A Dictionary Indexing Approach for EBSD

Using the Complete Pattern

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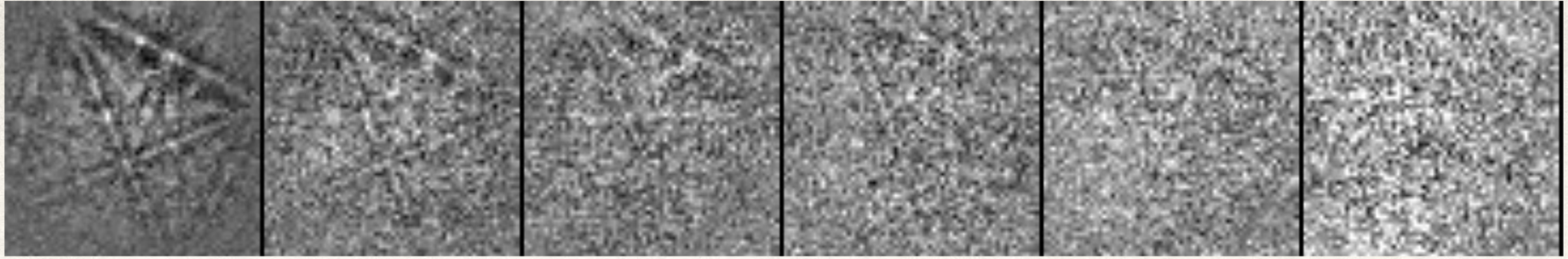
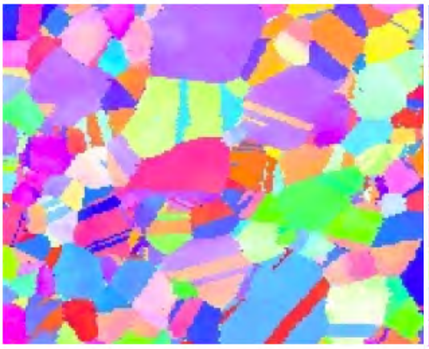
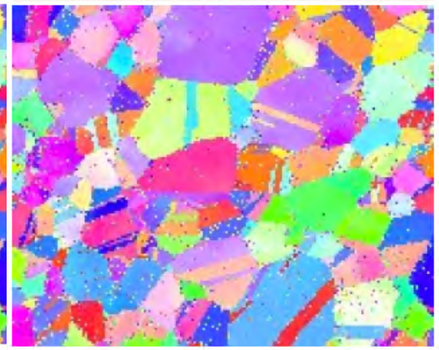
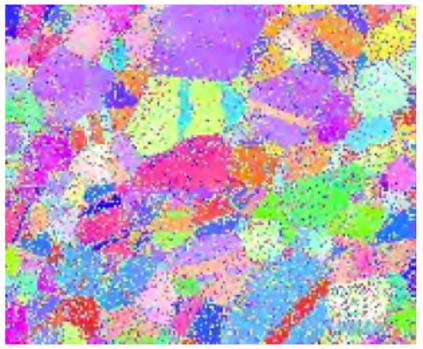
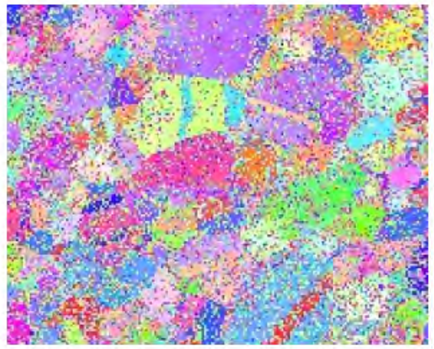
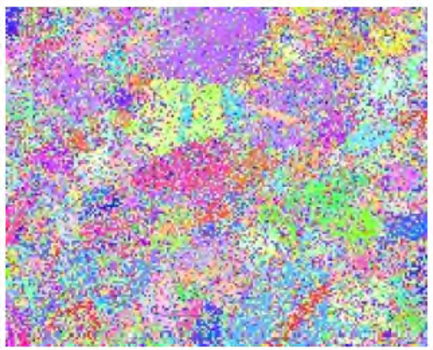
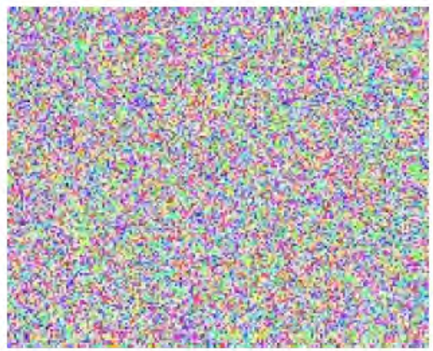
EBSD

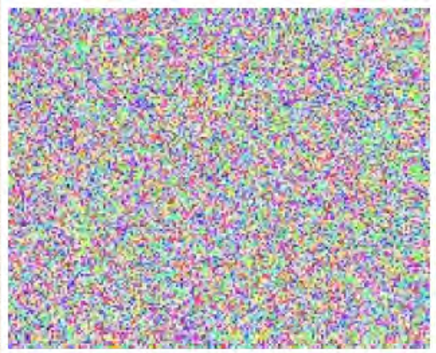
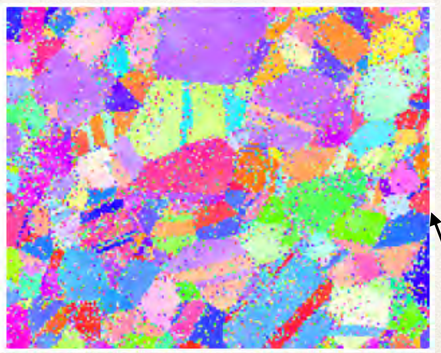


S. Wright; Ni 20kV

Conventional EBSD indexing is not robust against pattern noise…

99.1% 90.6% 60.2% 37.3% 19.4% 0.1%

Noisiest patterns have sufficient information to generate this IPF…

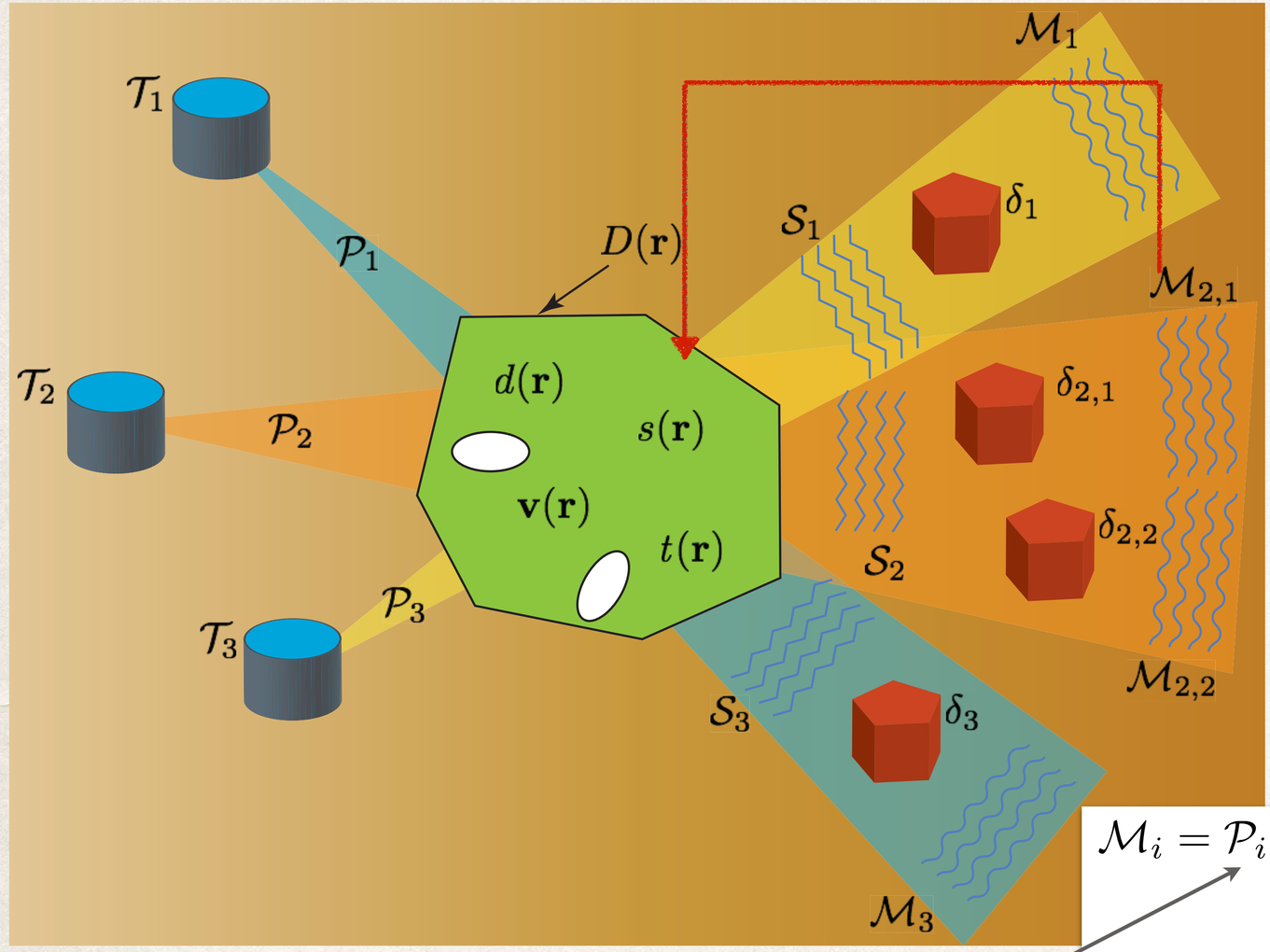
Outline

- How we view materials characterization
  - EBSD forward model and master pattern
- Dictionary Indexing
  - Methodology
  - Example Applications
- Beyond dictionary indexing… ***EMSphInx***
- Summary

The bigger picture of our approach

- Do we understand the underlying physics? Or are we just using a “black box”?
- Are we properly educating our students/postdocs in the use of these instruments?
- Do we have accurate quantitative models for all modalities?
  Can we predict the outcome of an observation?
- Do we know what the optimal acquisition conditions are?
  Are the manufacturer suggested settings really the best settings? If not, can we change them?
- Are we storing (can we store?) all the (raw) data for future processing
  and scientific validation?
- What does it take to “characterize a microstructure”?
  And how will we know that we have done a good job (the best possible job?) at this?

