Defect Metrology of Epitaxial Ge on Patterned Si Wafers using an Inline HRXRD Tool

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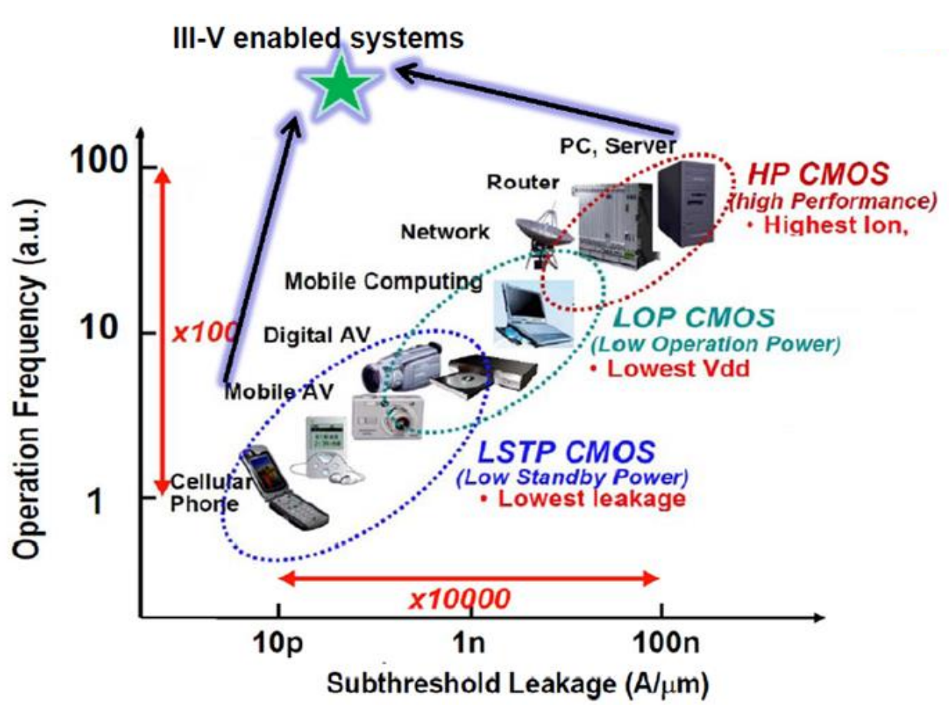
Abstract

The shift from the desktop to mobile computing devices puts ever increasing demands on CMOS technology to offer ever lower power consumption and higher performance. High mobility channel materials such as Ge and III-V are strong contenders to replace Si at the sub-10 nm technology nodes. The intrinsically higher carrier mobility and injection velocity of these materials have the potential to enable more aggressive scaling of the power supply voltage (V_{DD}) without compromising performance. These materials, however, must be integrated on Si substrates to take advantage of Si-based high-volume manufacturing (HVM) platforms. However, direct deposition of Ge or III-V on Si results in a highly defective material due to the large lattice mismatch with the Si substrate (> 4%). One promising integration approach is to use "aspect ratio trapping (ART)" where the mismatched material is grown within trenches patterned in SiO2 with aspect ratios sufficient to confine the dislocations to the lower part of the trench. With development, this is a promising approach to produce material with sufficiently low defect density for nanoelectronic devices. High-resolution X-ray diffraction (HRXRD) is an established technique for the characterization and metrology of epitaxial thin films such as Ge and III-V by the compound semiconductor industry and is also used for R&D and in-line process control in Si-based HVM. In this work we describe the use of an in-line X-ray metrology tool for the characterization of defectivity in Ge ART structures. The defect densities obtained using a novel "FastHRXRD" technique is compared to those using the more traditional reciprocal space mapping (RSM) method and are also shown to be consistent with those of transmission electron microscopy (TEM) performed on the same samples.

