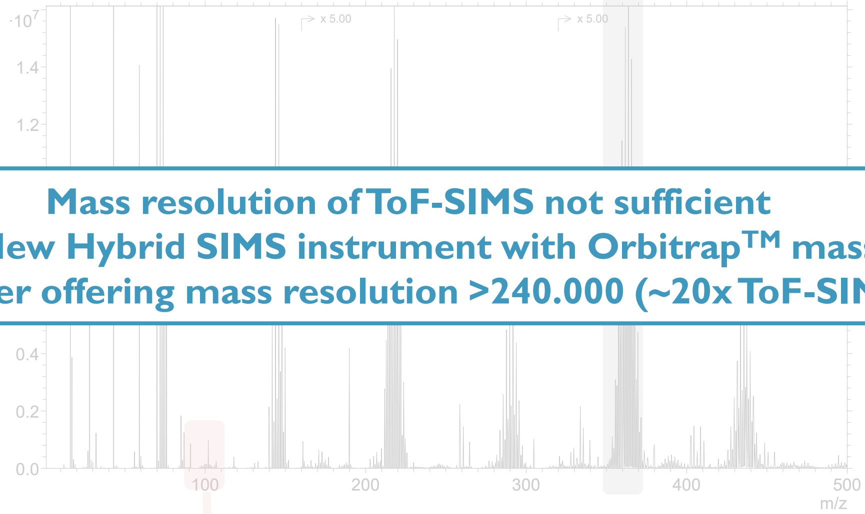
SF clusters $Ga_2^+/InGa^+$ & $Al_2^+/InAl^+$



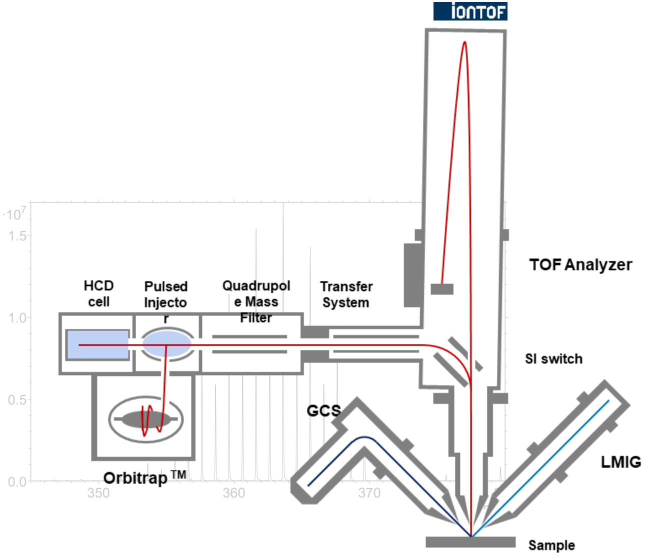
SIMS on new advanced devices

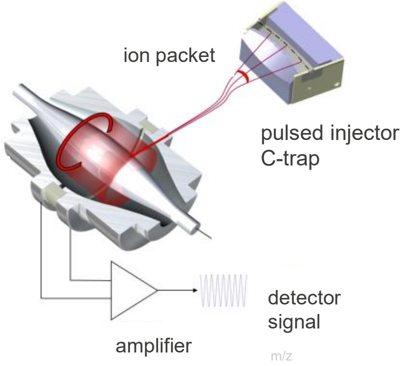
- Complex mass spectra of inorganic samples → <u>**high mass resolution**</u> required

ToF-SIMS spectrum
(M/ΔM > 7.000 @ ^{28}Si)



Mass resolution of ToF-SIMS not sufficient
→ New Hybrid SIMS instrument with Orbitrap™ mass analyzer offering mass resolution >240.000 (~20x ToF-SIMS)





extensive use of cluster ions in SF-SIMS → **mass interferences** represent a limitation for reaching low detection limits and unambiguous identification

Introduction

Context in the Semiconductor Industry

- Arsenic (As): Critical n-type dopant in advanced CMOS nodes
- Silicon-Germanium (SiGe): Key material for mobility enhancement

