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.

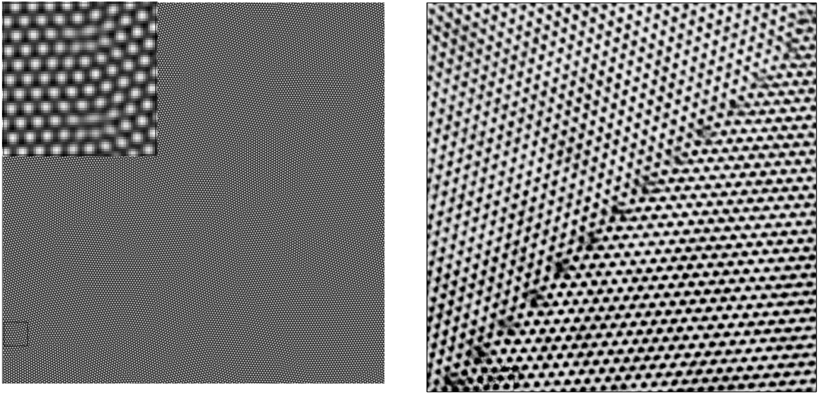

Figure : Left: A PFC image with a zoomed-in image detailing the part maked by a black rectangle. Right: A TEM-image in GaN. Courtesy of David M. Tricker.

Atomic material evolution:

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

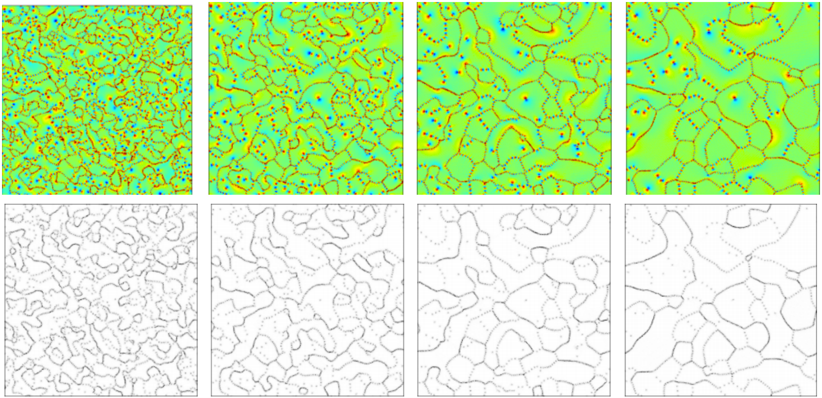

Figure : From top to bottom: time evolution of local volume distortion and grain boundaries.

Mathematical model

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

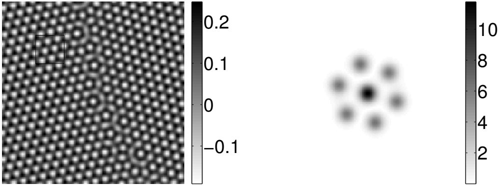

Figure : Left: An example of a crystal image. Right: Windowed Fourier transform at a local patch indicated by a rectangle.

Analysis goals:

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

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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 λ_1 and λ_2 are eigenvalues of $G(x)$.

A two-stage method

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

1^{st} stage

- Given a crystal image $f(x)$, apply the synchrosqueezed transforms to obtain initial information;

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- A variational approach to optimize G_0 outside the defect region;

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2^{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)

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

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Property

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

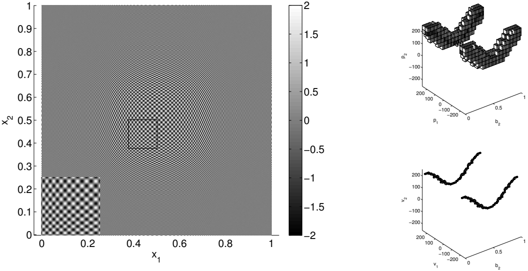


Figure : An example of a superposition of two 2D waves using 2D SSWPT.