Introduction

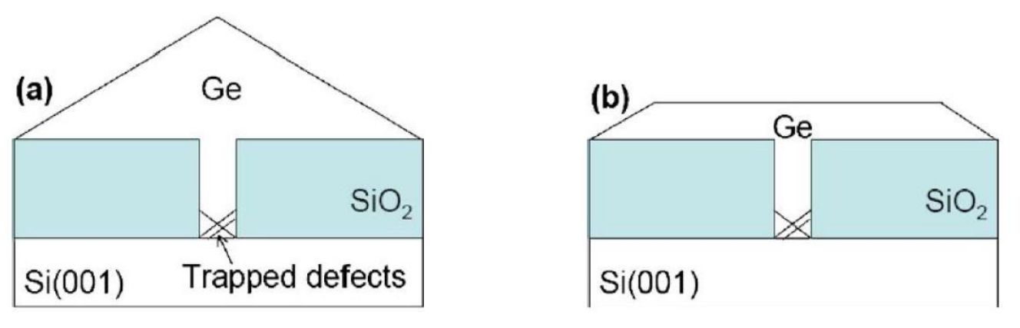
Property/ Material	Si	Ge	GaAs	$In_{0.53}Ga_{0.47}As$	InAs	Graphene
Eg (eV)	1.1	0.66	1.4	0.75	0.35	0*
μ_n (cm²/v-sec)	1,350	3,900	4,600	>8,000	40,000	>100,000
μ_p (cm²/v-sec)	480	1,900	500	350	<500	>100,000
m^*/m_o	0.165	0.12	0.067	0.041	0.024	<0.01
Lattice mismatch to Si	0	4%	4%	8%	12%	n.A
		pMOSFET		nMOSFET		

* Tunable but at cost of μ degradation

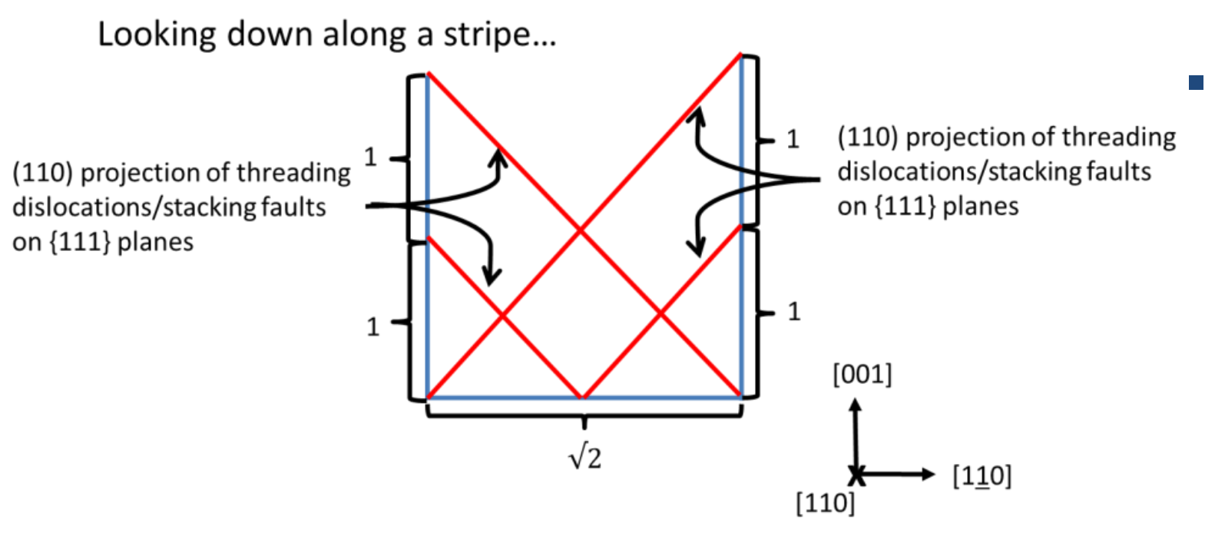


- Compound semiconductors have higher carrier mobility, narrower bandgap and lower effective mass than Si
- Ge & III-V FETs mitigate the performance and subthreshold leakage trade-off in Si CMOS
  - Excellent electrostatic integrity and scalability with robust control of short-channel effects
  - High speed performance at lower supply voltage
- Significant challenges for growth of Ge and III-Vs on Si
  - High mismatch (>4%) typically leads to highly defective films
  - Polar films on non-polar substrates -> anti-phase boundaries (APBs)