Analytical Challenges

- Accurate As profiling in SiGe (& Ge) is essential for device performance
- (ToF)SIMS suffers from mass interference between As and GeH
- High mass resolution needed for accurate As and Ge quantification

(structured samples – SF-SIMS)

Objectives of this Study

Compare SIMS detector technologies:

- ToF, Quadrupole, Magnetic Sector (MS), Orbitrap^{TM}
- Evaluate detection limit (dynamic range), mass resolution, sputter yield/rate

Advanced Approach

Apply Self-Focusing SIMS in Orbitrap^{TM}:

- Ultra-high mass resolution
- Localized profiling of low As levels in small SiGe structures
- Accurate quantification of As and Ge in SiGe

Problem statement

As in SiGe or Ge → main issue is mass resolution

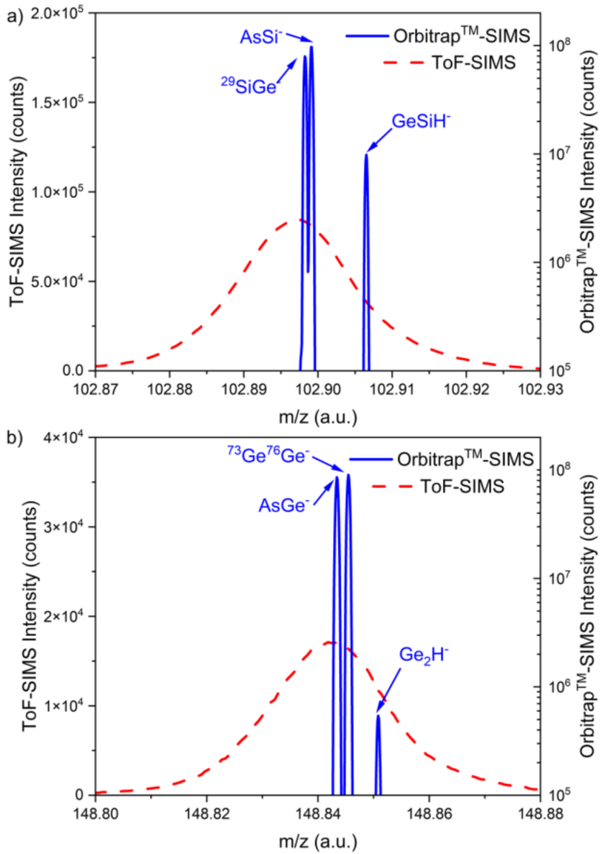
Nominal mass (m/z)	Signal 1 (& mass)	Signal 2 (& mass)	M/ΔM (mass resolution)
75	As (74.9221)	GeH (74.9296)	10.000
103	$As^{28}Si$ (102.8991)	$^{30}Si^{73}Ge$ (102.8978)	79.231
	$As^{28}Si$ (102.8991)	GeSiH (103.9065)	13.918
	$As^{28}Si$ (102.8991)	$^{29}SiGe$ (102.8982)	114.445
147	$^{72}GeAs$ (146.8442)	$Ge^{72}GeH$ (146.8516)	19.865
149	AsGe (148.8433)	Ge_2H (148.8507)	20.135
	AsGe (148.8433)	$^{73}Ge^{76}Ge$ (148.8454)	70.952
151	$^{76}GeAs$ (150.8435)	$^{76}GeGeH$ (150.8510)	20.134

Good performance for As analysis in SiGe requires:
- Good vacuum in the analysis chamber
- High mass resolution

