Frontiers of High Throughput Material Science

C. Lavoie, J. Jordan-Sweet, Conal Murray, Simone Raoux, B. Yang and Team...
Summary

- **Background and Challenge:**
  - Reduction trends → Increasing importance of materials
  - Feature size now → Increasing importance of surface/interfaces

- **IBM Current Synchrotron Capabilities:**
  - In situ phase formation during annealing
  - Full texture determination and phase identification through pole figure measurements

- **Example – Contacts to Si CMOS devices:**
  - Moving from yield to performance oriented integration
  - Importance of measuring in relevant dimensions

- **Future → more problems in sight**
  - Need for faster and easy to use characterization/optimization tools
  - Automation and remote access
End of Classical Scaling

Evolution of Predictions
Gate Width

Scaling now decreases performance
Performance gains now through innovations and materials improvements
Synchrotron X-Ray Diffraction

In Situ during annealing

Full texture determination
Pole figure Measurements

Can measure up to 4 samples/ hour
28 000 measurements over the past 15 years
IBM Device Contact Evolution

- **C54-TiSi₂**
- **NiSi** and **NiPtSi**
  - Low temperature formation \(\rightarrow\) Ni diffusion
  - But low temperature agglomeration (<600°C)
  - Stabilization through Pt additions and I/I
- **CoSi₂** - Important Si diffusion
  - Extreme sensitivity to oxygen

**Vacancies in Si**
- Void formation for size < 50nm

**NiSi (103) Pole Figure**

**Ni alloy - Si**
- Alloying for increased thermal stability

**ITRS predicted end of NiSi**

**C54-TiSi₂ Nucleation**
- Limited for < 0.25 um.
- Fixed through alloying with Nb or Ta

**Poly-Si Gate Width**
- 100 nm

**Resistance (arb. units)**
- 1 to 100

**Scattered Intensity or Resistance (arb. units)**
- 0 to 2

**Diffracted Angle**
- \(2\theta\) (deg)
- 0 to 50

**Technology Node (nm)**
- 250 to 15

**Figure**
- (a) Pure NiSi
- (b) Ni alloy - Si
Nickel Silicide Optimization

YIELD / RELIABILITY

Maintain Film Morphology
- Reduced film thickness
- Reduced dimensions

Reduce defectivity
1. Thermal instability
   → axiotaxy
2. Encroachment
   → fast diffusion of Ni on defects
3. Presence of theta phase in sequence
   → Roughness / fast growth of NiSi
4. Formation stress defects
   → Roughness in localized volumes
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Diffusion on DISLOCATIONS

Diffusion on EOR Defects

Standard Si orientation
45° wafer rotation
**Nickel Silicide Optimization**

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![Phase Sequence – 10 nm Ni / SOI](image_url)

- Ni
- \(\delta\)-Ni\(_2\)Si (013)
- \(\theta\)-Ni\(_2\)Si (110)
- NiSi
- \(\delta\)-Ni\(_2\)Si (020)

Temperature (°C)

- 3 °C/s in He

Roughness

Example: 100 nm Ni / Si(100)
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Ni Alloys

- Retard Agglomeration
- Retard NiSi$_2$ Formation
- Limit Axiotaxy

<table>
<thead>
<tr>
<th>Ti</th>
<th>V</th>
<th>Cr</th>
<th>Mn</th>
<th>Fe</th>
<th>Co</th>
<th>Ni</th>
<th>Cu</th>
<th>Zn</th>
<th>Ga</th>
<th>Ge</th>
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</thead>
<tbody>
<tr>
<td>Zr</td>
<td>Nb</td>
<td>Mo</td>
<td>Tc</td>
<td>Ru</td>
<td>Rh</td>
<td>Pd</td>
<td>Ag</td>
<td>Cd</td>
<td>In</td>
<td>Sn</td>
</tr>
<tr>
<td>Hf</td>
<td>Ta</td>
<td>W</td>
<td>Re</td>
<td>Os</td>
<td>Ir</td>
<td>Pt</td>
<td>Au</td>
<td>Hg</td>
<td>Tl</td>
<td>Pb</td>
</tr>
</tbody>
</table>

Limit Axiotaxy

- Pure Ni
- Ni 5% Pt
- Ni 10% Pt

Pole Figures

- Pure NiSi
- NiSi with Pt
Silicide Optimization

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**DEVICE PERFORMANCE**

ITRS 2009

Silicide to Si Contact resistivity ultimately becomes the dominant component of the overall parasitic resistance.