1^{st} stage: the synchrosqueezed transform (SST)

Local wave vector estimation

$$v_f(\xi, x) = \mathfrak{Re}\frac{\nabla_x W_f(\xi, x)}{2\pi i W_f(\xi, x)}.$$

Synchrosqeezed energy distribution of f

$$T_f(v, x) = \int |W_f(\xi, x)|^2 \delta(v_f(\xi, x) - v) d\xi.$$

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

$$\text{supp}(T_f(v, x)) \approx \text{supp}\left(\sum_{n \in \mathbb{Z}^2} \alpha(x)^2 |\widehat{s}(n)|^2 \delta\big(v - N\nabla(n \cdot \phi(x))\big)\right).$$

Intuitively,

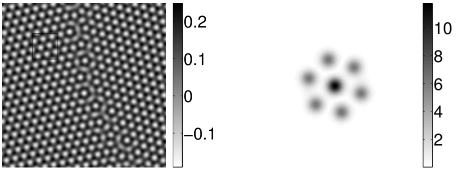
$$T_f(v, x) \approx \sum_{n \in \mathbb{Z}^2} \alpha(x)^2 |\widehat{s}(n)|^2 \delta\big(v - N\nabla(n \cdot \phi(x))\big).$$

1^{st} stage: estimate deformation gradient G_0

$$
\begin{aligned}
f(x) &= \sum_{k=1}^{M} \chi_{\Omega_k}(x)\left(\alpha(x) S\left(2\pi N\phi(x)\right) + c(x)\right) \\
&= \sum_{k=1}^{M} \chi_{\Omega_k}(x)\left(\sum_{n} \alpha(x)\widehat{S}(n) e^{2\pi i N n\cdot\phi(x)} + c(x)\right)
\end{aligned}
$$

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

$$
G_0(x) = \arg\min_{G} \sum_{j} \left\| v_j^{\text{est}}(x) - NGn_j \right\|^2 .
$$



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1^{st} stage: estimate defect region Ω_d

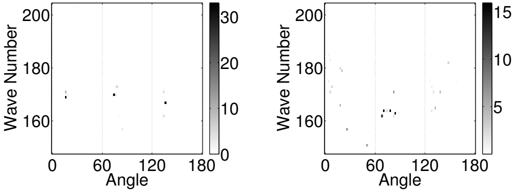

Figure : Left: $T_f(\xi, x)$ for x outside the defect region. Right: $T_f(\xi, x)$ for x inside the defect region.

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

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

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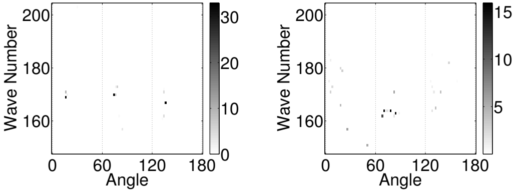

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  where $B_\delta(v_n^{\text{est}})$ denotes a small ball around v_n^{est}.
- $\text{mass}(x) := \sum_j w_j(x)$ will be close to 3 outside Ω_d, while its value will be much smaller than 3 inside Ω_d.

1^{st} stage: estimate defect region Ω_d

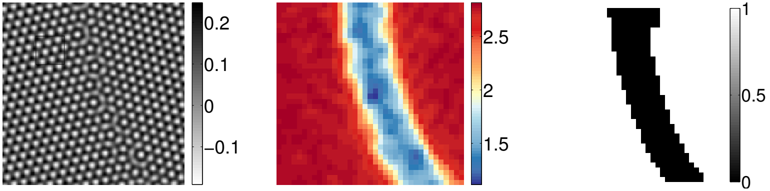

Figure : Left: Crystal image. Middle: mass(x). Right: Identified defect region Ω_d by thresholding.

2^{nd} stage: a variational model for an optimized G

Motivation

- G should minimize the elastic energy of the crystal system;
- $\operatorname{curl} G = b$ inside Ω_d, where b is a Burgers vector field.

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Variational model

$$\inf_{G:\Omega\to\mathbb{R}^{2\times 2}} \int_{\Omega\setminus\Omega_d} |G - G_0|^2 + W(G)\,\mathrm{d}y$$
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Neo-Hookean elastic energy

$$W(G) = \frac{\mu}{2}(|G|^2 - 2) + (\frac{\mu}{2} + \frac{\lambda}{2})(\det G - 1)^2 - \mu(\det G - 1).$$

2^{nd} stage: basic properties of the deformation gradient G

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

$$\operatorname{curl} G = \begin{pmatrix} \partial_{x_1} G_{12} - \partial_{x_2} G_{11} \\ \partial_{x_1} G_{22} - \partial_{x_2} G_{21} \end{pmatrix} = \begin{pmatrix} \partial_{x_2} \partial_{x_1} \phi_1 - \partial_{x_1} \partial_{x_2} \phi_1 \\ \partial_{x_2} \partial_{x_1} \phi_2 - \partial_{x_1} \partial_{x_2} \phi_2 \end{pmatrix} = 0;$$