Aspect Ratio Trapping & Samples

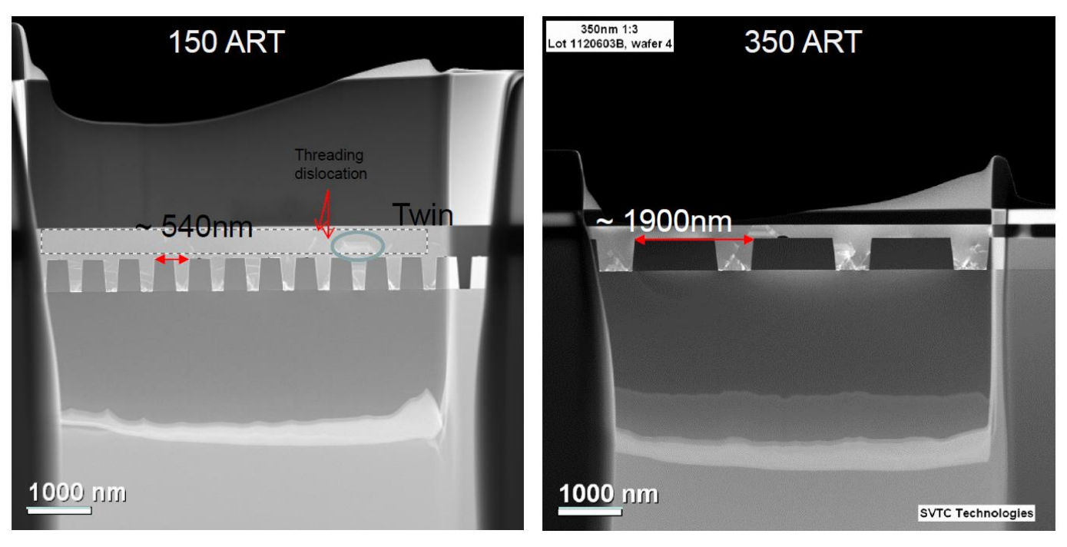


Schematic diagrams of ART structures after (a) Ge growth and overgrowth and (b) CMP [6]



- Aspect ratio (AR) requirement for dislocati trapping
  - Angle between projecti of threading segments and (001) surface is 55°
  - Need AR > $\sqrt{2} \approx 1.42$
  - Assumes defects on {11 planes and no dislocatic interactions
- For a given sidewall (oxid height, a narrower trench (150 nm) leads to a highe AR than a wider trench (350 nm) and hence bette dislocation trapping

- The ART samples were fabricated on 200 mm on-axis Si(001) substrates
- A 550 nm SiO_2 layer was first formed by thermal oxidation, followed by lithographic patterning and plasma dry etch
- Two samples (150 nm and 350 nm) with different pitches and aspect ratios were targeted

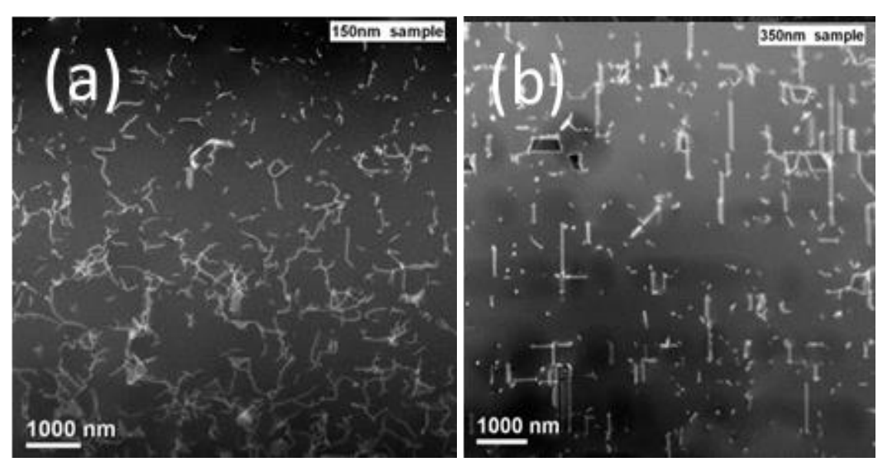


Cross section TEMs: (left) sample 150, (right) sample 350.