→ Blanket samples
→ Until certain level of As in SiGe

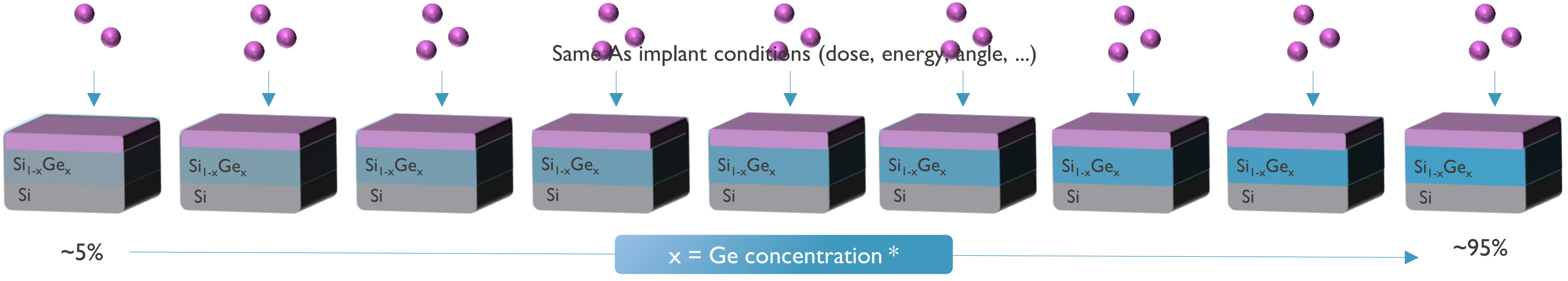
For patterned samples, where SF-SIMS is required:
- Cluster ions to be used
- Higher mass resolution needed

→ Insufficient mass resolution in ToF-, MS-, Quad-SIMS
→ Orbitrap™-SIMS has the required mass resolution



* certified by RBS

As implanted $Si_{1-x}Ge_x$



SIMS detectors on entire std series

- Quad-SIMS (Cs 2keV)
- MS-SIMS (Cs 2keV)
- ToF-SIMS (Bi1 15keV – Cs 2keV)
- Orbitrap™-SIMS (Cs 2keV)

Properties

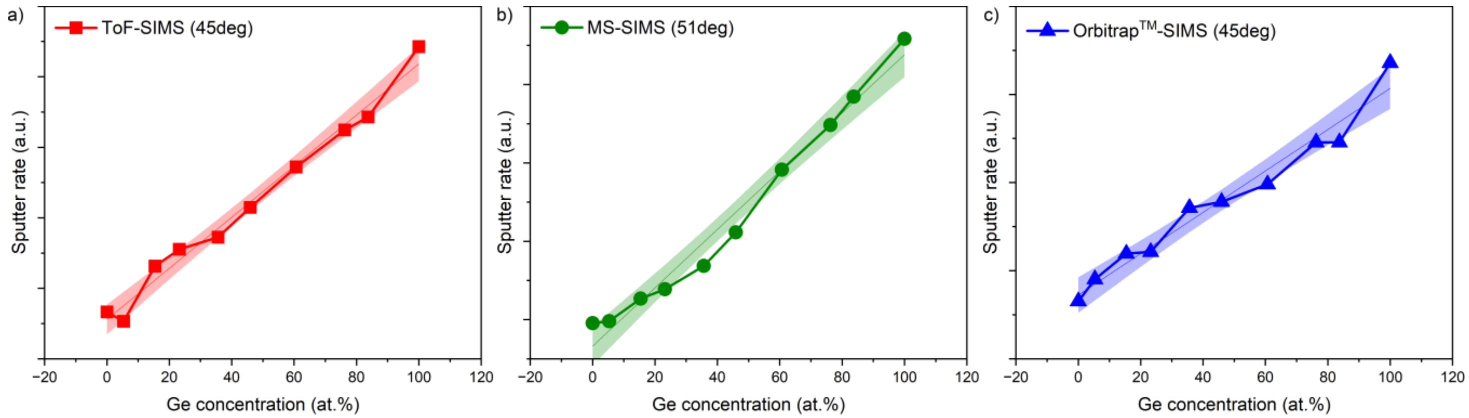
- Sputter rates (SR)
- Bulk intensities for SiGe quantification (^{70}Ge, ^{30}Si, Ge_2, SiGe)
- As detection limits (DL) in SiGe – various single and cluster ions
- Calibration curves for As quantification in SiGe

Application to patterned sample

- Ge quantification in SiGe small structures
- As dopant quantification in SiGe small structures

Comparison of SIMS detectors

Sputter Rates (normalized to current density)