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

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- In the defect region, curl $G \neq 0$;
- In the case of a dislocation, curl G gives the Burgers vector b;

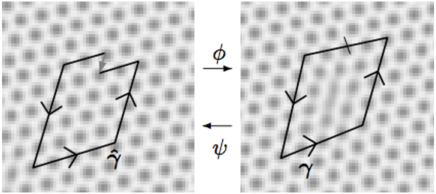
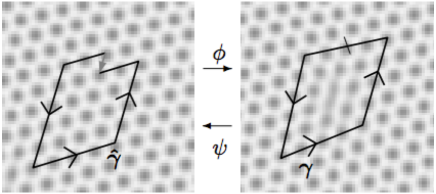


Figure : The curve γ around the dislocation (right) can be mapped back onto a curve $\hat{\gamma}$ in the reference latice by $\psi = \phi^{-1}$ (left). $\hat{\gamma}$ is no longer closed, the gap being the Burgers vector (gray arrow).

2^{nd} stage: basic properties of the Burgers vector b



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

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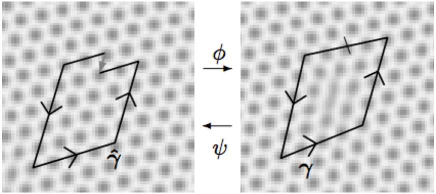

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- Recall that curl $G = 0$ on $\Omega \setminus \Omega_d$.

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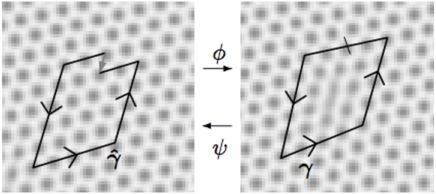

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- Recall that $\operatorname{curl} G = 0$ on $\Omega \setminus \Omega_d$.
- A discrete anolog
$$\tilde{b} = \begin{cases} 0 & \text{on } \Omega \setminus \Omega_d; \\ b/|\Omega_d| & \text{on } \Omega_d\,. \end{cases} \quad \to \quad \operatorname{curl} G = \tilde{b}$$

2^{nd} stage: basic properties of the Burgers vector b

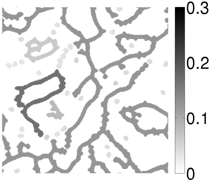
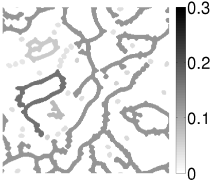


Figure : Identified defect region Ω_d and Ω_d^i. The grey scale indicates $|b_i|/|\Omega_d^i|$ on Ω_d^i.

- After the 1^{st} stage, we have G_0 and Ω_d;

2^{nd} stage: basic properties of the Burgers vector b



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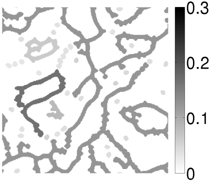

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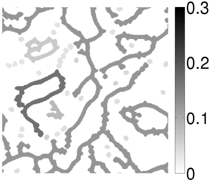
- Estimate the Burgers vector for each defect component Ω_d^i

$$b_i = \int_{\Omega_d^i} \operatorname{curl} G_0 dx.$$

2^{nd} stage: basic properties of the Burgers vector b



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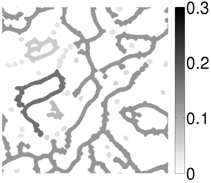

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- An ideal G should satisfy that $\operatorname{curl} G = b$.

2^{nd} stage: a variational model for an optimized G

Motivation

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

Variational model

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

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

No feasible set

- $\operatorname{curl} G = b$ well defined locally;
- $\operatorname{curl} G = b$ inconsistent globally;

2^{nd} stage: basic properties of the deformation gradient G

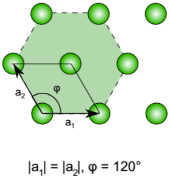

Figure : 2D Bravais lattice of the hexagonal crystal.