Our view of the (characterization) world…



Characterization is an inverse problem.

Most inverse problems are ill-posed…

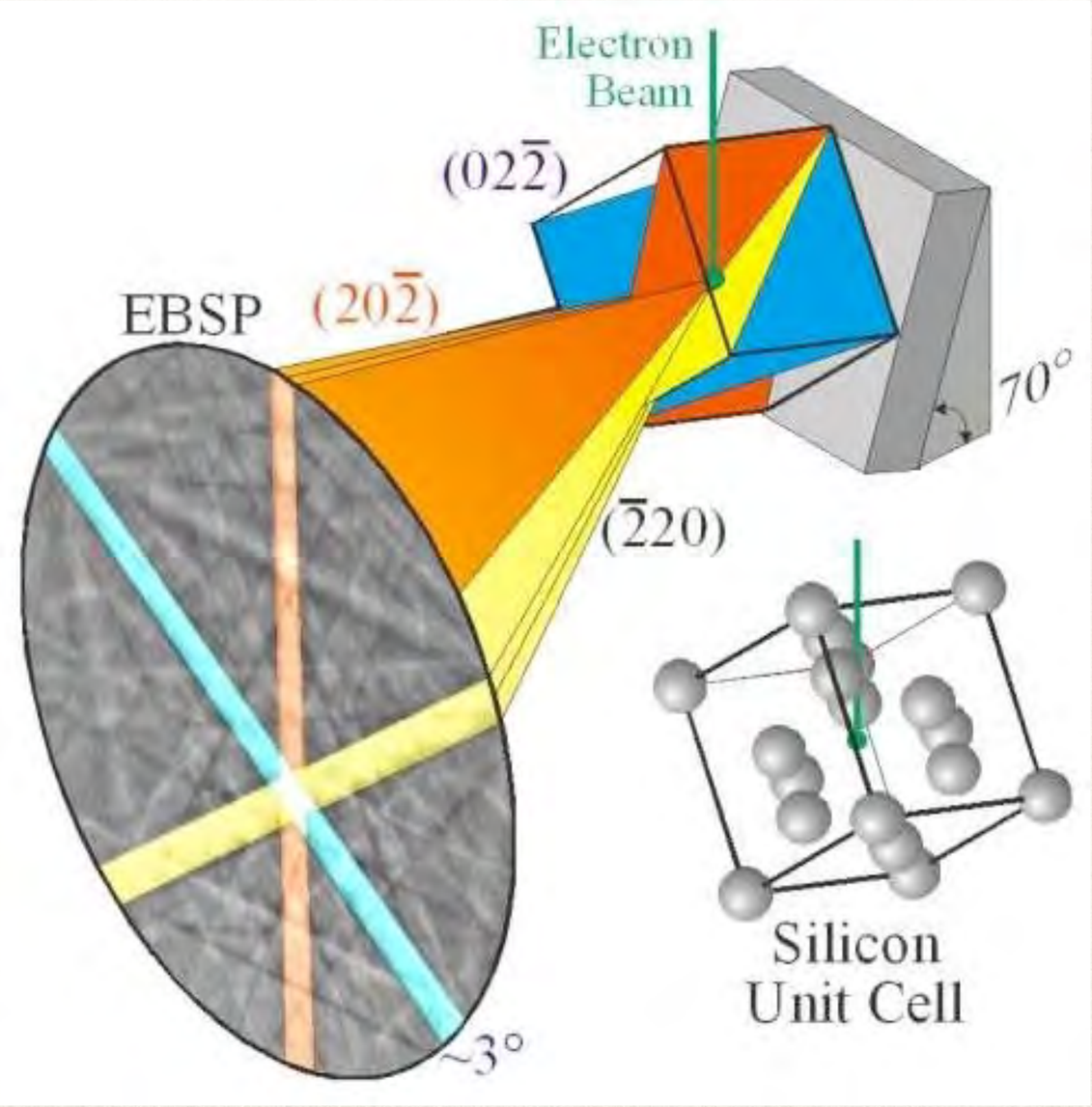
So, some form of regularization is needed…

Forward models are a strong form of regularization

$$\mathcal{M}_i = \mathcal{P}_i\left[\underbrace{D(\mathbf{r}), s(\mathbf{r}), \boldsymbol{\nu}(\mathbf{r}), t_{jk}(\mathbf{r}), \ldots}_{\text{unknown}}; \underbrace{T_i(\mathbf{r},\theta); \tau_i(\mathbf{r},\theta')}_{\text{can be modeled}}; \text{noise terms}\right]$$

Generalized forward projector (physics-based)

EBSD Forward Model



http://www.ifw-dresden.de/institutes/ikm/organisation/dep-31/methods/electron-back-scatter-diffraction-ebsd

- **Stochastic component:**
  - Monte Carlo model using Continuous Slowing Down Approximation to predict spatial, energy, and depth distributions for BSEs
- **Deterministic component:**
  - Dynamical scattering model using Scattering Matrix or Bloch wave approaches to predict distribution of BSEs with respect to crystal reference frame
- **Detector component:**
  - Geometrical model for detector (pattern center etc.) and crystal orientation (Euler angles etc.)

Scattering Model

$$P(\hat{\mathbf{k}}) = \sum_{n \in \mathrm{A.U.}} P_n(\hat{\mathbf{k}}) \qquad P_n(\hat{\mathbf{k}}) = \sum_{j \in \mathcal{S}_n} \sigma_j \int_{E_{\min}}^{E_{\max}} \mathrm{d}E \int_0^{z_0(E)} \mathrm{d}z \, \bar{\lambda}_{\hat{\mathbf{k}}}(E, z) \left| \Psi_{\hat{\mathbf{k}}}(\mathbf{r}_j; E, z) \right|^2$$

Rutherford scattering cross section

Integration over energy

Integration over depth

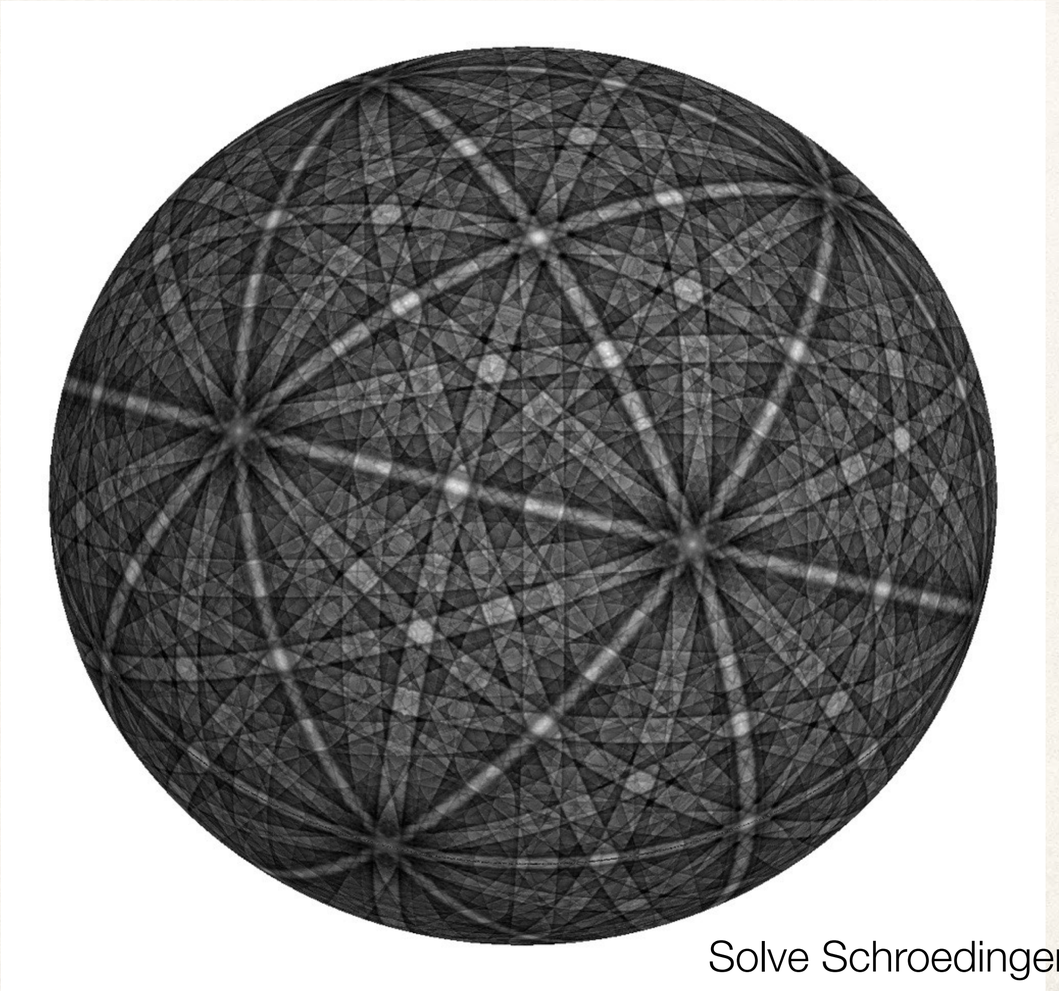
Probability of BSE escaping from depth *z* with energy *E* traveling in direction **k**