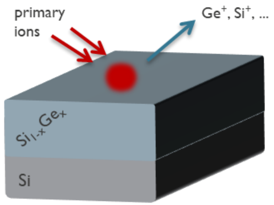


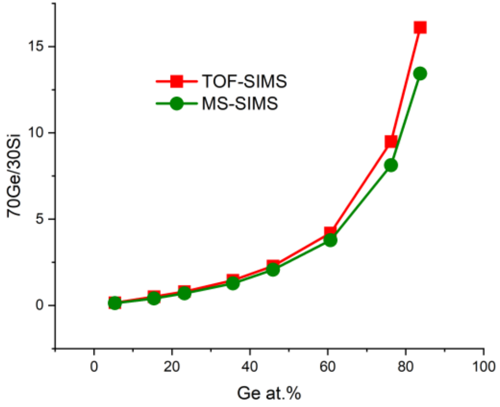
- Similar trends of the sputter rates across mass analyzers, Cs 2keV sputter beam used in all cases
- Linear increase of the sputter rates with increasing Ge concentration in SiGe

Comparison of SIMS detectors

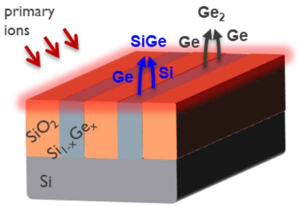
Ge quantification in SiGe – calibration curves (SIMS & SF-SIMS)

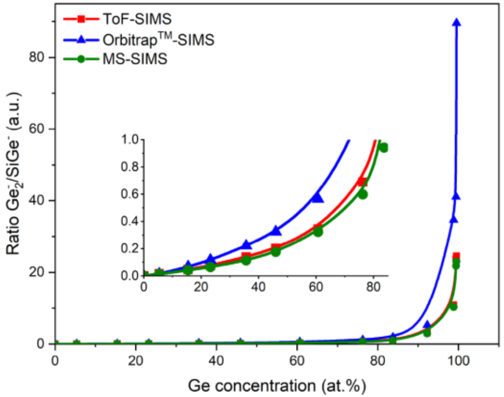
Blanket samples





Patterned samples (SF-SIMS)



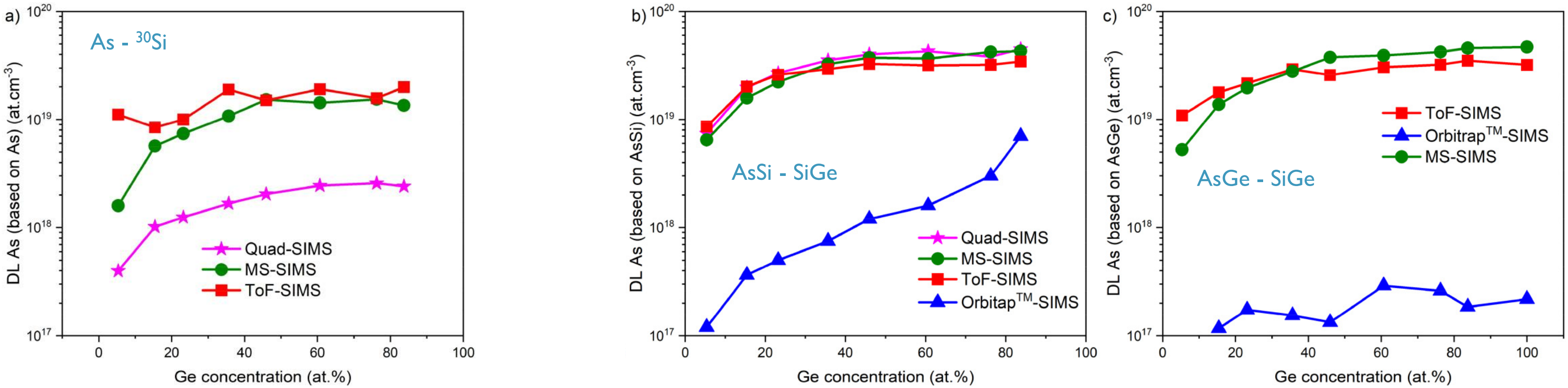


- Ratio of single ions ($^{70}Ge^-$ and $^{30}Si^-$) vs Ge content
- Similar calibration curves in TOF and MS

