A two-stage method for crystal image analysis via synchrosqueezed transforms (SSTs) and variational optimization

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Atomic crystal image analysis:
Crystal segmentations, crystal rotations, crystal defects, crystal deformations.

Figure: Left: A PFC image with a zoomed-in image detailing the part marked by a black rectangle. Right: A TEM-image in GaN. Courtesy of David M. Tricker.
Atomic material evolution:

Crystallization, Ostwald ripening, or processes of elastic and plastic deformation

Figure: From top to bottom: time evolution of local volume distortion and grain boundaries.
Mathematical model

\[ f(x) = \sum_{k=1}^{M} \chi_{\Omega_k}(x) (\alpha(x)S(2\pi N \phi(x))) + c(x). \]

**Figure**: Left: An example of a crystal image. Right: Windowed Fourier transform at a local patch indicated by a rectangle.
Analysis goals:

\[ f(x) = \sum_{k=1}^{M} \chi_{\Omega_k}(x) (\alpha(x) S (2\pi N \phi(x)) + c(x)). \]

- Grain segmentation \( \Omega_k \) and grain boundary \( \partial \Omega_k \);
Analysis goals:

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- Grain segmentation \( \Omega_k \) and grain boundary \( \partial \Omega_k \);
- Smooth deformation \( \phi(x) \) or its gradient \( G(x) = \nabla \phi(x) \in \mathbb{R}^{2\times2} \).
Analysis goals:

\[
f(x) = \sum_{k=1}^{M} \chi_{\Omega_k}(x) \left( \alpha(x) S \left( 2\pi N \phi(x) \right) + c(x) \right).
\]

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- Smooth deformation \( \phi(x) \) or its gradient \( G(x) = \nabla \phi(x) \in \mathbb{R}^{2\times 2} \);
- Polar decomposition \( G(x) = R_{\theta(x)} P(x) \) gives the angle of crystal rotation \( \theta(x) \);
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- \( \det(P(x)) - 1 \) indicates the volume distortion of \( G(x) \).
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- \( \det(P(x)) - 1 \) indicates the volume distortion of \( G(x) \);
- \( |\lambda_1(x) - \lambda_2(x)| \) characterizes the difference of the principal stretches of \( G(x) \), where \( \lambda_1 \) and \( \lambda_2 \) are eigenvalues of \( G(x) \).
A two-stage method

\[ f(x) = \sum_{k=1}^{M} \chi_{\Omega_k}(x) (\alpha(x) S (2\pi N\phi(x)) + c(x)) \]

1st stage

- Given a crystal image \( f(x) \), apply the synchrosqueezed transforms to obtain initial information;
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1st stage

- Given a crystal image \( f(x) \), apply the synchrosqueezed transforms to obtain initial information;
- Estimate defect region \( \Omega_d = \bigcup_k \partial \Omega_k \) and initial deformation gradient \( G_0 \);
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1st stage

- Given a crystal image \( f(x) \), apply the synchrosqueezed transforms to obtain initial information;
- Estimate defect region \( \Omega_d = \bigcup_k \partial \Omega_k \) and initial deformation gradient \( G_0 \);
- Use 2D band-limited synchrosqueezed wave packet transform for better efficiency;
A two-stage method

\[ f(x) = \sum_{k=1}^{M} \chi_{\Omega_k}(x) (\alpha(x) S(2\pi N \phi(x)) + c(x)) \]

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2\textsuperscript{nd} stage

- A variational approach to optimize \( G_0 \) outside the defect region;
A two-stage method

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2\textsuperscript{nd} stage

- A variational approach to optimize \( G_0 \) outside the defect region;
- Better agreeing with physical understanding of the deformation field;
$1^{st}$ stage: the synchrosqueezed transform (SST)

\[
\begin{align*}
\text{SS} + \text{ a wave packet transform} & = 2\text{D SSWPT (Y. and Ying, SIIMS 13)} \\
\text{SS} + \text{ a general curvelet transform} & = 2\text{D SSCT (Y. and Ying, SIMS 14)}
\end{align*}
\]
$1^{st}$ stage: the synchrosqueezed transform (SST)

SS+ a wave packet transform = 2D SSWPT (Y. and Ying, SIIMS 13)
SS+ a general curvelet transform = 2D SSCT (Y. and Ying, SIMS 14)

**Property**

Suppose $W_f(\xi, x)$ is a phase-space transform of $f$ with a frequency variable $\xi$ and a spatial variable $x$, then the SST $T_f(\xi, x)$ of $W_f(\xi, x)$ is a sharpened phase-space representation.