Probability of finding electron at position **r**

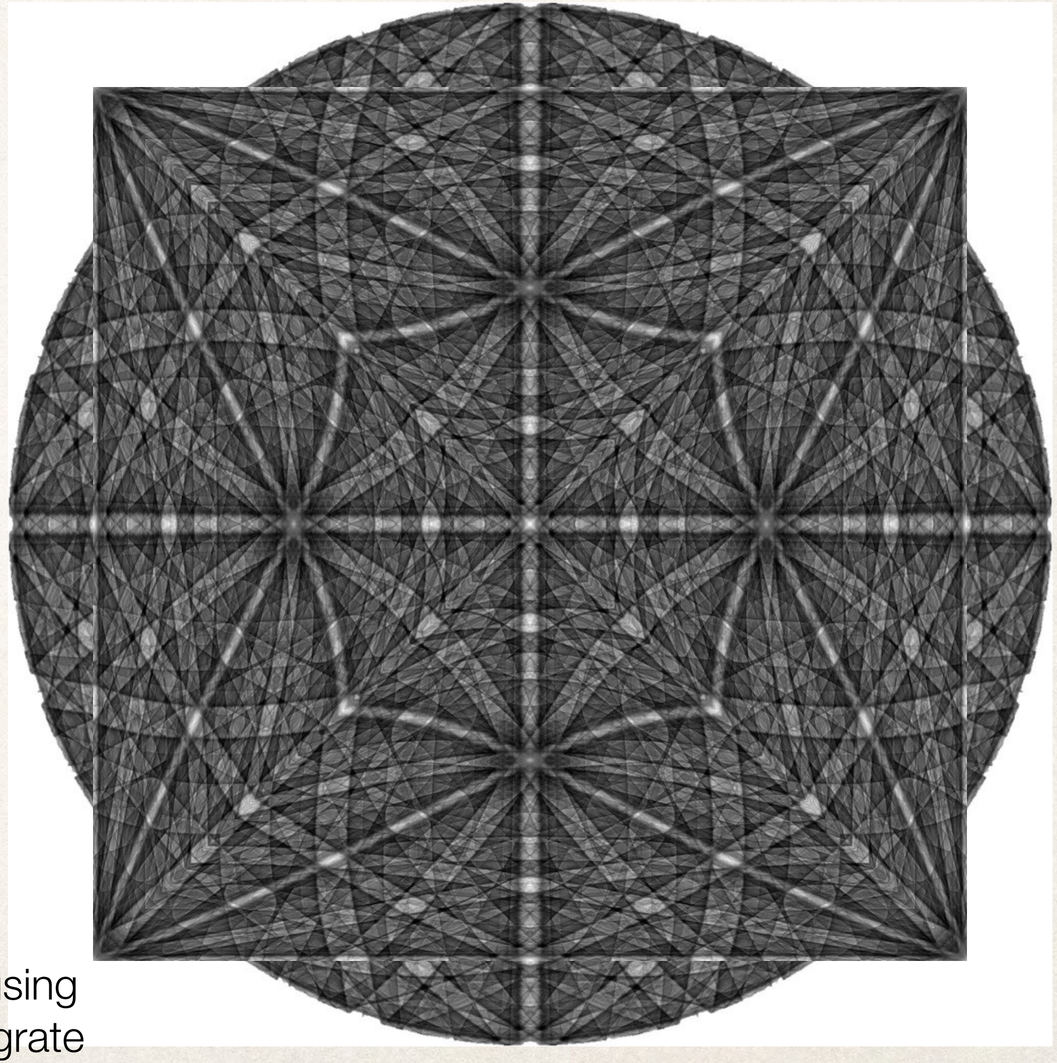
$$\bar{\lambda}_{\hat{\mathbf{k}}}(E, z) \equiv \frac{\lambda_{\hat{\mathbf{k}}}(E, z)}{N z_0(E)(E_{\max} - E_{\min})}$$

from Monte Carlo simulations

EBSD Forward Model: Dynamical Scattering

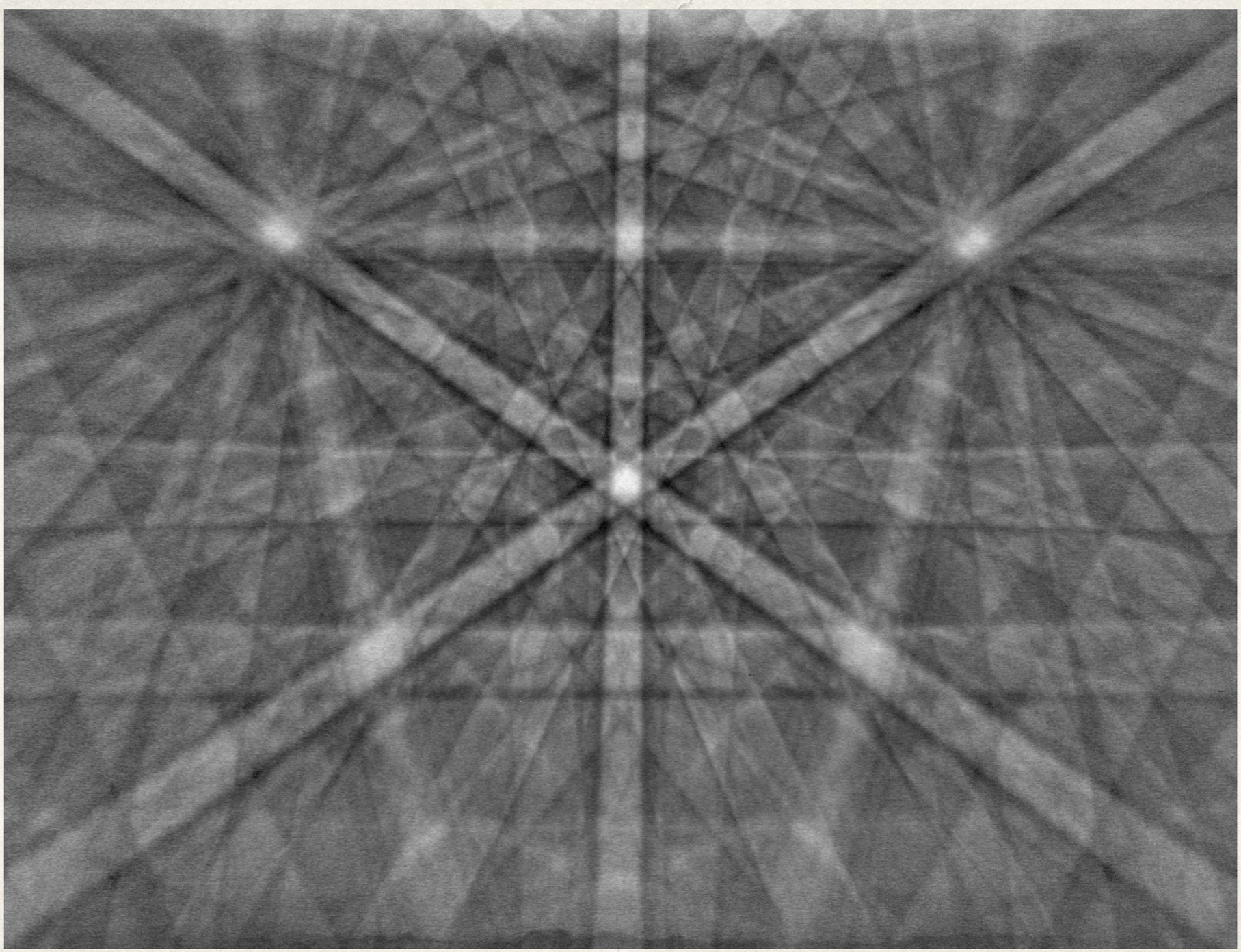


Ni
30 kV



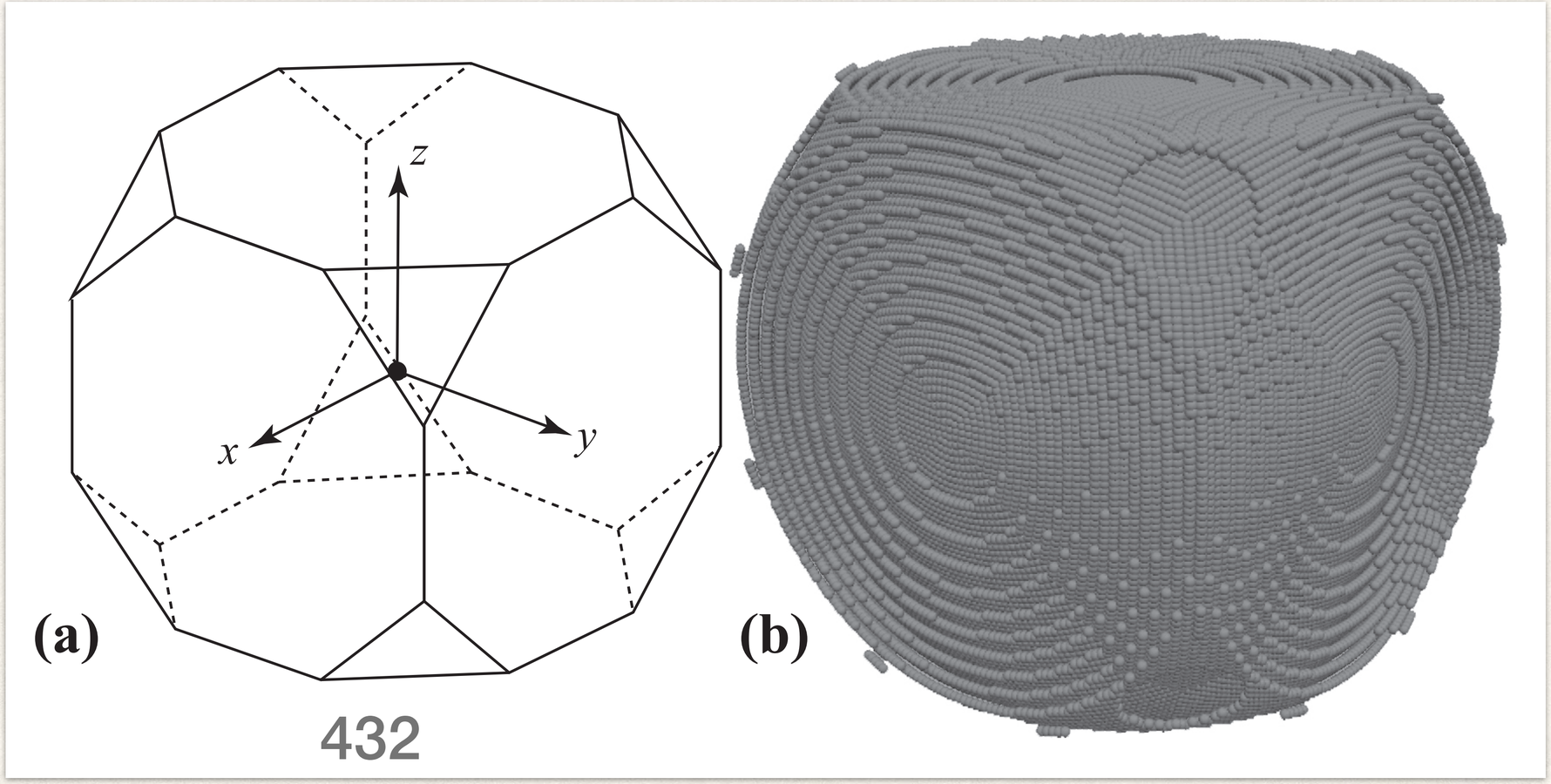
Solve Schroedinger equation using Bloch wave approach and integrate over depth of interaction volume