- Ratio of cluster ions (Ge_2^- and $SiGe^-$) vs Ge content
- Similar calibration curves in ToF and MS
- Higher sensitivity in Orbitrap™ (especially at high Ge%)

Comparison of SIMS detectors

Arsenic detection limits and dynamic ranges



- As detection limit (and dynamic range) limited by mass resolution in ToF-, MS- (& Quad-) SIMS

  (single ions As and ^{30}Si)

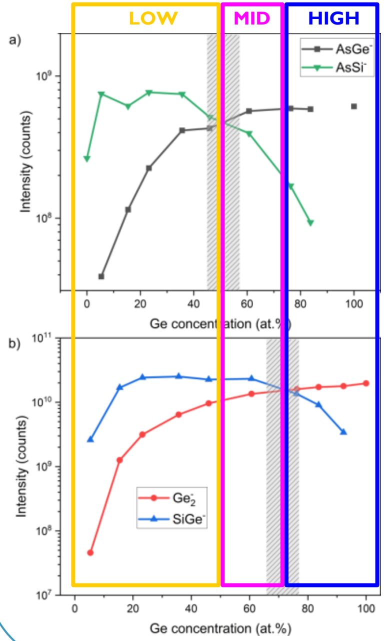
- As detection limit (and dynamic range) limited by mass resolution in ToF-, MS- (& Quad-) SIMS
- High mass resolving power of Orbitrap™-SIMS allows much better As detection limit (and dynamic range)
- More than 1 order of magnitude better in Orbitrap™-SIMS

  (cluster ions AsSi, AsGe, SiGe for SF-SIMS application)

Arsenic dopant quantification – Orbitrap™-SIMS

Arsenic dopant quantification – calibration curves (SF-SIMS)

As response vs Ge content in SiGe



Peak intensities of

a) dopant selective peaks $AsSi^-$ and $AsGe^-$

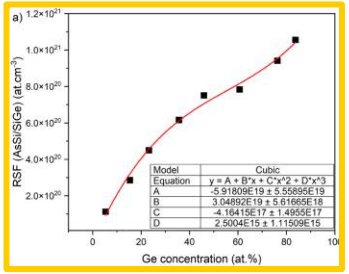
b) b) matrix selective signals $SiGe^-$ and Ge_2^-