**Figure:** An example of a superposition of two 2D waves using 2D SSWPT.
1st stage: the synchrosqueezed transform (SST)

Local wave vector estimation

\[ v_f(\xi, x) = \Re e \frac{\nabla_x W_f(\xi, x)}{2\pi i W_f(\xi, x)}. \]

Synchrosqueezed energy distribution of \( f \)

\[ T_f(\nu, x) = \int |W_f(\xi, x)|^2 \delta(v_f(\xi, x) - \nu) d\xi. \]

Theorem: (Y., Lu and Ying, 14)

\[ \text{supp}(T_f(\nu, x)) \approx \text{supp} \left( \sum_{n \in \mathbb{Z}^2} \alpha(x)^2 |\hat{s}(n)|^2 \delta(\nu - N \nabla(n \cdot \phi(x))) \right). \]

Intuitively,

\[ T_f(\nu, x) \approx \sum_{n \in \mathbb{Z}^2} \alpha(x)^2 |\hat{s}(n)|^2 \delta(\nu - N \nabla(n \cdot \phi(x))). \]
1\textsuperscript{st} stage: estimate deformation gradient $G_0$

\[ f(x) = \sum_{k=1}^{M} \chi_{\Omega_k}(x) \left( \alpha(x) S(2\pi N \phi(x)) + c(x) \right) \]

\[ = \sum_{k=1}^{M} \chi_{\Omega_k}(x) \left( \sum_{\alpha} \alpha(x) \hat{S}(n)e^{2\pi i N n \cdot \phi(x)} + c(x) \right) \]

1. Pre-determine reference lattice $n_j$ of interest;
2. Apply the SST to estimate $N n_j \cdot \phi(x)$ and denote them as $v^\text{est}_j(x)$;
3. Solve

\[ G_0(x) = \arg \min_G \sum_j \| v^\text{est}_j(x) - N G n_j \|^2. \]

\[ \begin{array}{c}
\includegraphics[width=0.4\textwidth]{crystal_image.png}
\end{array} \]

\[ \begin{array}{c}
\includegraphics[width=0.4\textwidth]{fourier_transform.png}
\end{array} \]

\textbf{Figure :} Left: An example of a crystal image. Right: Windowed Fourier transform at a local patch indicated by a rectangle.
1\textsuperscript{st} stage: estimate defect region $\Omega_d$

\[ w_n(x) = \frac{\int_{B_\delta(v_n^{\text{est}})} T_f(v, x) \, dv}{\int_{\arg v \in [(n-1)\pi/3, n\pi/3]} T_f(v, b) \, dv} , \]

where $B_\delta(v_n^{\text{est}})$ denotes a small ball around $v_n^{\text{est}}$.

Figure: Left: $T_f(\xi, x)$ for $x$ outside the defect region. Right: $T_f(\xi, x)$ for $x$ inside the defect region.
1\textsuperscript{st} stage: estimate defect region $\Omega_d$

Figure: Left: $T_f(\xi, x)$ for $x$ outside the defect region. Right: $T_f(\xi, x)$ for $x$ inside the defect region.