Sample label	Pitch (nm)	Oxide height (nm)	Trench length (um)	Aspect ratio	Coalesced layer thickness (nm)
150 nm	540	550	100	3:1	500
350 nm	1900	550	100	1:1	230

TEM Analysis

- Plan-view and cross-sectional TEMs were collected to provide complementary information about defect distribution
  - cross-sectional orientation imaged along the [110] ART axis direction gives a defect profile in the Ge from the top coalesced layer down to the bottom of the trench
  - plan-view orientation imaged normal to the surface along the [001] direction reports defects residing throughout the thickness of the TEM sample, which is on the order of 100 nm, therefore mainly revealed the defects reside in the coalesced layer
- Two types of defects were detected in the TEM images: stacking faults (SFs), which have a "boxy" appearance, and threading dislocations (TDs), which look like wavy lines on the images
  - plan-view TEMs show that threading dislocations are dominant in the narrower trench sample, whereas SFs are dominant in the wider trench sample
  - The trench width also impacts the thickness of the coalesced Ge after CMP.

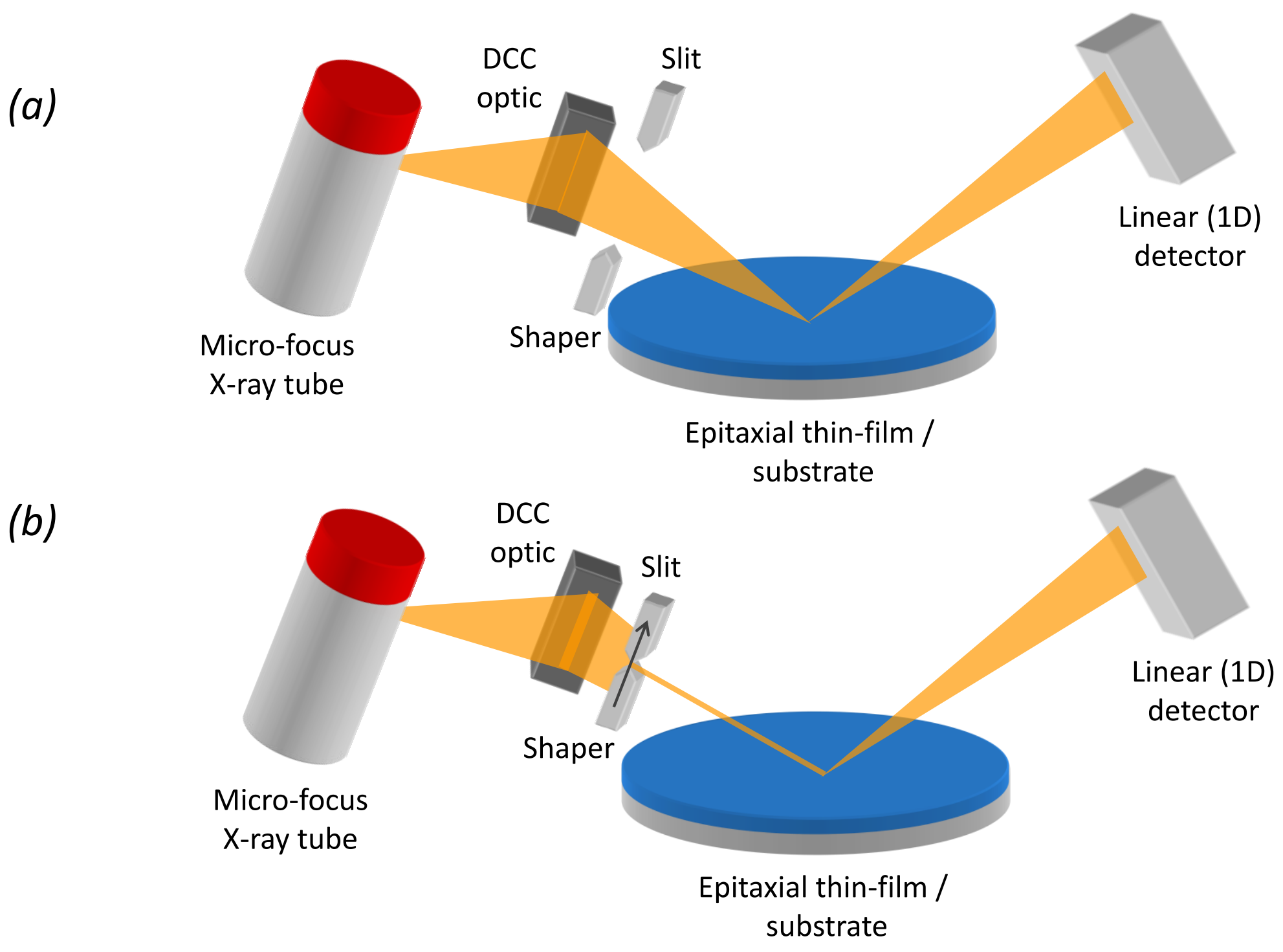


ADF-STEM micrographs of plan–view TEMs (a) sample 150, (b) sample 350.

Sample	*Defect density (cm^{-2})*
150	Cross section: 2.2 x 10^8 in top 100nm and $3x10^9$ for the coalesced Ge film Plan view: total $2x10^9$
350	Cross section: 0 in top 100nm and 2x10 ^{9} for the coalesced Ge film Plan-view: total $1.7x10^9$ (TD $3.6x10^8$, SF $1.3x10^9$)