Si [111]



Cubochoric sampling of SO(3)

Cubic, N=100 -> 333,227 sampling points



D. Rosca, A. Morawiec, and M. De Graef. “A new method of constructing a grid in the space of 3D rotations and its applications to texture analysis”. *Modeling and Simulations in Materials Science and Engineering* 22, 075013 (2014)

Pattern Matching Engine: dot products

- convert each experimental/dictionary pattern into a column vector
  - e.g., 60x60 EBSD pattern results in a 3,600-component vector
- normalize this vector (length = 1)

Dictionary: $\hat{\mathbf{w}}_k \quad (1 \ldots k \ldots N_d)$

Experiment: $\hat{\mathbf{v}}_j \quad (1 \ldots j \ldots N_e)$

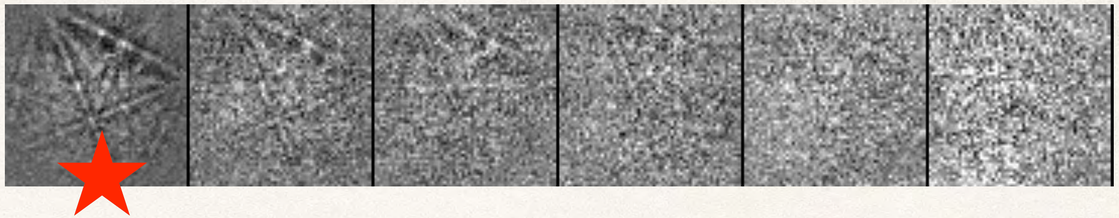
large numbers!

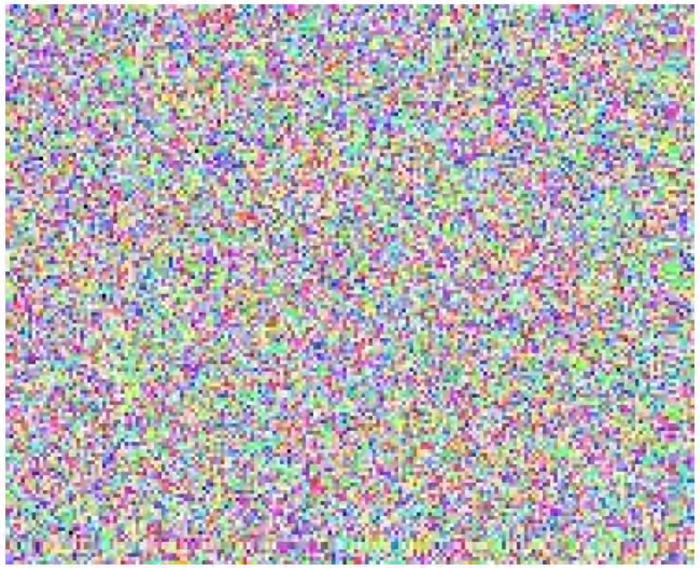
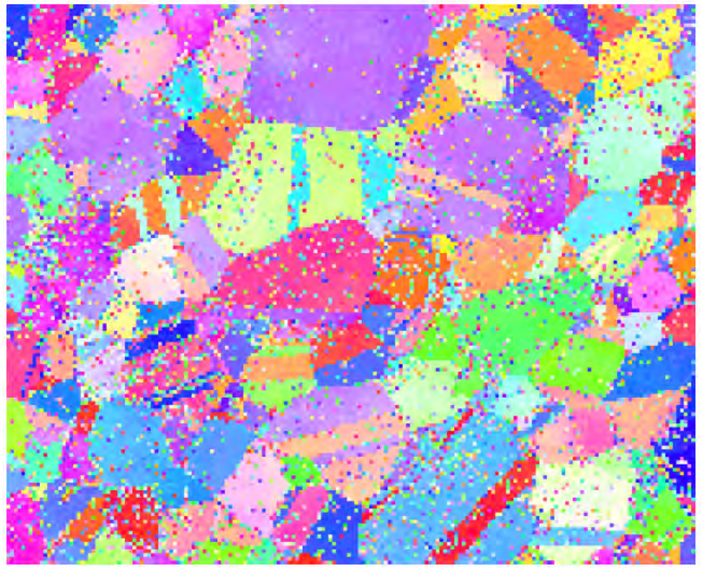
For each experimental pattern j, compute a vector of dot products:

$$\hat{\mathbf{d}}_j = (\hat{\mathbf{v}}_j \cdot \hat{\mathbf{w}}_1, \hat{\mathbf{v}}_j \cdot \hat{\mathbf{w}}_2, \ldots, \hat{\mathbf{v}}_j \cdot \hat{\mathbf{w}}_{N_d})$$

Sort the entries and keep the top 30-40 or so;
largest dot product = best match

Robustness against noise



CI Index Rate	OIM Analysis Result	Dictionary Result
0.1		

Derived maps

Average dot product map

(Fo)

Confidence Index map

(Fo)

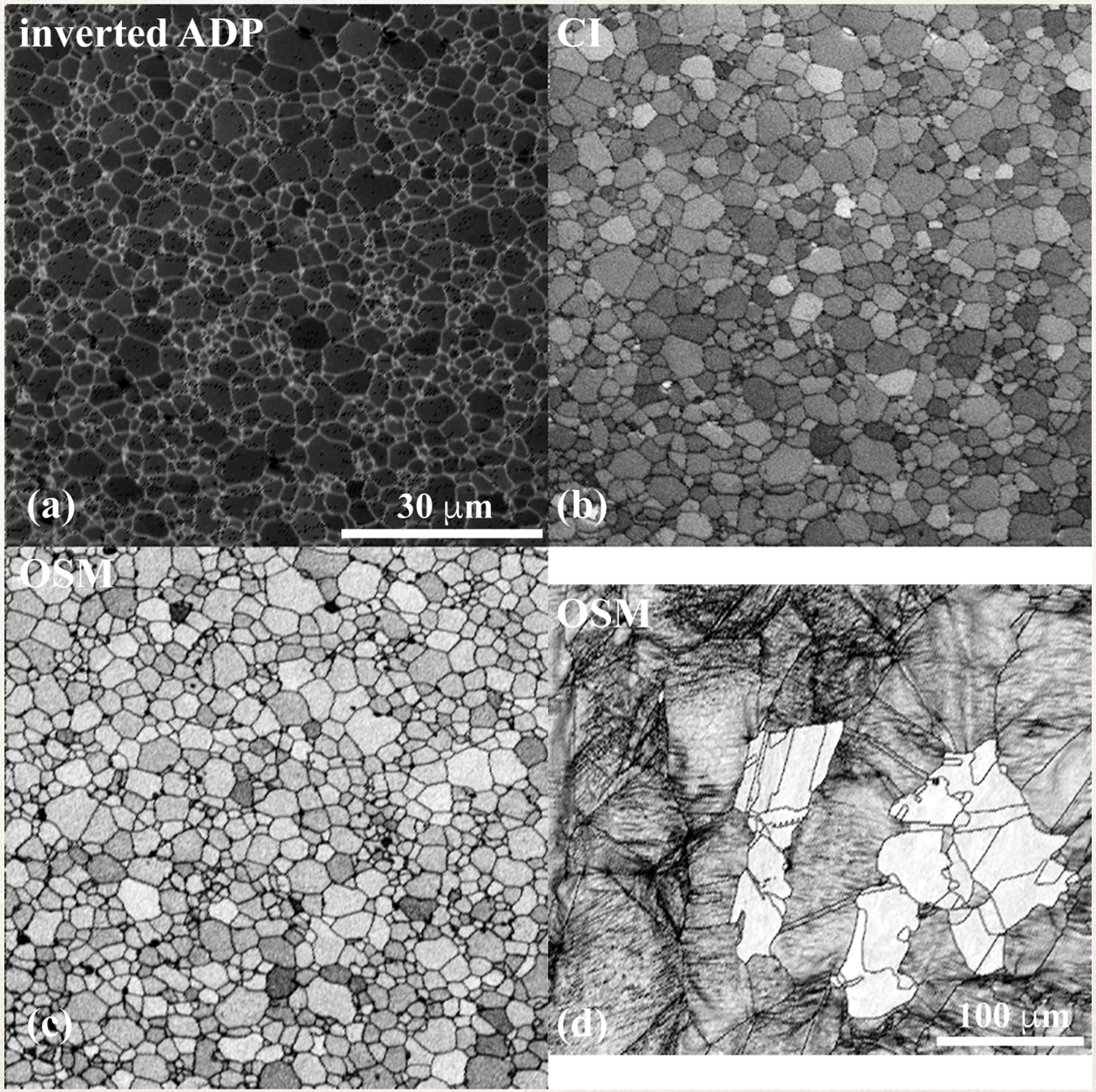
Orientation Similarity map

(Fo)