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where $B_\delta(v_{n}^{\text{est}})$ denotes a small ball around $v_{n}^{\text{est}}$.

\[ \text{mass}(x) := \sum_j w_j(x) \] will be close to 3 outside $\Omega_d$, while its value will be much smaller than 3 inside $\Omega_d$. 
1\textsuperscript{st} stage: estimate defect region $\Omega_d$

Figure: Left: Crystal image. Middle: $\text{mass}(x)$. Right: Identified defect region $\Omega_d$ by thresholding.
2\textsuperscript{nd} stage: a variational model for an optimized $G$

Motivation

- $G$ should minimize the elastic energy of the crystal system;
- $\text{curl } G = b$ inside $\Omega_d$, where $b$ is a Burgers vector field.
2nd stage: a variational model for an optimized $G$

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Variational model

\[
\inf_{G: \Omega \rightarrow \mathbb{R}^{2 \times 2}} \int_{\Omega \setminus \Omega_d} |G - G_0|^2 + W(G) \, dy
\]

s.t. $\text{curl } G = b$

where $|\cdot|$ denote the Frobenius norm and $W$ is the elastic stored energy density.
2nd stage: a variational model for an optimized $G$

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Neo-Hookean elastic energy

$$W(G) = \frac{\mu}{2} (|G|^2 - 2) + \left(\frac{\mu}{2} + \frac{\lambda}{2}\right)(\det G - 1)^2 - \mu(\det G - 1).$$
2nd stage: basic properties of the deformation gradient $G$

- In the grain interior, $G$ is locally continuous and curl-free:

$$\text{curl } G = \left( \frac{\partial x_1 G_{12}}{\partial x_1} - \frac{\partial x_2 G_{11}}{\partial x_1} \right) \left( \frac{\partial x_1 G_{22}}{\partial x_1} - \frac{\partial x_2 G_{21}}{\partial x_1} \right) = \left( \frac{\partial x_2}{\partial x_1} \phi_1 - \frac{\partial x_1}{\partial x_2} \phi_1 \right) = 0;$$

- In the defect region, $\text{curl } G \neq 0$;

- In the case of a dislocation, $\text{curl } G$ gives the Burgers vector $b$;

Figure: The curve $\gamma$ around the dislocation (right) can be mapped back onto a curve $\hat{\gamma}$ in the reference lattice by $\psi = \phi - 1$ (left). $\hat{\gamma}$ is no longer closed, the gap being the Burgers vector (gray arrow).
2nd stage: basic properties of the deformation gradient $G$

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2nd stage: basic properties of the Burgers vector \( b \)

Let \( B \) be the area covering a defect with the boundary \( \gamma \), then

\[
\int_B \text{curl} \, G \, dx = \int_{\partial B} G n^\perp \, dx = \int_0^1 G(\gamma(t)) \dot{\gamma}(t) \, dt = \int_0^1 \dot{\gamma} \, dt = \hat{\gamma}(1) - \hat{\gamma}(0)
\]

implies

\[
\int_B \text{curl} \, G \, dx = b.
\]
$2^{nd}$ stage: basic properties of the Burgers vector $b$

- Let $B$ be the area covering a defect with the boundary $\gamma$, then
  \[
  \int_B \text{curl } G \, dx = \int_{\partial B} Gn^\bot \, dx = \int_0^1 G(\gamma(t)) \dot{\gamma}(t) \, dt = \int_0^1 \dot{\gamma} \, dt = \hat{\gamma}(1) - \hat{\gamma}(0)
  \]
  implies
  \[
  \int_B \text{curl } G \, dx = b.
  \]

- Recall that curl $G = 0$ on $\Omega \setminus \Omega_d$. 

2\textsuperscript{nd} stage: basic properties of the Burgers vector $b$

\begin{itemize}
  \item Let $B$ be the area covering a defect with the boundary $\gamma$, then

  \[\int_B \text{curl } G \, dx = \int_{\partial B} G n^\perp \, dx = \int_0^1 G(\gamma(t)) \dot{\gamma}(t) \, dt = \int_0^1 \dot{\gamma} \, dt = \dot{\gamma}(1) - \dot{\gamma}(0)\]

  implies

  \[\int_B \text{curl } G \, dx = b.\]

  \item Recall that $\text{curl } G = 0$ on $\Omega \setminus \Omega_d$.

  \item A discrete analog

  \[\tilde{b} = \begin{cases} 
  0 & \text{on } \Omega \setminus \Omega_d; \\
  b/|\Omega_d| & \text{on } \Omega_d.
  \end{cases} \quad \rightarrow \quad \text{curl } G = \tilde{b}
  \]
\end{itemize}
2nd stage: basic properties of the Burgers vector $b$

**Figure**: Identified defect region $\Omega_d$ and $\Omega_d^i$. The grey scale indicates $|b_i|/|\Omega_d^i|$ on $\Omega_d^i$.