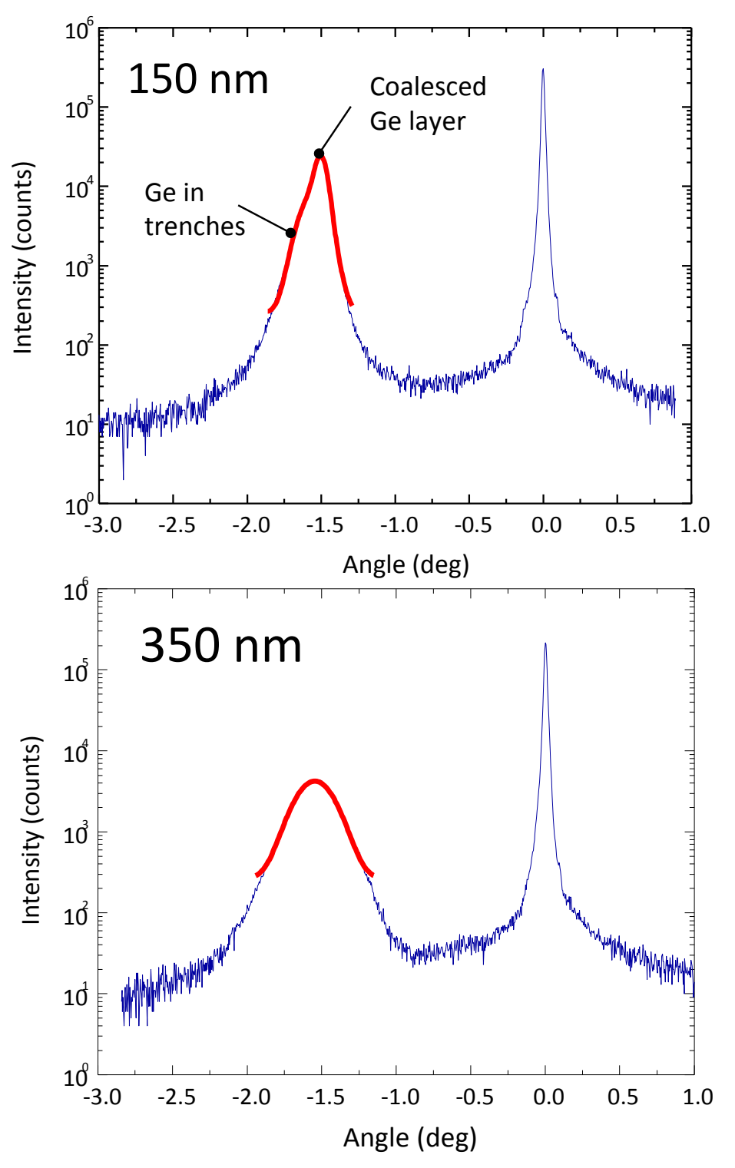
HRXRD Analysis

- HRXRD measurements were done using a Jordan Valley JVX7200 X-ray metrology tool
  - 50W micro-focus Cu X-ray tube and doubly curved crystal (DCC) optic used to produce a convergent beam focused on the sample. Beam has a convergence angle of ~4 deg and a small spot-size of ~60 µm
  - Linear (1D) detector measures the entire diffracted / reflected intensity in parallel
  - Data from small test pads on product wafers can be collected with a dramatic reduction in measurement time (about 10x) compared to conventional parallel beam diffractometers with a similar spot size
  - Fully automated measurement and analysis with various loadport options and SECS/GEM and 300 mm software
- Measurements of the symmetric 004 Bragg reflection were done using the FastHRXRD mode in which the incident beam slit was opened wide and the diffracted intensity distribution was acquired simultaneously in about 30 s
- Additionally, reciprocal space maps (RSMs) were collected by:
  - Creating a pseudo parallel beam using a narrow slit to reduce the incident beam divergence to about 0.02 deg
  - Scanning the position of this slit in the beam to adjust the incidence angle from -3 to +1 deg with respect to the substrate peak position without changing the spot position on the sample
  - Acquiring the intensity over a range of about 4 deg with the 1D detector at each step



