PRISMA, APS-U- R&D BEAMLINE, PTYCHOGRAPHY, VELOCIPROBE…

Stefan Vogt

Associate Division Director, X-ray Science Division, Advanced Photon Source
Principal Science Advisor, APS upgrade
Adj. Assoc. Professor, Feinberg School of Medicine, Northwestern University
COHERENT DIFFRACTIVE IMAGING

**Lensless method**

Resolution $\sim \lambda / \text{angular size}$ limited only by wavelength and signal

- Two-step process: record coherent diffraction pattern, recover object structure numerically (iterative phase retrieval)
- Sensitive to phase as well as absorption of the specimen
- Get 3D by tomographic methods; no depth of field limit
- But: must assume some information to recover phase, e.g. known object extent or illumination profile

---

WHAT IS PTYCHOGRAPHY?
WHAT IS PtyCHOGRAPHY?

X-ray beam

lens

sample

diffraction pattern
WHAT IS PTYCHOGRAPHY?
FROM DIFFRACTION PATTERN TO IMAGE: PHASE RETRIEVAL

- Iterate between real & reciprocal space
- Reconstruct sample, beam (composed of coherent modes)
CRYO-PYTCHOGRAPHY & XRF OF CHLAMYDOMONAS REINHARDTII

- 5.2keV, 70nm ZP, 167x151 Cartesian grid
- 0.5s exposure, 6.5h measurement
- white spots beam damage (not careful)
- ~20 nm resolution

=> Beautiful structural visualization, strong contrast

Junjing Deng et al., PNAS 2015

TXM: Hummel et al, PLOS One, 2012
Chip structures

The IARPA RAVEN Program
(Rapid Analysis of Various Emerging Nanoelectronics)

Ptychography-based Rapid Imaging of Nano-structures with Multi-layer Assemblies (PRISMA)
## RAVEN/RAVEN: Goals/Metrics

<table>
<thead>
<tr>
<th>Metric</th>
<th>Phase-1 per BAA</th>
<th>Phase 2</th>
<th>Phase 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>IC Area</td>
<td>1 cm²</td>
<td>1 mm²</td>
<td>1 cm²</td>
</tr>
<tr>
<td>Duration/Goal</td>
<td>24 months – Develop Test Bench Tool</td>
<td>24 months – Develop Test Bench Tool</td>
<td>24 months – Develop Alpha Prototype</td>
</tr>
<tr>
<td>Time</td>
<td>80 days to acquire images and reconstruct all circuit layers with &gt;90% accuracy</td>
<td>80 days to acquire images and reconstruct all circuit layers with &gt;90% accuracy</td>
<td>40 days to acquire images and reconstruct all circuit layers with 100% accuracy</td>
</tr>
<tr>
<td>Lateral Resolution</td>
<td>20 nm</td>
<td>20 nm</td>
<td>≤ 10 nm</td>
</tr>
<tr>
<td>Vertical Resolution</td>
<td>20 nm</td>
<td>20 nm</td>
<td>≤ 10 nm</td>
</tr>
<tr>
<td>Metal Layers</td>
<td>≤ 13</td>
<td>≤ 13</td>
<td>≤ 13</td>
</tr>
<tr>
<td>Reproducibility</td>
<td>-</td>
<td>-</td>
<td>95%</td>
</tr>
<tr>
<td>Test Articles</td>
<td>Bare die ≥ 14 nm feature size</td>
<td>Bare die ≥ 14 nm feature size</td>
<td>Bare die, 10 nm feature size</td>
</tr>
<tr>
<td>IC Thickness</td>
<td>≥ 50 μm</td>
<td>≥ 50 μm</td>
<td>50 - 200 μm</td>
</tr>
</tbody>
</table>

Both resolution and timing are very challenging goals/metrics. To meet them, it requires special imaging equipment (monochromator, microscope, detector, etc.), a powerful x-ray source with substantial photon flux, and powerful advanced computing resources.

10x10x0.1mm³ => 10PB @ 1 byte greyscale
Early Data on 22 nm Technology

Sockel LGA 1150, 3MB Cache, 22nm, 53Watt, inkl. GMA HD Grafikkern (350/1100 MHz GPU), Intel HD, inkl. Cooler

Paul Scherrer Institute

Inhomogeneous polishing trying to remove copper layer and interconnects

Copper & interconnects
Active layer
Silicon

~10 µm cylinder
Early Data on 22 nm Technology

Paul Scherrer Institute
Early Data on 22 nm Technology

3D resolution 14.6 nm
DOI:10.1038/nature21698

Normal incidence tomography, limited to small sample volumes.