- After the 1st stage, we have $G_0$ and $\Omega_d$;
2nd stage: basic properties of the Burgers vector $b$

Figure: Identified defect region $\Omega_d$ and $\Omega_d^i$. The grey scale indicates $|b_i|/|\Omega_d^i|$ on $\Omega_d^i$.

- After the 1st stage, we have $G_0$ and $\Omega_d$;
- Devide $\Omega_d$ into connected components $\Omega_d^i$;
2\textsuperscript{nd} stage: basic properties of the Burgers vector $b$

**Figure:** Identified defect region $\Omega_d$ and $\Omega_d^i$. The grey scale indicates $|b_i|/|\Omega_d^i|$ on $\Omega_d^i$.

- After the 1\textsuperscript{st} stage, we have $G_0$ and $\Omega_d$;
- Devide $\Omega_d$ into connected components $\Omega_d^i$;
- Estimate the Burgers vector for each defect component $\Omega_d^i$

\[
    b_i = \int_{\Omega_d^i} \text{curl} \ G_0 \, dx.
\]
2\textsuperscript{nd} stage: basic properties of the Burgers vector \( b \)

\textbf{Figure} : Identified defect region \( \Omega_d \) and \( \Omega_d^i \). The grey scale indicates \( |b_i|/|\Omega_d^i| \) on \( \Omega_d^i \).

- After the 1\textsuperscript{st} stage, we have \( G_0 \) and \( \Omega_d \);
- Devide \( \Omega_d \) into connected components \( \Omega_d^i \);
- Estimate the Burgers vector for each defect component \( \Omega_d^i \)
  \[ b_i = \int_{\Omega_d^i} \text{curl} \ G_0 \, dx. \]
- Define
  \[ b = \begin{cases} 
  0 & \text{on } \Omega \setminus \Omega_d; \\
  b_i/|\Omega_d^i| & \text{on } \Omega_d^i.
  \end{cases} \]
$2^{nd}$ stage: basic properties of the Burgers vector $b$

**Figure:** Identified defect region $\Omega_d$ and $\Omega_d^i$. The grey scale indicates $|b_i|/|\Omega_d^i|$ on $\Omega_d^i$.

- After the 1$^{st}$ stage, we have $G_0$ and $\Omega_d$;
- Devide $\Omega_d$ into connected components $\Omega_d^i$;
- Estimate the Burgers vector for each defect component $\Omega_d^i$
  \[ b_i = \int_{\Omega_d^i} \text{curl } G_0 \, dx. \]

- Define
  \[ b = \begin{cases} 
    0 & \text{on } \Omega \setminus \Omega_d; \\
    b_i/|\Omega_d^i| & \text{on } \Omega_d^i.
  \end{cases} \]

- An ideal $G$ should satisfy that $\text{curl } G = b$. 
2nd stage: a variational model for an optimized $G$

Motivation

- $G$ should minimize the elastic energy of the crystal system;
- $\text{curl } G = b$ inside $\Omega_d$.

Variational model

$$\inf_{G: \Omega \to \mathbb{R}^{2 \times 2}} \int_{\Omega \setminus \Omega_d} |G - G_0|^2 + W(G) \, dy$$

s.t. $\text{curl } G = b$

where $|\cdot|$ denote the Frobenius norm and $W$ is the elastic stored energy density.

No feasible set

- $\text{curl } G = b$ well defined locally;
- $\text{curl } G = b$ inconsistent globally;
2\textsuperscript{nd} stage: basic properties of the deformation gradient $G$ 

\begin{center}
\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{hexagonal_crystal_lattice.png}
\caption{2D Bravais lattice of the hexagonal crystal.}
\end{figure}
\end{center}

Locally point group invariance

- Rotational symmetry of 2D Bravais lattice of the hexagonal crystal;
2\textsuperscript{nd} stage: basic properties of the deformation gradient $G$

Figure: 2D Bravais lattice of the hexagonal crystal.