Locally point group invariance

- Rotational symmetry of 2D Bravais lattice of the hexagonal crystal;

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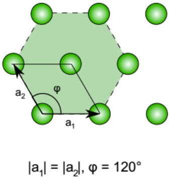

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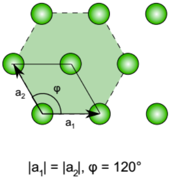

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- Rotational symmetry of 2D Bravais lattice of the hexagonal crystal;
- Point group $P \subset SO(2)$ comprises all those rotations which leave the reference lattice invariant;
- Non-uniqueness of G to describe crystal deformation (G and RG for $R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

2^{nd} stage: basic properties of the deformation gradient G

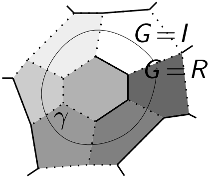
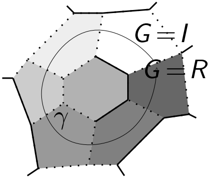


Figure : Along a closed path γ traversing a sequence of crystal grains, the deformation gradient G changes continuously from I to $R \neq I$. The gray shade indicates the local crystal orientation from the identity I (white) to R (dark gray). Dots represent point dislocations; lines indicate high angle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

2^{nd} stage: basic properties of the deformation gradient G



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- Globally inconsistency of G leads to curl $G \neq 0$ outside the defect region Ω_d. Conflict!

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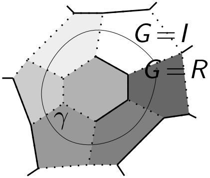

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- Globally inconsistency of G leads to curl $G \neq 0$ outside the defect region Ω_d. Conflict!
- Introduce a jump set S across which G is allowed to jump by a point group element,

$$G^- = RG^+ \text{ for some } R \in P \,,$$

where G^- and G^+ denote the value of G on either side of S.

2^{nd} stage: a variational model for an optimized G

Motivation

Consider point group invariance

2^{nd} stage: a variational model for an optimized G

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Consider point group invariance

New variational model

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

Numerical solution:

Optimized by a nonlinear projected conjugate gradient method

Numerical example 1

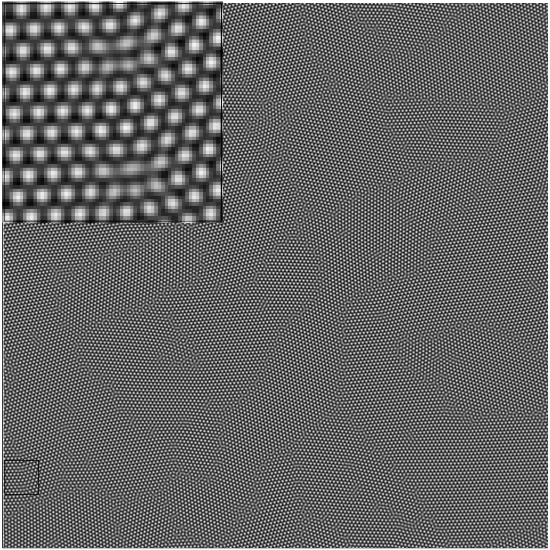


Figure : A noiseless PFC image; a zoomed-in image detailing the rectangle part.

Numerical example 1

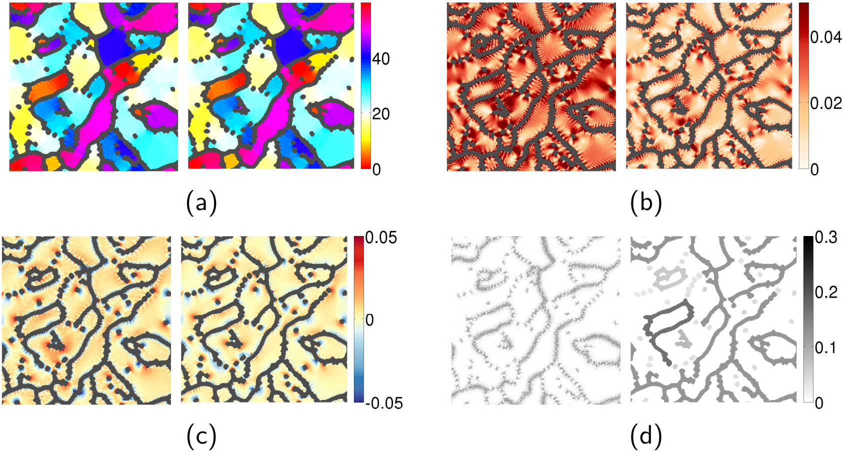


Figure : (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.