Paul Scherrer Institute
PRISMA Program - Overview

TEAM DESCRIPTION
Performers:
• USC’s Information Sciences Institute (ISI) and Dep. of Electrical Engineering – Prime
• Northwestern University’s EE Dept. - Sub
• Stanford University’s EE Dept. - Sub
• Paul Scherrer Institute (PSI) - Sub
Collaborators:
• Intel Corporation
• Argonne’s Advanced Photon Source (APS)

APPROACH
• Non-destructive X-ray IC imaging of 1 cm\(^2\) bare die up to 50 µm thick.
• Coherent Diffraction Imaging (Ptychography) X-ray and novel HPC algorithms.
• Use of IC collateral/available information to tune the imaging process parameters, and expedite the image acquisition process.
• Construction of a CDI-tailored microscope, detector, and high-efficiency FZPs.

EXPECTED RESULTS
• PHASE-1:
  ➢ 2D and 3D X-ray imaging of 1 mm\(^2\) bare IC die.
  ➢ Establishment/completion of a RAVEN-centric X-ray endstation at ANL’s APS.
  ➢ Imaging algorithms and HPC infrastructure.
• PHASE-2 & 3:
  ➢ 2D and 3D imaging of 1 cm\(^2\) bare IC die up to 50 µm thick.
  ➢ Full engagement of integrated X-ray endstation at ANL’s APS for experiments.

SCHEDULE AND STATUS
• IC specimens for initial experiments currently available (Intel-provided).
• Initial X-ray endstation and companion instrumentation currently available.
• Initial experiments: June, 2017 (starting).
• Completion of RAVEN-centric X-ray endstation 24 months ACA (end of Phase-1).
• Integration of PSI-provided instrumentation at ANL’s APS: 32 months ACA.
• Phase-2 & -3 experiments: Starting 36 mos. ACA

1. Argonne APS collaboration/involvement in PRISMA is “GFE” per BAA’s instructions.
PRISMA@APS

- Prisma will access APS through either CDT or PUP
- Early access (2017 & 2018) on existing instrumentation (Velociprobe - up to 30% of available time)
  - Early experiments and data
  - Develop / prototype analysis pipeline
- Build new beamline with APS/APS-U/Prisma resources
  - Prisma will be installed at sector 28 of APS
    - Assembling package for procurement of hutches at Sector 28
    - Expect award by 6/30/2017
- Prisma @ S28 Online 2019
  - 30% beamtime dedicated to Prisma
  - Planning to optimize for high stability, high flux
  - H-DMM planned
THE VELOCIProbe
Early Access: Velociprobe

Goal:
- To push speed limit for scanning, while retaining high stability and position control
- Ptychography: 10 nm and below
- Fluorescence: 50 nm and below

Note: focus on 2D images, but tomography capable (not laminography)

Concept:
- Ultra-stable granite coarse stages
- Fast scanning of zone plate
- Low-noise, high-bandwidth, interferometer-encoded control
VELOCIPROBE INSTALLED AT 2-ID-D

- 2-ID-D and 2-ID-E operate in parallel
- 2-ID-D:
  - Microfluorescence: 100-200 nm beam
  - New velociprobe instrument
- 2-ID-E: Microfluorescence: 300 nm beam
- Shared beam defining slits
- 2x 3.3cm Undulator (collinear)
- Mirror (Si, Rh, Pt stripes)
- For 2-ID-D: DCM & DMM
First experiments

Optics
- Zone plate: 180 um diameter, 50 nm outmost width
- Beam stop: 65 um
- OSA: 30 um

Scans
- 40 nm step size
- 50 ms /point
- 8 keV x-rays

Ge particles
- Highly promising anode materials for lithium-ion batteries.
- Particle size: 500 nm – 5 um

Reconstruction
- Ptychographic image: 12.5 nm resolution
- Focused beam: 58 nm FWHM

Reconstruction: 19.2 nm resolution
VELOCIPROBE TIMELINE:

- Installed in January 2017
- Initial commissioning 2017-1 cycle (Feb-Apr)
- 2017-2 (Jun-Aug): continue commissioning + friendly 1\textsuperscript{st} users
  - Prisma 3-6 days as required

Tentative plan 2017-2:
- May 31\textsuperscript{st} – June 5\textsuperscript{th} : commissioning
- June 13\textsuperscript{th} – June 19\textsuperscript{th} : commissioning
- July 8\textsuperscript{th} – July 14\textsuperscript{th} : Prisma
- July 25\textsuperscript{th} – July 31\textsuperscript{st} : tbd
- August 9\textsuperscript{th} – 22\textsuperscript{nd} : tbd

- 2017-3 (Oct-Dec): open to GU
  - Prisma 3-6 days as required
- 2018-1: GU, Prisma 3-6 days as required
- 2018-2: GU, Prisma 3-4 weeks as required
- 2018-3: GU, Prisma 4-5 weeks as required
  - ‘end’ of prisma CDT at 2-ID
- 2019-1: sector 2 down for canting (change from original plan)
- 2019-2: sector 2 commissioning (LN2 mono, HDCM, …), friendly users
- 2019-3: GU operations
Key points during phase 1

- developing data analysis pipeline, up to 20Gb/s for phase 1, 60Gb/s for phase 2 & 3
- ZPs are chromatic lenses – how well do they work for ptychography with a multilayer monochromator?
  - Alternatives: capillary optic; narrow bandwidth multilayer
- ZP parameters (size and beam divergence)?
- Tradeoff flux vs degree of spatial coherence?
- Tradeoff illumination area vs sampling frequency?
- Acquire data in ‘tiles’ – what is the ideal tile size (100x100 um²) for acquisition, processing, etc?