3 regime

Low ≤ 50 at. % Ge

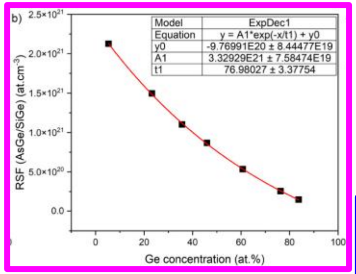
Mid 50-70 at. % Ge

High ≥70 at. % Ge



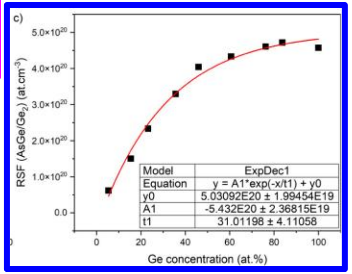
AsSi/SiGe

Calibration curves for As quantification in SiGe



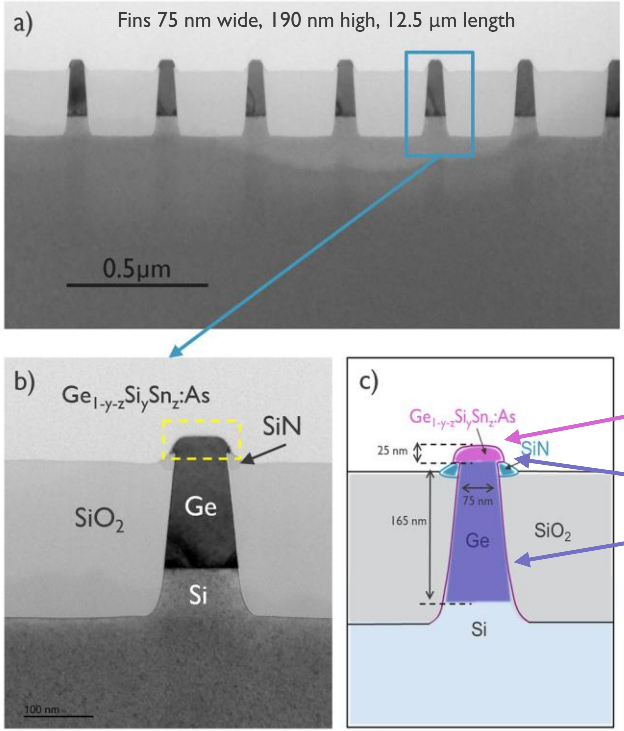
AsGe/SiGe

$AsGe/Ge_2$



Patterned sample

$Si_{0.08}Ge_{0.90}Sn_{0.02}$:As fins



As dopant quantification in SiGe(Sn):As fin region ?

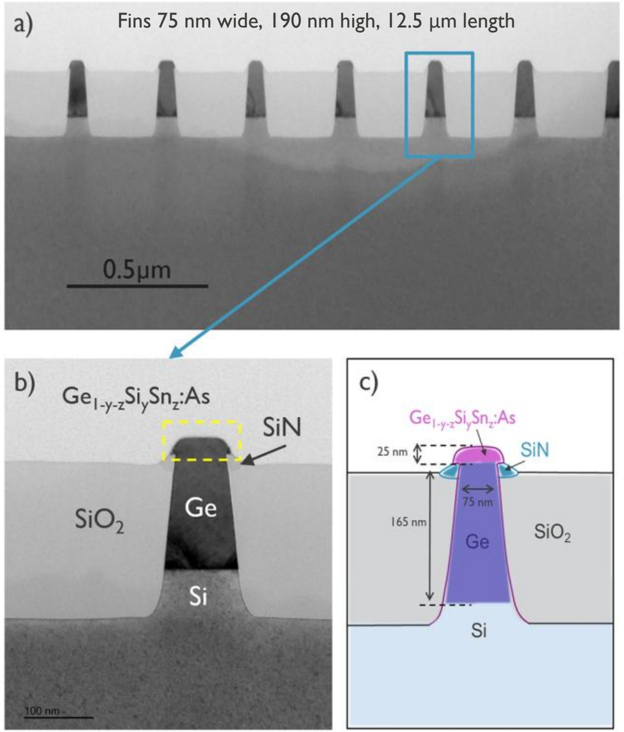
Fin bulk composition = Ge concentration in SiGe(Sn) and Ge ?

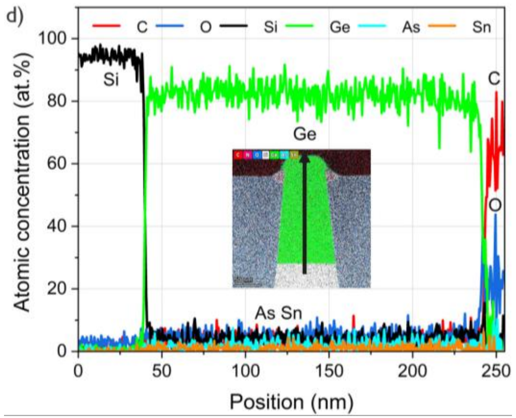
Patterned sample

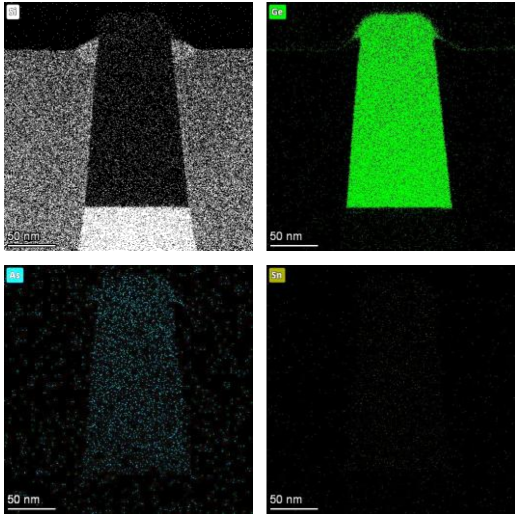
$Si_{0.08}Ge_{0.90}Sn_{0.02}$:As fins

Fin bulk composition = Ge concentration in SiGe(Sn) and Ge ?

