Towards Automatic Control of STEM Microscopes

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1. Introduction
Why is automatic control needed in electron microscopy?

- STEM applications:
  - material science research
  - nanotechnology
  - biology

- STEM operation requires repetitive manual tasks.
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Research goals

- This work is part of the CONDOR project at the Embedded Systems Institute (www esi nl)

- Its goal: To develop flexible, quantitative, nano-measuring STEMs

- DCSC research goals:
  - Modeling framework for image-based STEM control
  - Image-based sensor for defocus control
  - Introduce STEMs as a new application area
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  • Modeling framework for image-based STEM control
  • Image-based sensor for defocus control
  • Introduce STEMs as a new application area
2. STEM operation

Principle of operation

- A thin electron beam is generated with a FEG and an objective aperture.
- The beam can be displaced by deflector coils.
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- The upper objective lens forms a small probe (5nm).
- Its scattering forms a diffraction pattern (DP).
- The DP is projected on dark (HAADF) or bright (BF) field sensors.
- The image is formed by rastering the probe.
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Image formation process

- Image formation assumptions:
  - All lenses are ideal except the objective lens.
  - The specimen is thin (20nm).
  - Images are formed on a plane orthogonal to the optical axis.
2. STEM operation

Image formation process (cont.)

- Images record the wave, $\psi$, of the electrons exiting the specimen:

$$\psi : \mathbb{R}^2 \times \mathbb{R} \rightarrow \mathbb{R}$$

$$(r, t) \mapsto \psi(r, t) = \phi(r)p(r, t)$$

where

- $\phi(r)$: specimen’s transmittance function
- $p(r, t)$: point spread function
2. STEM operation

Image formation process (cont.)

\[ p(r, t) \triangleq \mathcal{F}^{-1} \left\{ A(q) e^{j\pi (0.5C_s \lambda^3 |q|^4 - \Delta f(t) \lambda |q|^2)} \right\} \]

- \( A(q) \) models the objective aperture.
- \( C_s \) and \( \Delta f(t) \) are the strengths of the lens aberrations.
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![Diagram of STEM operation](image)
2. STEM operation

Image formation process (cont.): Image models

- **Bright field images**: $I_{bf}(r, t) = |\phi(r) \ast p(r, t)|^2$

- **Diffractograms**: $I_{dif}(q, t) = |\mathcal{F}\{I_{bf}(r, t)\}|^2$
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Framework goal

- To enable image-based STEM control
  - deflector coils, objective lens, specimen holder

- Example: microscope alignment:
  - Force the electrons to fly parallel to the optical axis
  - Correctly position the electron probe and the specimen
  - Regulate optical aberrations (e.g., defocus regulation)
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Modeling framework

- Models for each block are not readily available.
- First-principles modeling may not be feasible.
- Model identification is preferred.

As an initial approach, consider defocus regulation.

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Modeling framework (cont.): Defocus regulation

- Objective: $|Δf(t) - Δf_{ref}| < ε$, $∀t ∈ ℝ^+$, $ε > 0$. 
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Modeling framework (cont.): Defocus regulation

- Objective: $|\Delta f(t) - \Delta f_{ref}| < \epsilon$, $\forall t \in \mathbb{R}^+$, $\epsilon > 0$. 

![Diagram of STEM modeling framework]
4. Defocus Sensor

Sensor properties

- Defocus is measured in two steps

1. An experimental bright-field image (EBFI) is acquired.
2. An estimate, $\Delta \hat{f}(t)$, is computed from the image.
   - A defocus guess, $\Delta f_g(t)$, is needed.

- Assumptions

  - $\Delta f(t)$ is constant during the image acquisition.
  - EBFI acquisition and processing takes $\tau$ sec.
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Sensor properties (cont.)

- This leads to:

\[
\Delta \hat{f}(t) = \begin{cases} 
\Delta f(0), & t \in [0, \tau), \\
h(\Delta f(n\tau), \Delta \hat{f}(n\tau)), & t \in [(n + 1)\tau, (n + 2)\tau), 
\end{cases} 
\]

\[n = 0, 1, \ldots,\]

where the **sensor function** \( h : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R} \) with action

\[h : (\Delta f, \Delta f_g) \mapsto \Delta \hat{f} = h(\Delta f, \Delta f_g),\]

describes the estimation algorithm.
4. Defocus Sensor

The estimator

- The estimator was developed by Coene & Denteneer.
  - It uses experimental diffractograms of amorphous materials.
    - $\phi(r)$ is modeled as a zero mean i.i.d. process.
    - Their expected value is
      $$\mathbb{E}\{I_{dif}(\bar{q}, t)\} = \delta(\bar{q}) + 4[\kappa A(\bar{q}) \sin(\chi(\bar{q}, t))]^2.$$
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4. Defocus Sensor

The estimator (cont.)

- Ideal zero location: solve for $\ell$ in

$$0.5C_s \lambda^3 \ell_i^4 - \Delta f(t) \lambda \ell_i^2 = n_i.$$

- If $\hat{\ell}_i$ are estimates from data, then $\hat{\Delta f}$ is found by minimizing

$$J = \sum_{i=1}^{N_r} |0.5 \hat{C}_s \lambda^3 \hat{\ell}_i^4 - \hat{\Delta f} \lambda \hat{\ell}_i^2 - n_i|^2$$
4. Defocus Sensor

The estimator (cont.)

- The whole procedure was then automated.

- It was tested on 6 calibrated EBFI
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<table>
<thead>
<tr>
<th>Operator $\Delta f_{op}$</th>
<th>Automated Estimator $\Delta \hat{f}$ for $\Delta f_g = \Delta f_{op} - 50\text{nm}$</th>
<th>Automated Estimator $\Delta \hat{f}$ for $\Delta f_g = \Delta f_{op} + 100\text{nm}$</th>
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<tbody>
<tr>
<td>158.3nm</td>
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<td>288.5nm</td>
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<tr>
<td>350.1nm</td>
<td>357.5nm</td>
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The estimator (cont.): The sensor function $h$

- Multiple EBFI are needed to characterize $h$.
  
- Not practical. Instead: simulated diffratograms (SD).
  
  - 50 sets of 15 SD with $\Delta f \in [70\text{nm}, 350\text{nm}]$
  
  - $\hat{\Delta f}$ was estimated using $\Delta f_g \in [-180\text{nm} + \Delta f, 180\text{nm} + \Delta f]$.  

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The estimator (cont.): The sensor function $h$ (cont.)

\[ \Delta \hat{f} \text{ for } \Delta f_g \leq \Delta f \]

\[ \Delta \hat{f} \text{ for } \Delta f_g \geq \Delta f \]

$\Delta \hat{f} = 1.0296 \Delta f - 2.6806n$m
4. Defocus Sensor

The estimator (cont.): The sensor function $h$ (cont.)

- Results: When $\Delta f \in [100\text{nm}, 350\text{nm}]$ and $\Delta f_g > \Delta f$

  \[ h(\Delta f, \Delta f_g) = 1.0296\Delta f - 2.6806 \times 10^{-9} \]

  - This was obtained via linear data fit.
    
    - Maximum fit error of 9.28nm.
    
    - Thus: $|\Delta \hat{f} - \Delta f| < 7.68\text{nm}$

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Conclusions

- STEMs are complex machines in need of automation.
  - They constitute a new challenging application area.

- A new control-oriented STEM modeling framework was introduced, together with an image-based defocus sensor.
  - Research is ongoing to improve the sensor response.
  - The sensor has been used to identify the objective lens model.