Schematic diagrams of the Jordan Valley (a) convergent beam, FastHRXRD setup and (b) pseudo-parallel beam setup for measuring for reciprocal space maps (RSMs). A convergent X-ray beam and linear (1D) detector are used to provide rapid, small-spot measurements on product wafers.

- Symmetric 004 reflection measured with the X-ray beam perpendicular to the ART trenches
  - Typical measurement time ~30 s
  - Angular position of Ge layer peak affected by strain relaxation of material
  - Full width at half max (FWHM) can be used to assess material quality
- Diffraction signal from sample 150 is asymmetric and modeled as two Gaussian peaks
  - Weaker, broader component to the left from relaxed Ge material in the trenches
  - Stronger, narrower peak due to the coalesced Ge layer
  - Coalesced layer has small in-plane tensile strain ε_{xx} = 0.19% due to mismatch of CTE between Ge and SiO_2
- Diffraction signal from sample 350 modeled as a single Gaussian peak
  - Much thinner coalesced Ge layer



FastHRXRD diffraction data collected with the X-ray beam perpendicular to the trenches (a) top: sample 150 and (b) bottom: sample 350. The X-axis shows the angular deviation from the Bragg angle of the Si substrate.

- Defect density in the Ge from the HRXRD data was estimated using the simple model proposed by Ayers [10], which relates the FWHM of the omega rocking curve, β (rad), to the threading dislocation density, *D* (cm^{-2})