As dopant quantification in SiGe(Sn):As fin region ?







- Si and As backgrounds throughout the whole fin
- Sn not detected
- No distinction between SiGe(Sn) and Ge regions

Patterned sample

$Si_{0.08}Ge_{0.90}Sn_{0.02}$:As fins

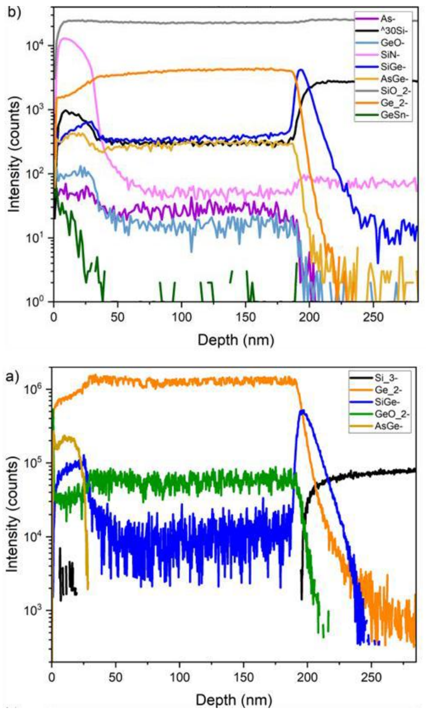
Fin bulk composition = Ge concentration in SiGe(Sn) and Ge ?

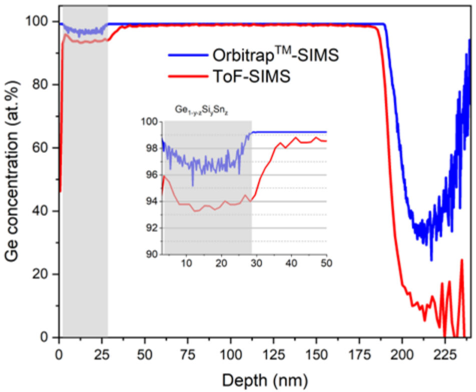
As dopant quantification in SiGe(Sn):As fin region ?

SF-SIMS Ge calib curves

ToF-SIMS

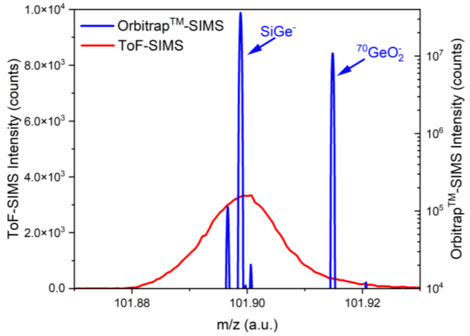
Orbitrap™-SIMS





Orbitrap™-SIMS → Ge ~97 at.% at the top

ToF-SIMS → Ge ~94 at.% at the top



Source of error in ToF-SIMS → mass interference between $SiGe^-$ and $^{70}GeO_2^-$ signals at m/z ~102 due to the presence of oxygen contamination in the fin