Orientation Similarity map

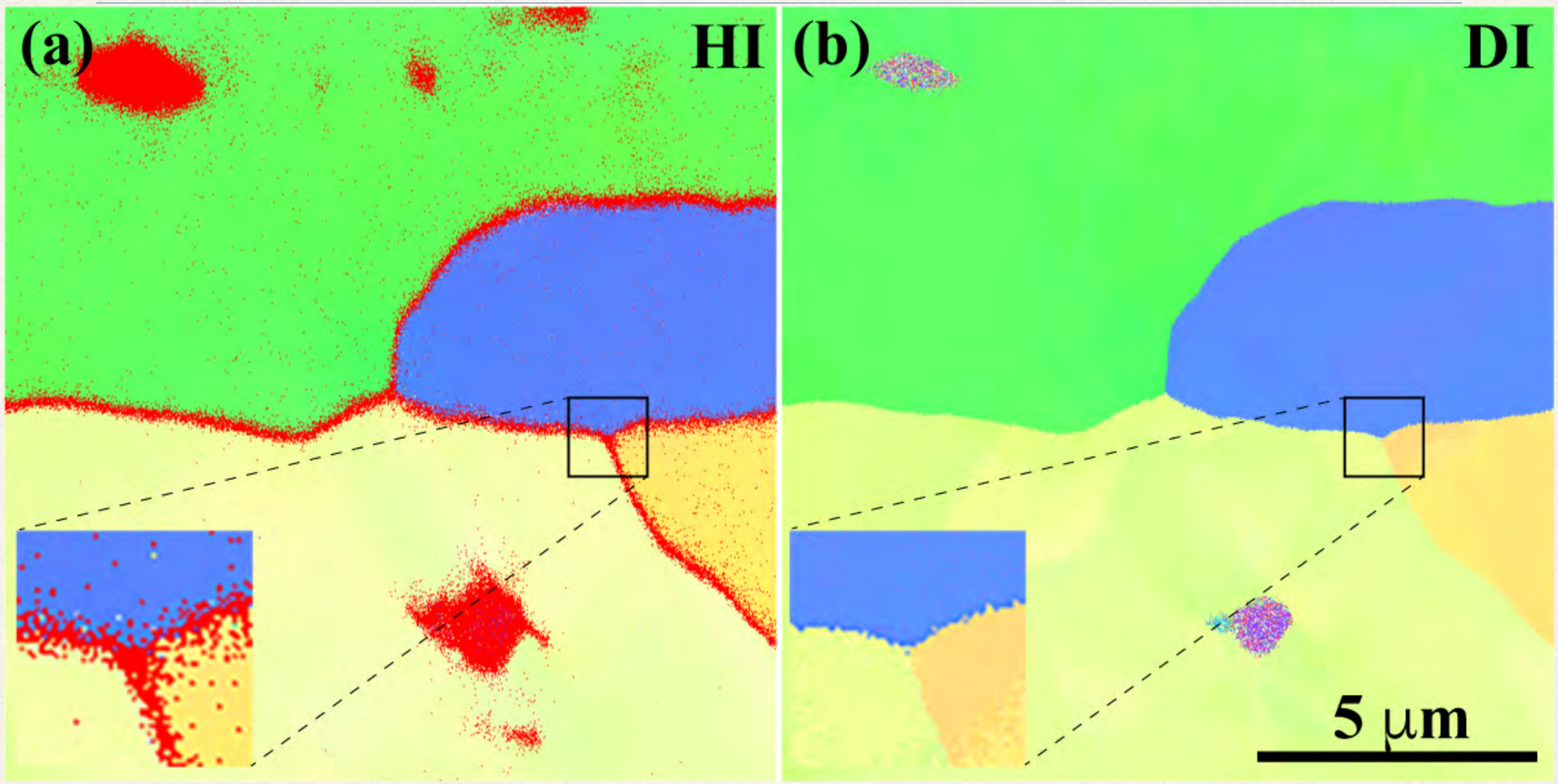
(partially recrystallized Cu)

Fo = Forsterite Mg_2SiO_4

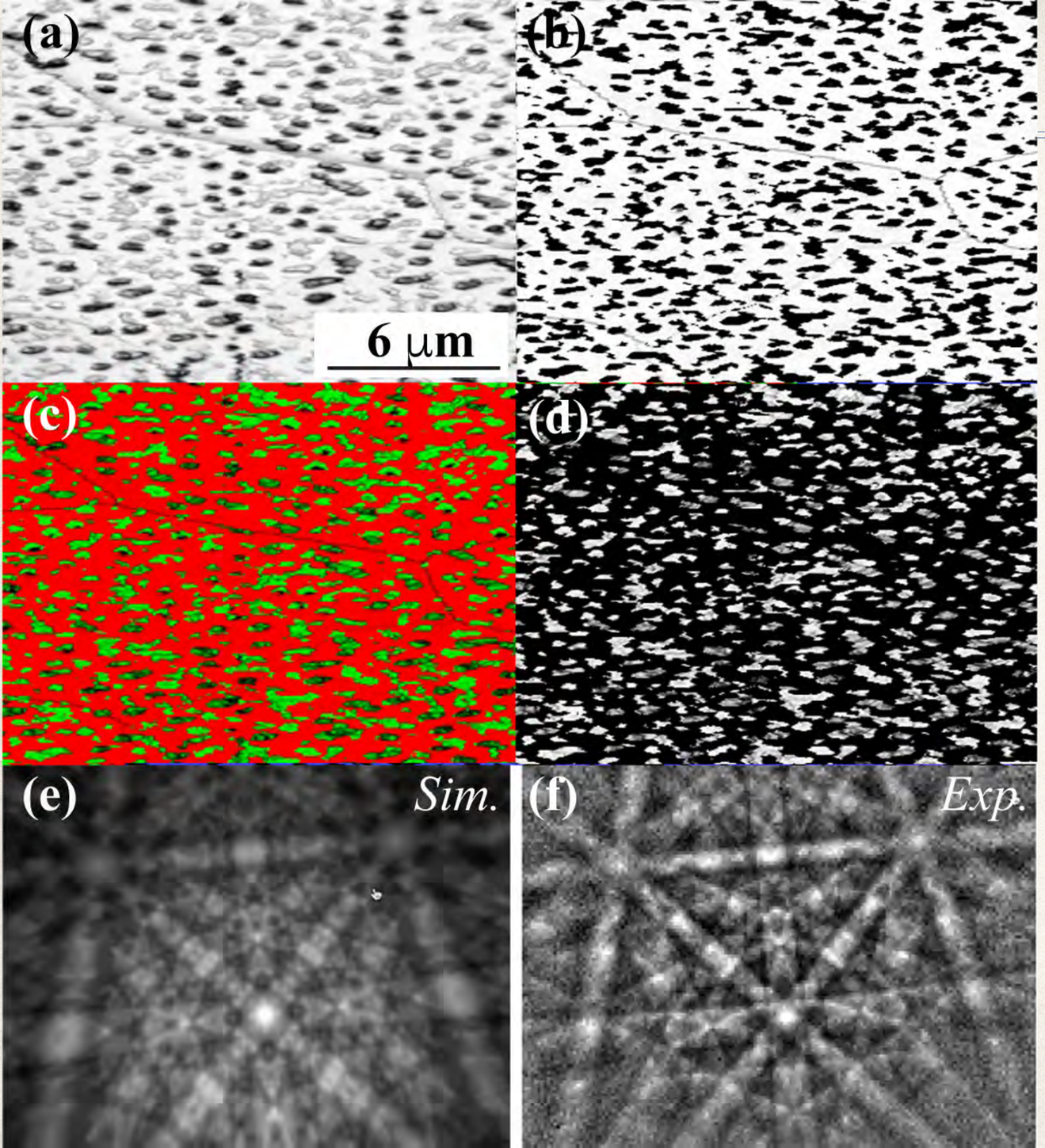


Shot-peened Al; collaboration U. Manchester

Overlap patterns



Note: There are no bad/missing points in the DI approach… hence, no need for in-painting or any other post-processing "correction" approaches…

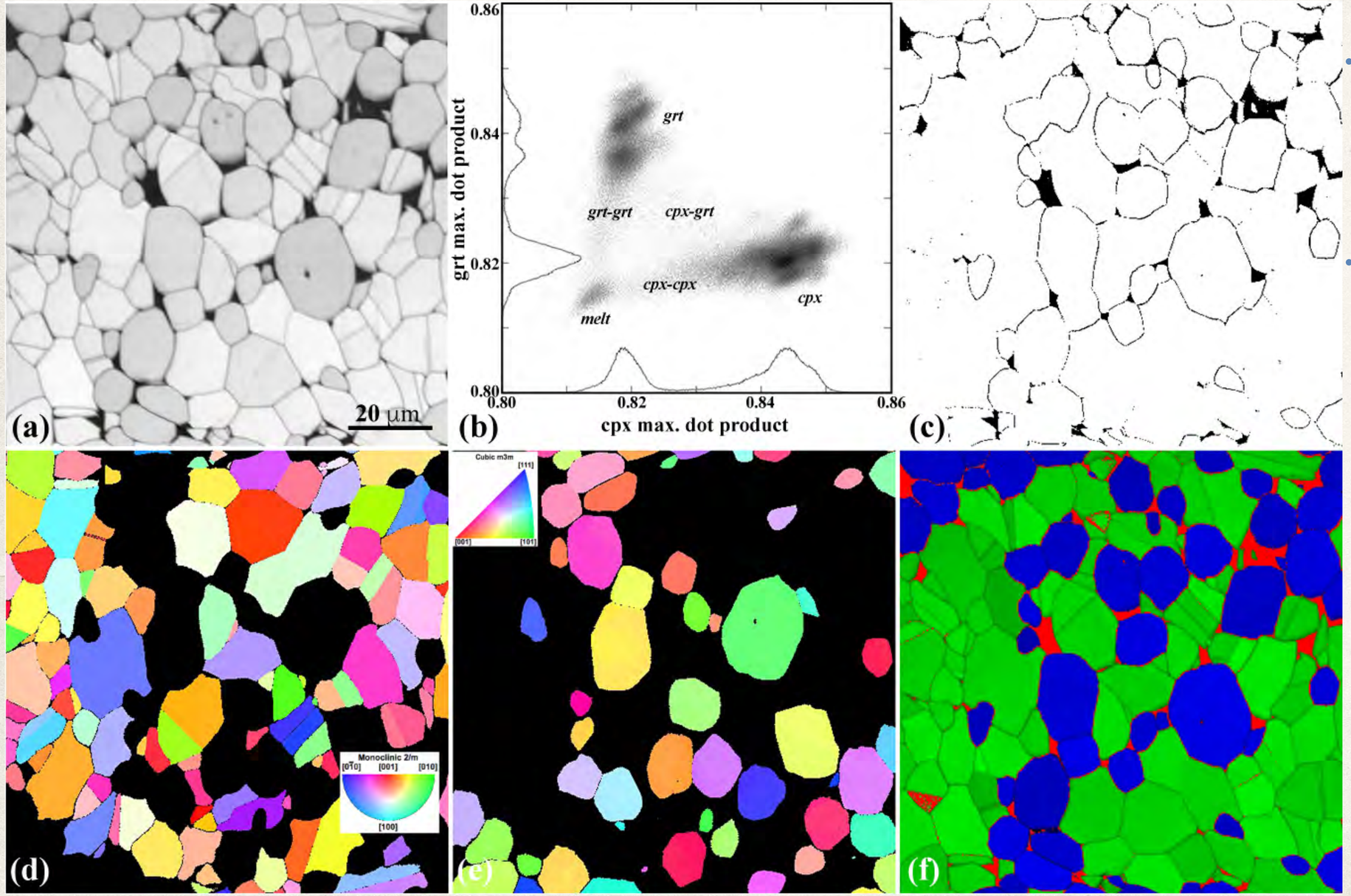


Similar crystal structures

- De-wetted Ag on poly-Ni substrate (7 keV, 40 nm step size)
- (a) ADP; (b) Ni OSM; (d) Ag OSM; (c) phase map (Ni red, Ag green); (e) experimental, (f) simulated patterns for Ag.