Locally point group invariance

- Rotational symmetry of 2D Bravais lattice of the hexagonal crystal;
- Point group $P \subset SO(2)$ comprises all those rotations which leave the reference lattice invariant;
2nd stage: basic properties of the deformation gradient $G$

- Rotational symmetry of 2D Bravais lattice of the hexagonal crystal;
- Point group $P \subset SO(2)$ comprises all those rotations which leave the reference lattice invariant;
- Non-uniqueness of $G$ to describe crystal deformation ($G$ and $RG$ for $R \in P$).

Figure: 2D Bravais lattice of the hexagonal crystal.

Locally point group invariance
2\textsuperscript{nd} stage: basic properties of the deformation gradient $G$

Figure: Along a closed path $\gamma$ traversing a sequence of crystal grains, the deformation gradient $G$ changes continuously from $I$ to $R \neq I$. The gray shade indicates the local crystal orientation from the identity $I$ (white) to $R$ (dark gray). Dots represent point dislocations; lines indicate high angle grain boundaries. Along the path $\gamma$ all grains are connected by low angle grain boundaries.
2\textsuperscript{nd} stage: basic properties of the deformation gradient $G$

Figure: Along a closed path $\gamma$ traversing a sequence of crystal grains, the deformation gradient $G$ changes continuously from $I$ to $R \neq I$. The gray shade indicates the local crystal orientation from the identity $I$ (white) to $R$ (dark gray). Dots represent point dislocations; lines indicate high angle grain boundaries. Along the path $\gamma$ all grains are connected by low angle grain boundaries.

- Globally inconsistency of $G$ leads to $\text{curl } G \neq 0$ outside the defect region $\Omega_d$. Conflict!
2\textsuperscript{nd} stage: basic properties of the deformation gradient $G$

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure.png}
\caption{Along a closed path $\gamma$ traversing a sequence of crystal grains, the deformation gradient $G$ changes continuously from $I$ to $R \neq I$. The gray shade indicates the local crystal orientation from the identity $I$ (white) to $R$ (dark gray). Dots represent point dislocations; lines indicate high angle grain boundaries. Along the path $\gamma$ all grains are connected by low angle grain boundaries.}
\end{figure}

- Globally inconsistency of $G$ leads to curl $G \neq 0$ outside the defect region $\Omega_d$. \textbf{Conflict!}
- Introduce a jump set $S$ across which $G$ is allowed to jump by a point group element,
  \[ G^- = RG^+ \text{ for some } R \in P, \]
  where $G^-$ and $G^+$ denote the value of $G$ on either side of $S$. 

2nd stage: a variational model for an optimized $G$

Motivation
Consider point group invariance
2\textsuperscript{nd} stage: a variational model for an optimized $G$

Motivation
Consider point group invariance

New variational model

$$
\min_{G: \Omega \rightarrow \mathbb{R}^{2 \times 2}} \int_{\Omega \setminus \Omega_d} |G - G_0|^2 + W(G) \, dy \\
\text{s. t.} \quad \text{curl} \ G = b \text{ on } \Omega \setminus S, \quad G^-(G^+)^{-1} \in P \text{ on } S,
$$

Numerical solution:
Optimized by a nonlinear projected conjugate gradient method
Numerical example 1

Figure: A noiseless PFC image; a zoomed-in image detailing the rectangle part.
Numerical example 1

Figure: (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.
Numerical example 2

Figure: A noisy PFC image; a zoomed-in image detailing the rectangle part.
Numerical example 2

Figure: (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.
Numerical example 3

Figure: A TEM-image in GaN. Courtesy of David M. Tricker
Figure: (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.
Numerical example 4

Figure: A photograph of a bubble raft with large disorders and blurry boundaries. Courtesy to Barrie S. H. Royce.
Numerical example 4

Figure: (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.
Figure: A TEM-image of Sigma 99 tilt grain boundary in Al. Courtesy of National Center for Electron Microscopy in Lawrence Berkeley National Laboratory.
Numerical example 5

Figure: (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.
Future work

- Establish new optimization model for $G$ inside the defect region $\Omega_d$;
- Consider more complicated crystal images;
- Design fast optimization method.