Numerical example 2

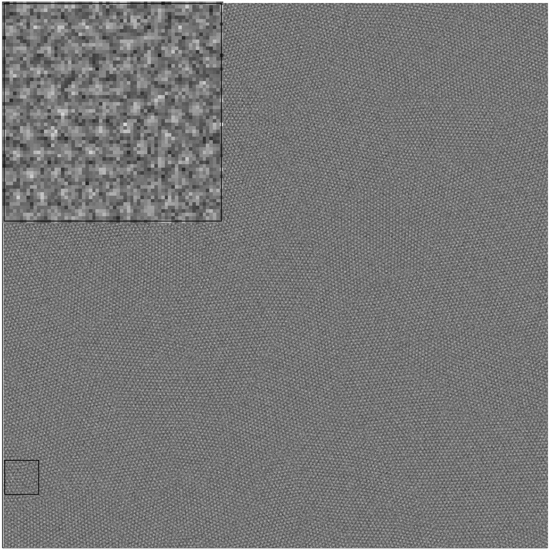
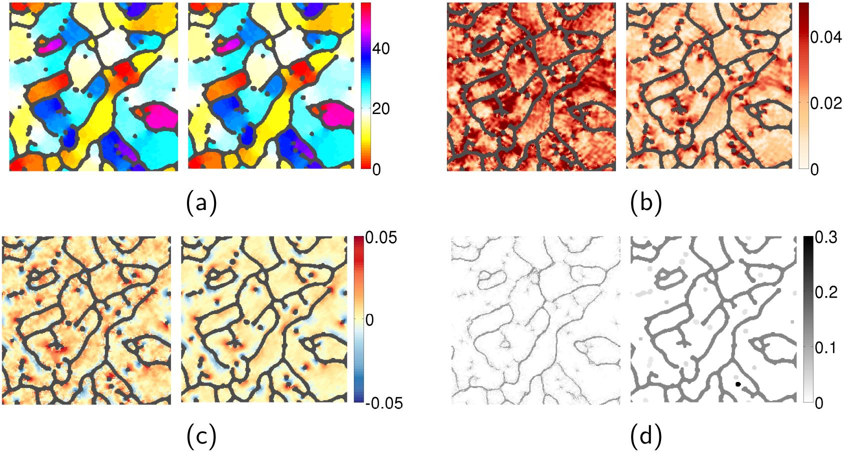


Figure : A noisy PFC image; a zoomed-in image detailing the rectangle part.

Numerical example 2



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Numerical example 3

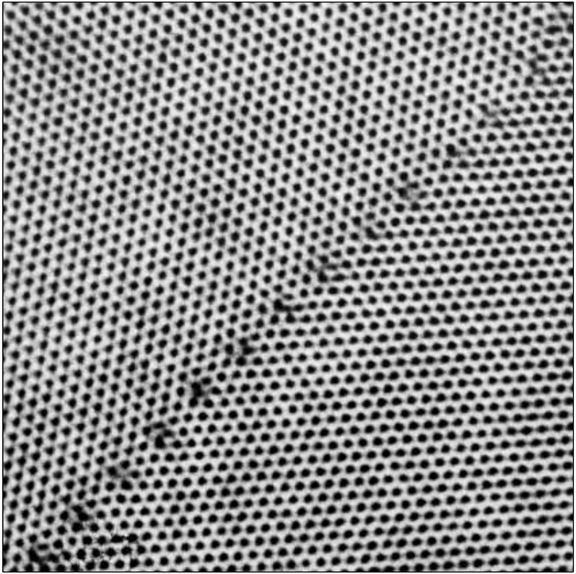
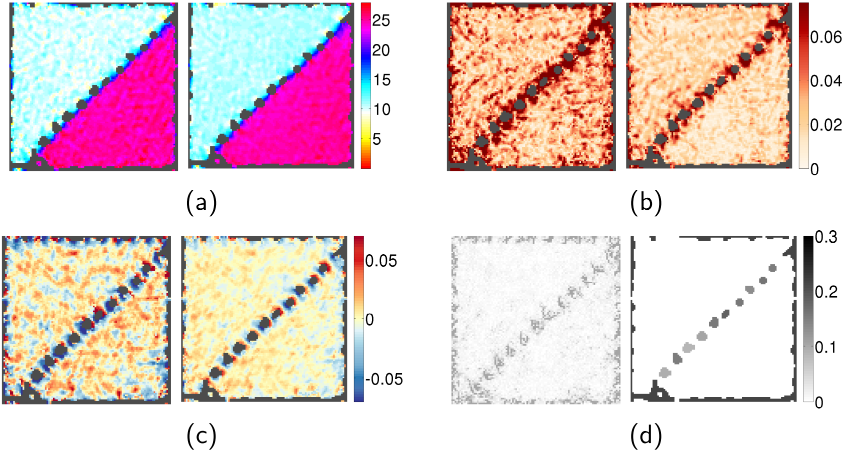