Collaboration with Dominique Chatain (Univ. Marseille, France)

Multi-phase Materials

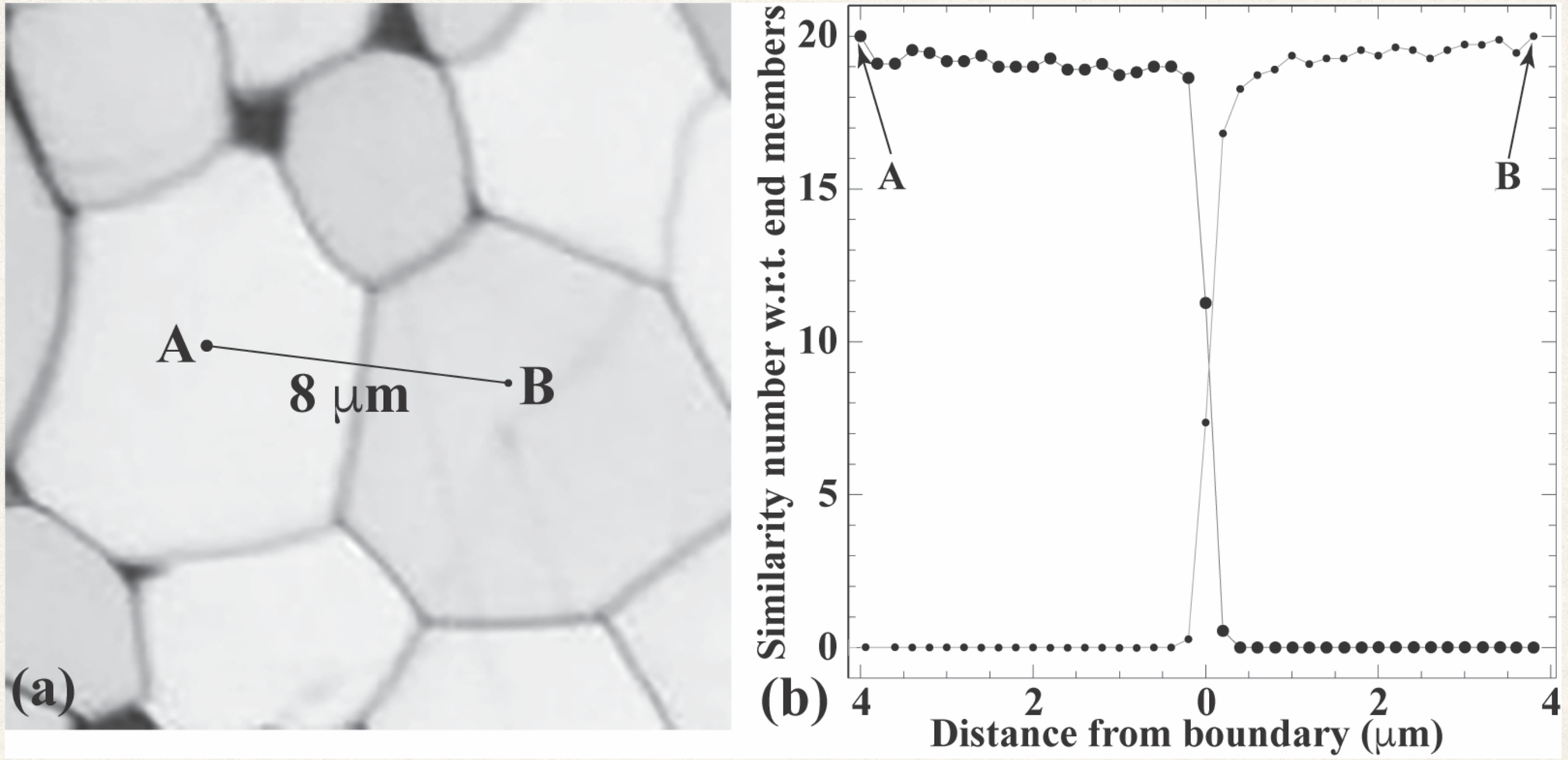


- garnet (cubic)
  clino-pyroxene (monoclinic)
  amorphous (glassy) phase

- (a) ADP map; (b) dot product joint histogram; (c) glassy region; (d) and (e) [001] IPF maps; (f) phase map (garnet blue, cpx green, glassy phase red)

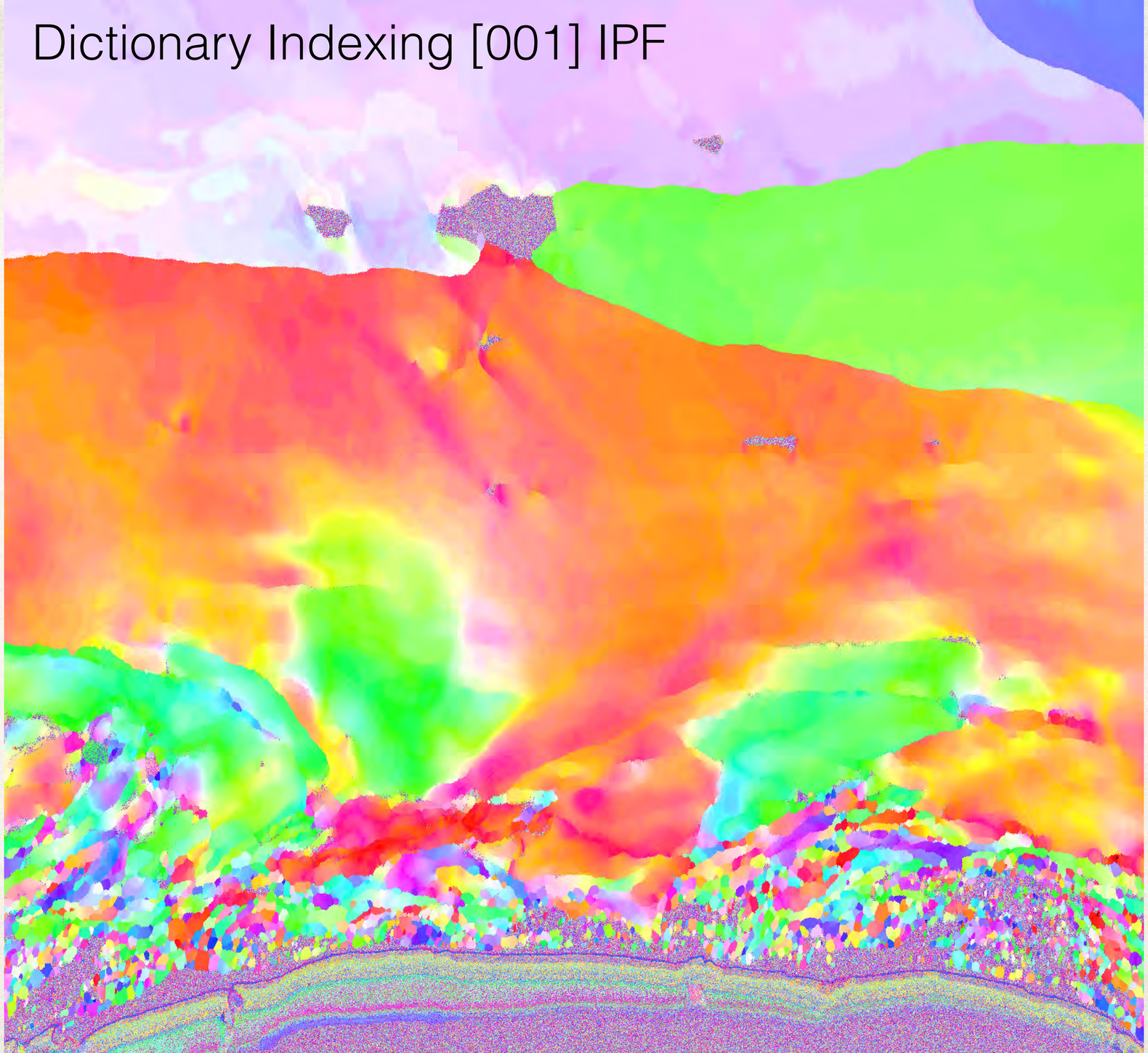
Collaboration with Katharina Marquardt (Imperial College)