Patterned sample

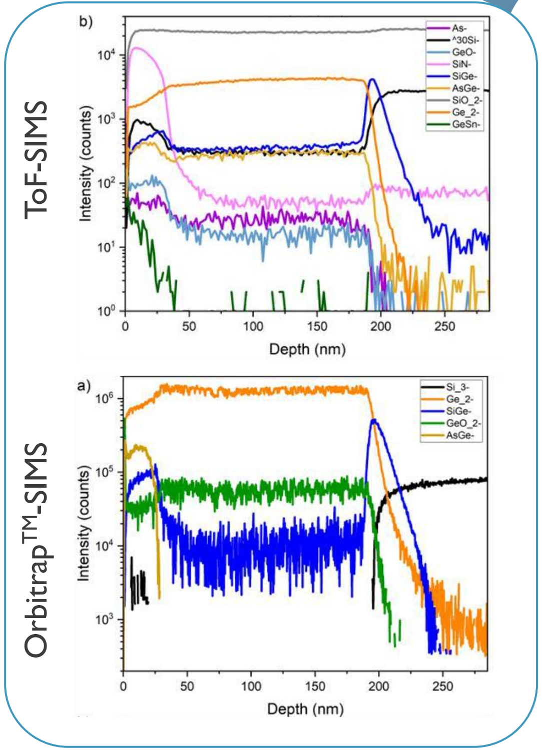
$Si_{0.08}Ge_{0.90}Sn_{0.02}$:As fins

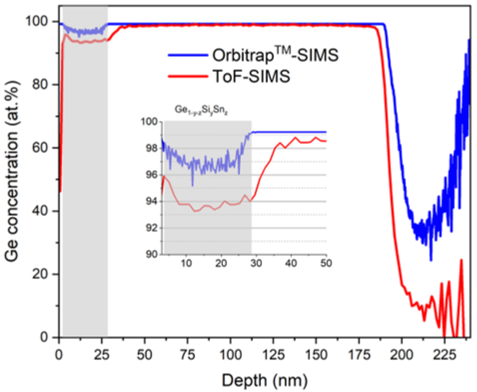
Fin bulk composition = Ge concentration in SiGe(Sn) and Ge ?

As dopant quantification in SiGe(Sn):As fin region ?

SF-SIMS Ge calib curves

SF-SIMS As calib curves





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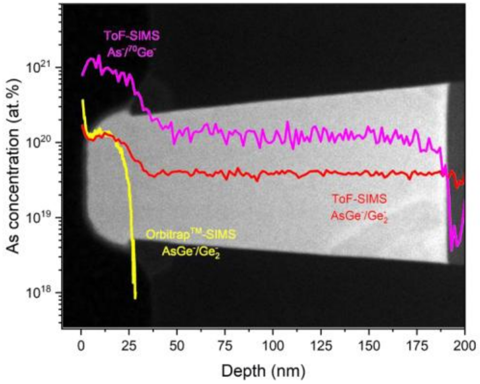

- Physically correct top-only As distribution in SiGe fin with Orbitrap™-SIMS using $AsGe^-/Ge_2^-$ (yellow curve)
- Wrong As concentration at the top and fake high background As tail far below doped region with ToF-SIMS using $As^-/^{70}Ge^-$ (magenta curve)
- Large error in As quantification in both top and bulk using ToF-SIMS using $AsGe^-/Ge_2^-$ (red curve)

Summary

- As quantification in SiGe and Ge requires high mass resolution to avoid peak interferences
- Orbitrap™-SIMS allows to reach required mass resolution to avoid peak interferences
- Using Self-Focusing SIMS in the Orbitrap™-SIMS, accurate As dopant quantification in SiGe and Ge is possible in small volumes and structured samples such as fins, GAA and cFETs
- Further improvement is to lower down the Cs sputter energy in OrbitrapTM-SIMS to reach better depth resolution required for advanced semiconductor devices such as cFETs

NPL National Physical Laboratory

Zhou Y et al.. J. Vac. Sci. Technol. A 42, 053208 (2024)

#6 Alexis Franquet / Orbitrap™-SIMS for Accurate Quantification of Arsenic in SiGe Across Blanket and Fin-Type Geometries

#45 Rita Tilmann / Quantification of P-doped Si in Advanced and confined Semiconductor Structures Using TOFSIMS, Orbitrap™-SIMS, and Self-Focusing SIMS

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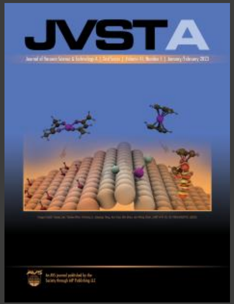

Orbitrap™-SIMS for accurate quantification of arsenic in SiGe across blanket and fin-type geometries
Rita Tilmann ; Alexis Franquet ; Alexandre Merkulov ; Lennaert Wouters ; Clement Porret ; Alexander Pirkl ; Paul van der Heide
J. Vac. Sci. Technol. A 44, 033402 (2026)
https://doi.org/10.1116/6.0005245