Figure : A TEM-image in GaN. Courtesy of David M. Tricker

Numerical example 3



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Numerical example 4

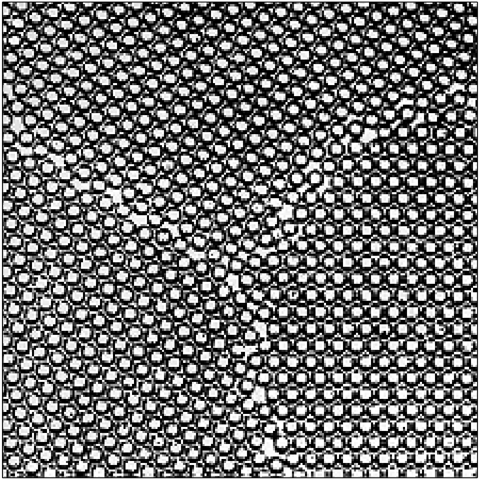

Figure : A photograph of a bubble raft with large disorders and blurry boundaries. Courtesy to Barrie S. H. Royce.

Numerical example 4

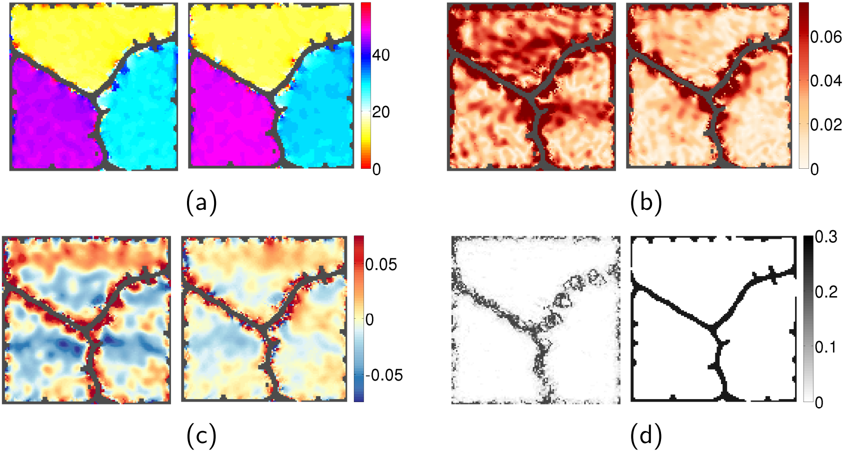

Figure : (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.

Numerical example 5

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

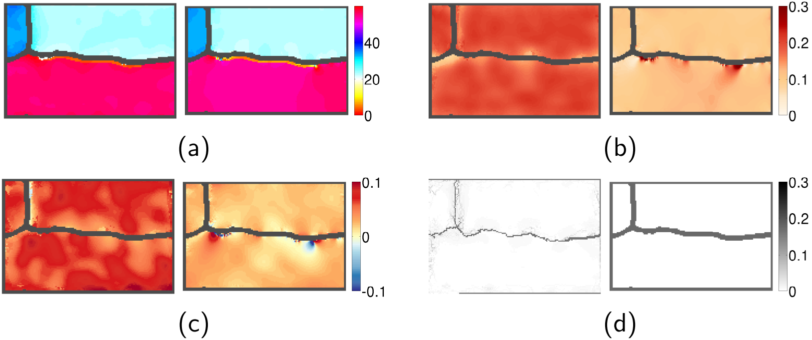

Figure : (a)-(d): the comparison of its initial and optimized crystal orientations, difference of principal stretches, volume distortion, and the curl of the inverse deformation gradient.

Future work

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