Grain boundary location



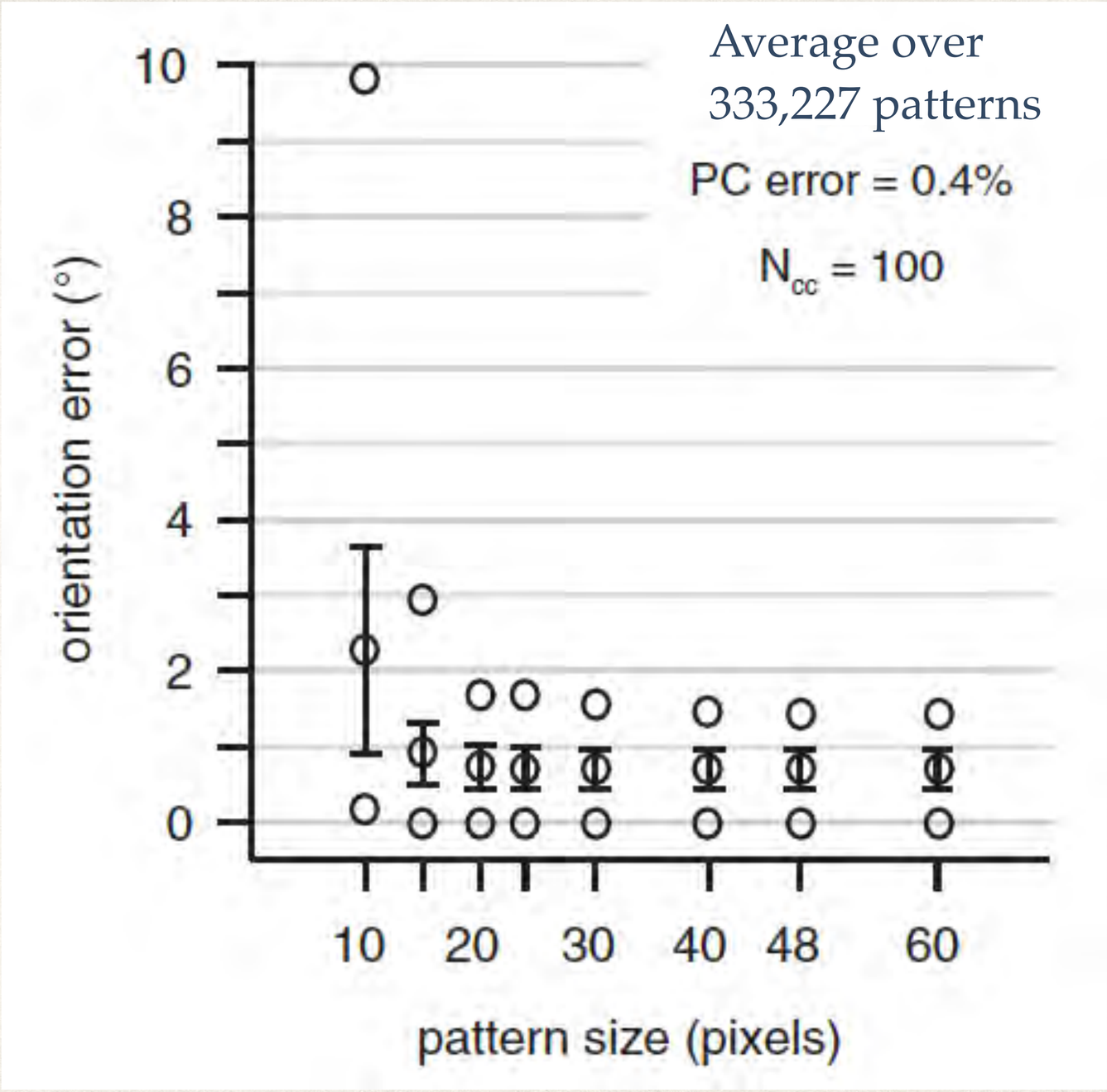
- OSM map allows for determination of GB location with sub-pixel accuracy

Shot-peened Al;
coll. U. Manchester



56x52 microns

So, how many pattern pixels do we really need?

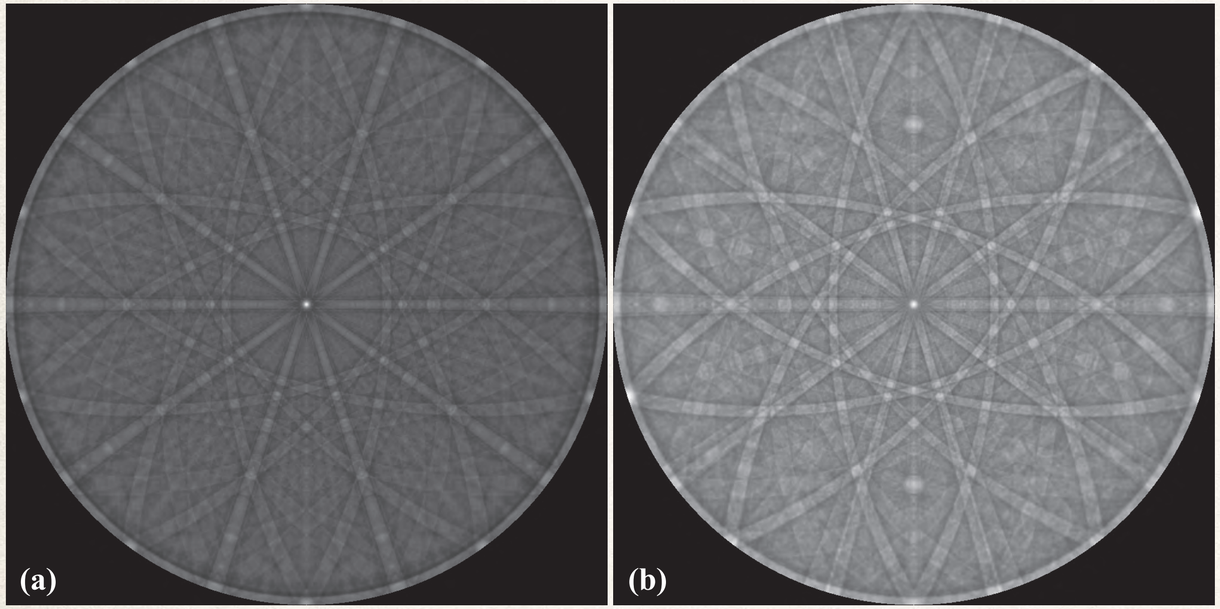


15x15 is sufficient for dictionary indexing !

F. Ram, S. Singh, S.I Wright and De Graef. "Error Analysis of Crystal Orientations Obtained by the Dictionary Approach to EBSD Indexings", Ultramicroscopy, 181, 17-26 (2017)

Quasicrystals ?

$Al_{70}Ni_{15}Co_{15}$

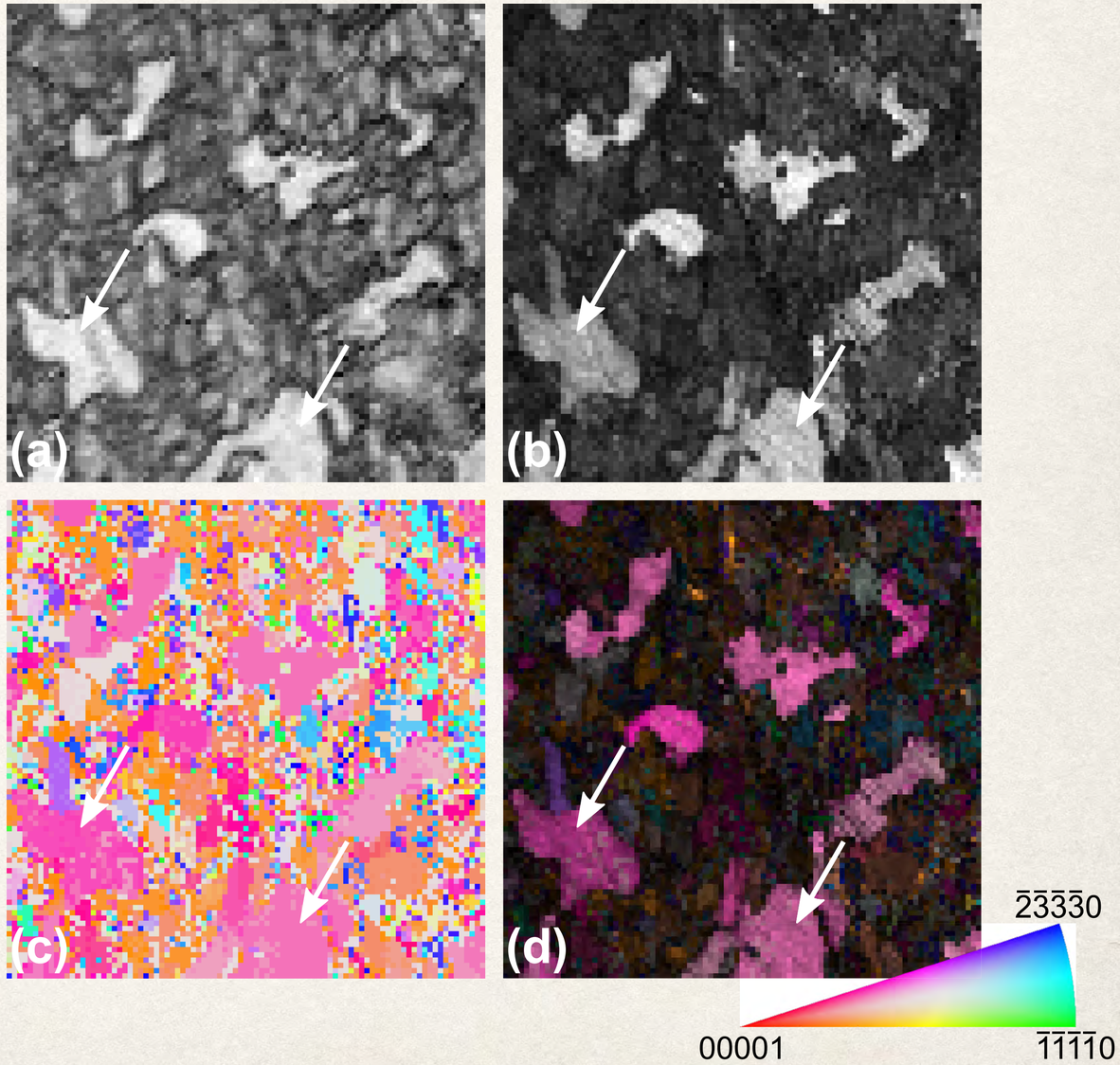


2D

$P10_5/mmc$

Approximant

Co_4Al_{13}



Availability: EMsoft

- All code is open source
  - EMsoft mostly written in fortran-90, with bits in C++ and OpenCL
  - BSD-2 license (completely open)
- Central location for all EMsoft-related links

http://vbff.materials.cmu.edu/EMsoft

Moving beyond dictionary indexing

- Strengths:
  - Robust against noise;
  - Always provides a solution (far less clean-up needed afterwards);
  - No issues with overlapping patterns;
  - Provides additional map types (e.g., OSM).
- Drawbacks:
  - execution time inversely proportional to rotational point group order;
  - brute force approach (each experimental pattern is tested against every dictionary pattern);
  - Requires significant computational resources (multi-CPU + GPU)

http://vbff.materials.cmu.edu/EMsoft

NEW: Spherical Indexing

- Instead of computing individual dictionary patterns, we back-project the experimental patterns onto the Kikuchi sphere and perform a spherical correlation; this results directly in the Euler angles for the experimental pattern.