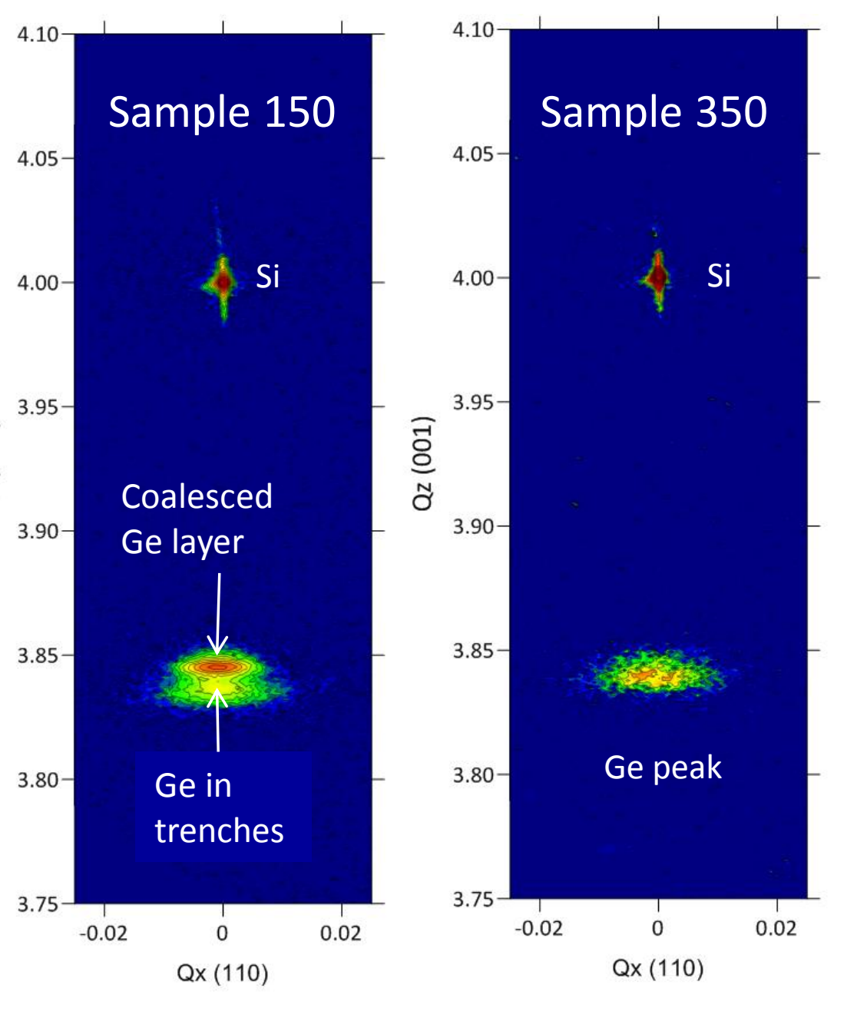
$$D \sim \frac{\beta^2}{4.36b^2}$$

where b = a/2 <110> (~ 4 Å) is the magnitude of the dislocations' Burgers vector

- *D* provides an estimate of the volume averaged defect density in the Ge under the assumption that threading dislocations are the dominant defects.
- β is defined for an ω-scan on a conventional diffractometer and not the peak width in the FastHRXRD data
  - but for reasonably thick (> 100 nm), defective layers the difference is small
- Defect density obtained by HRXRD and TEM are in reasonable agreement

Sample	*FWHM (deg) [Defect density (cm^{-2})]*
150	Coalesced layer: 0.093 [3.8 x 10^8] Trench layer: 0.205 [1.9 x 10^9]
350	0.255 [2.8 x 10^9]

- Defect density in the coalesced layer of sample 150 is one order of magnitude lower than that in the trench area, indicating defect reduction by ART



Reciprocal space maps (RSMs) around the symmetric 004 Bragg reflection from Si measured using a JVX7200 X-ray metrology tool.

- Symmetric 004 reciprocal space maps (RSMs) measured for both samples
  - Used mainly for R&D applications
  - Provides more information than FastHRXRD measurements, but the acquisition time can be long (>1 h)
- RSM for sample 350 shows that the Ge peak broadening in the FastHRXRD measurements is due to scattering in the Qx direction
  - due to tilts induced by the defects at the bottom of the trenches
- For sample 150 there is also broadening of the Ge peak in the Qz direction
  - result of the different lattice parameters of the material in the trenches and the coalesced material
- Defect densities estimated from Qx widths are within 10% of those obtained using FastHRXRD data

Summary & Conclusion

We have demonstrated the capability of an inline HRXRD metrology tool to monitor the defect density of ART samples by studying Ge ART samples with different pitches and aspect ratios. The defect density extracted from FastHRXRD is comparable to the values obtained using RSMs and TEM analysis. With a typical measurement time of ~30 seconds, this tool provides fast and non-destructive feedback to support optimization of the ART processes in the R&D phase; it is also expected to enhance fabrication yield. This study demonstrates that the trench width in the Ge ART can affect defect type and density, as well as thickness of the coalesced Ge layer. In particular, when the Ge trench width is increased from 150 nm to 350 nm, the dominant defect type changes from threading dislocations to stacking faults. The post-CMP coalesced Ge layer also becomes thinner as the trench is widened.

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