Reduction of this contact resistivity requires:
1. Max dopant concentration in Si
2. Reduction in barrier heights through substrate or contact modifications
3. Possible use of Schottky contacts (also used for junctions)?
**Contact Resistance – $R_C$**

In most measurements, $R_C \rightarrow$ part of overall resistance

Other R elements are known $\rightarrow R_C$ inferred

\[
\rho_c = \frac{k}{qA^*T} \cdot c_{FE} \cdot \exp\left[\frac{\phi_b}{E_{00}}\right]
\]

\[
E_{00} = \frac{h}{4\cdot\pi} \cdot \sqrt{\frac{N_d}{\varepsilon_s \cdot m_t}}
\]

\[
\rho_c \sim \exp\left[\frac{\Phi_B}{(N)^{1/2}}\right]
\]

$\Phi_b$ : Schottky barrier height

$N$ : Dopant density
Barrier Heights – Metal Silicides Binary compounds

- Process window established and contact R tested
- NiPt silicide can be engineered to ~ 50 meV of band edge
How about sizes and texture?

\[ \rho_c = \frac{k}{qA^*T} \cdot c_{FE} \cdot \exp \left( \frac{\phi_B}{E_{00}} \right) \]

\[ E_{00} = \frac{h}{4 \cdot \pi} \cdot \sqrt{\frac{N_d}{\varepsilon_s \cdot m_t}} \]

- In most measurements, \( R_c \) → part of overall resistance
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\[ \rho_c \sim \exp \left[ \left( \frac{\Phi_B}{N^{1/2}} \right) \right] \]

\( \Phi_B \): Schottky barrier height
\( N \): Dopant density
Type of textures

Random texture

Fiber texture

Axiotaxial texture

Epitaxial texture

MOST STABLE FILM

Highly Anisotropic Material

- Different interface orientation have different diffusion behavior and Schottky barriers
- Huge anisotropy may cause grain growth, voiding and texture changes
- Different texture components will have different agglomeration and stressing behaviors

Young's Modulus

<table>
<thead>
<tr>
<th></th>
<th>Coefficient of thermal expansion (10^{-6})</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>+ 42</td>
</tr>
<tr>
<td>b</td>
<td>- 43</td>
</tr>
<tr>
<td>c</td>
<td>+34</td>
</tr>
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</table>

b-axis shows thermal contraction

Recent Developments

- **Full texture determination**

- **Analysis and Fitting software**
  - Full fit of all planes and diffraction angles

Unambiguous phase indexation and grain orientation:

Ni-Pt / Si-Ge

6 hours → 640 pole figures
Recent Developments

- **New Test Site** - large enough for xray beam
  - (~3 x 5 mm chiplets various dimensions reaching below 30 nm)

  - PHASE FORMATION
  - STRESS
  - TEXTURE

Silicide phase formation temperature increases for decreasing linewidths.
NiSi texture in nano-dimensions

Pt was used to eliminate axiotaxy in NiSi. With narrow dimensions, axiotaxy returns
Requirements for the Future Microelectronics Industry

- Applicable to wide range of materials
- Fast acquisition and analysis → must get more in shorter time
  - Less access time
  - Shorter learning cycles
- Straightforward Techniques and Analysis
  - Multiple potential users if learning/analysis is rapid
- Timely access
  - Need to solve problems as they appear. Regular window for access.
- Remote Access
  - IBM Research → world wide.
  - Regular web access → train more engineers.
X20C upgrade → CLS Brockhouse and NSLS-II

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Time-resolved XRD for phase transformations and texture evolution in thin films and nanostructures

Three in-situ probes in real time: resistivity, XRD and light scattering
Robotic sample changing, automated pumpdown and purge with purified gases
Rapid thermal annealing up to 1100°C

<table>
<thead>
<tr>
<th>Fast linear detector for phase transformations</th>
<th>MMPAD area detector for fast texture evolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>640 pixels, 80mm long</td>
<td>512x256 pixels,</td>
</tr>
<tr>
<td>$10^7$ max cps</td>
<td>$10^8$ dynamic range,</td>
</tr>
<tr>
<td>30 msec readout</td>
<td>20-500 fps (1.5 msec readout)</td>
</tr>
</tbody>
</table>

Matlab script analysis:
integrated or peak-fitted regions vs temperature or time,
derivatives for transition temps,
Avrami analysis,
conversion of pole figures to ODF?
tie-in to PDF files for phase ID?

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θ

2θ

chamber

added partial chi arc

flange clamping apparatus, slides in and out to remove flange on chamber for sample changing

2 rails for guiding flange clamping apparatus
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