- Design / develop hutch (S28) for phase 2
PRISMA ENDSTATION @ S28 (APS-U R&D BL)
Sector 28 timeline:
- September 2017: award of hutch procurement
- 2017/2018: construction
- Oct 2018: shielding verification of FOE
- Oct-Dec 2018:
  - installation of BL optics (monos, etc)
  - begin commissioning
- Feb-Apr 2019: ready for installation of Prisma endstation instrument
Status of the End Station Instrument

Sample scanner and rotation

Interferometry

Paul Scherrer Institute
EIGER detector: Characteristics

Single-photon counting with hybrid pixel detectors: No background and no readout noise, high dynamic range.

Key parameters:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pixel size</td>
<td>75 x 75 (\text{um}^2)</td>
</tr>
<tr>
<td>Counter</td>
<td>4/8/12 bit</td>
</tr>
<tr>
<td>Chip frame rate</td>
<td>23/12/8 kHz</td>
</tr>
<tr>
<td>Dead time between frames</td>
<td>3 (\text{us})</td>
</tr>
<tr>
<td>Min. threshold (high frame rate)</td>
<td>4.5-5 keV</td>
</tr>
<tr>
<td>Threshold dispersion (after trimming)</td>
<td>&lt; 50 eV</td>
</tr>
<tr>
<td>Noise</td>
<td>350-700 eV RMS</td>
</tr>
</tbody>
</table>

Paul Scherrer Institute
DATA ACQUISITION CONSIDERATIONS:

- Assume detector operates at 13kHz: 1.1e9 measurements / day, or 2.25e10 measurements in 20 days.
- Distance between measurement spots: 0.66 microns
  \[
  \text{Distance} = \frac{10\times 10000}{\sqrt{2.25\times 10^{10}}} = 0.66
  \]
  This assumes we need 10 projections, each of which is 10x10 mm
- 66% overlap: 2 micron spot size, 50% overlap 1.3 um spot size, 5 nm resolution, 10 keV

<table>
<thead>
<tr>
<th>Oversample</th>
<th>probe size (um)</th>
<th>pixel</th>
<th>distance (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5</td>
<td>2.0</td>
<td>1400</td>
<td>4.23</td>
</tr>
<tr>
<td>3.8</td>
<td>1.3</td>
<td>1000</td>
<td>3.85</td>
</tr>
<tr>
<td>5</td>
<td>2.0</td>
<td>2000</td>
<td>6.05</td>
</tr>
<tr>
<td>5.4</td>
<td>1.3</td>
<td>1400</td>
<td>4.23</td>
</tr>
</tbody>
</table>
POTENTIAL APPROACHES

‘easier to implement’:

- Reconstruct local 2D patches, say 50x50 um = 5700 measurements, 
  = 8.6 GB in 0.45s
- Throw away data
- Stitch 2D patches into one large 2D projection
- Reconstruct global 3D data set based on ~10 full projections

Better quality reconstruction ?

- Reconstruct local 3D volumes, local tomography based on ptychography, eg, 50x50umx10 projections= 57000 measurements, 
  86GB in 4.5s.
- Throw away data
- Stitch 3D patches into final 3D dataset.
REASONING

- $2.1M in equipment money
  - Includes hutch to be used for CHEX later
- 2 FTEs starting in year 2,3
- Helps us push technology and methods that will be directly relevant for APS-U
  - Consistent, fast data handling
  - Data analysis
  - Lensless imaging

no commitment after 5 years
APS MBA UPGRADE

Brightness vs. x-ray energy

- Brightness increases of 100x and more compared to what we have today
- Micro/nanoprobes directly brightness driven
  ⇒ possible to get nearly 100% of APS flux into a 0.3x0.25 um spot!!!
  ⇒ 5nm and below for elemental mapping and with CDI/Ptychography

This upgrade will revolutionize scanning probe microscopies…
ACKNOWLEDGEMENTS

- J. Deng, C. Roehrig et al, Microscopy group, Argonne
- V. De Andrade, Imaging group, Argonne
- J. Damoulakis et al, USC
- D. Gursoy, Computational X-ray Science Group, Argonne
- Youssef Nashed, Ollie Cossairt, Aggelos Katsagelos, Northwestern
- Piero Pienetta, SLAC
- Chris Jacobsen, APS/NU
- Tony Levi, Richard Leahy, USC
- Oliver Bunk, Mirko Holler et al, PSI

Financial support:
- Department of Energy (Basic Energy Science)
- National Institutes of Health (NIBIB, NIGMS)
Thanks!