- In principle, this is independent of crystal symmetry; in practice we get a faster algorithm if we include hard-coded symmetry aspects;

- Goal: keep DI strengths and remove most drawbacks.

- Secondary goal: provide real-time indexing.

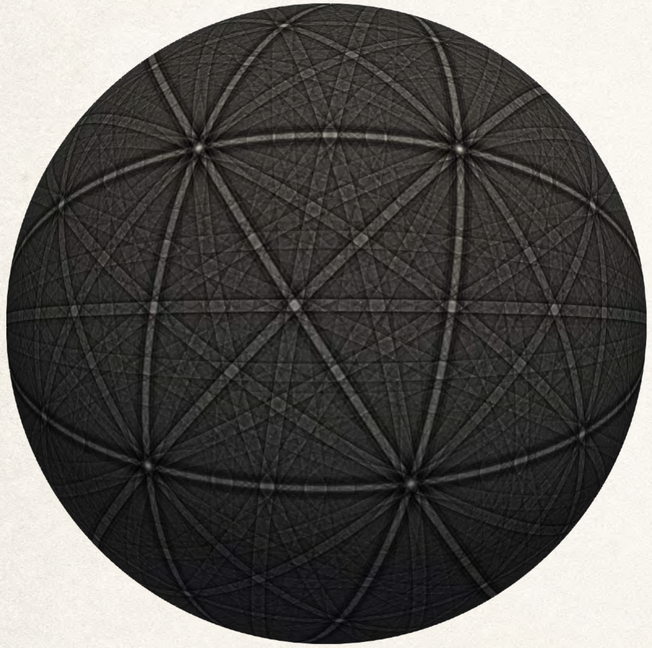
http://vbff.materials.cmu.edu/EMsoft

EMSphInx

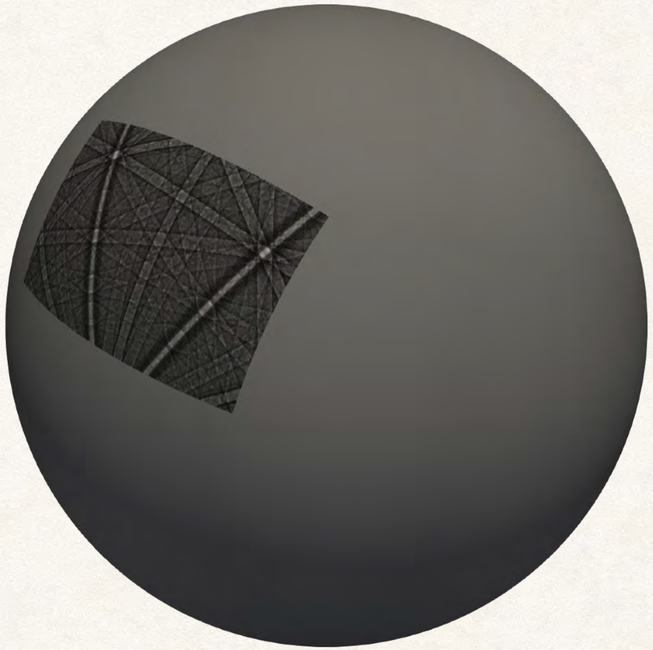
- Compute the spherical harmonic transform of the master pattern
- Back-project the experimental pattern onto the sphere, scale, and pad with zeroes; apply the spherical harmonic transform
- Cross-correlate the two transforms; this results in a 3D intensity array in Euler space.
- Find the location of the maximum intensity, taking into account crystallographic symmetry; that results in the orientation
- Refine the orientation by finding the peak more accurately.

http://vbff.materials.cmu.edu/EMsoft

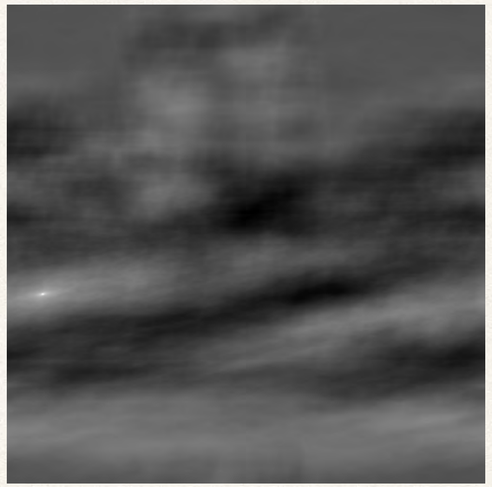
Efficient EBSD Master Pattern Indexing



$f(x)$



$g(x)$



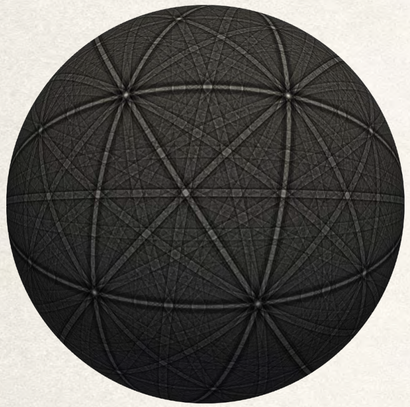
Orientation Space

$$\mathscr{F}^{-1}\left\{\overline{\mathscr{F}\{f\}}\mathscr{F}\{g\}\right\}$$

$\mathscr{F}$ On the sphere?

Spherical Harmonic Transformation

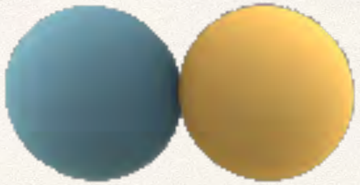
max l = bandwidth



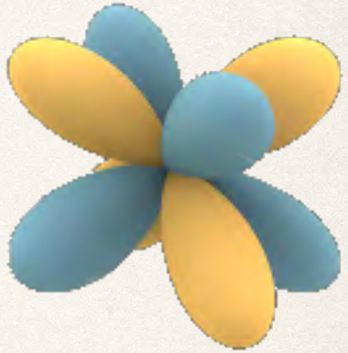
= a^0_0

+ a^1_0

+ a^1_1



... + a^l_m



	Fourier Transform	Spherical Harmonic Transform
Forward	$\mathscr{F}$	$\hat{f}^l_m \triangleq \mathscr{S}\{f(\theta,\phi)\} = \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} f(\theta,\phi)\overline{Y^l_m(\theta,\phi)}\sin\theta d\phi d\theta$
Inverse	$\mathscr{F}^{-1}$	$f(\theta,\phi) = \sum_{m=-l_{max}}^{l_{max}}\sum_{l=\lvert m\rvert}^{l_{max}} \hat{f}^l_m Y^l_m(\theta,\phi)$
Basis	$\exp(-2\pi i x\xi)$	$Y^l_m(\theta,\phi) = \sqrt{\frac{(2l+1)!(l-1)!}{4(l+m)!}} P^l_m(\cos(\theta))\exp(im\phi)$

Wikimedia commons

Spherical Cross Correlation

Spherical Cross Correlation for a Single Rotation

$$(f \star g)(R) \triangleq \int_{\theta,\phi} f(\theta,\phi)\overline{g(\theta_R,\phi_R)}d\phi d\theta$$
$$= \sum_{l,m,n} \hat{f}(l,m)\overline{\hat{g}(l,n)}D^l_{m,n}(R)$$

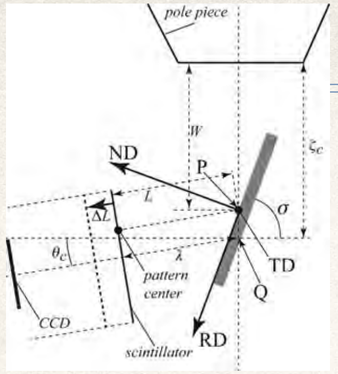
$$D^j_{k,m}(\alpha,\beta,\gamma) = d^j_{k,m}(\beta)\exp(im\alpha)\exp(ik\gamma)$$

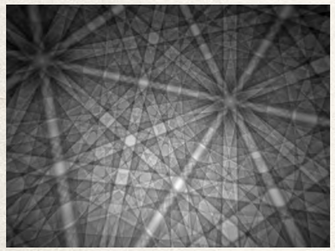
$$d^j_{k,m}(\beta) = \sqrt{\frac{(j+k)!(j-k)!}{(j+m)!(j-m)!}}\cos\left(\frac{\beta}{2}\right)^{k+m}\sin\left(\frac{\beta}{2}\right)^{k-m}P^{k-m,k+m}_{j-k}(\cos(\beta))$$

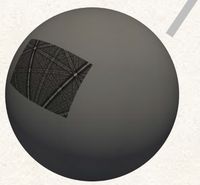
O(n^5) → n^3 ln(n)

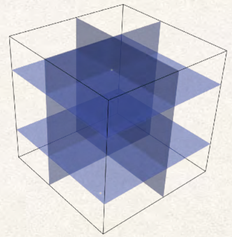
$$(f\star g)(\alpha,\beta,\gamma) = \mathscr{F}^{-1}\left\{\sum_l \hat{f}(l,m)\overline{\hat{g}(l,n)}d^l_{m,k}\left(\frac{\pi}{2}\right)d^l_{k,n}\left(\frac{\pi}{2}\right)\right\}\left(\alpha+\frac{\pi}{2},\beta+\pi,\gamma+\frac{\pi}{2}\right)$$

Indexing Algorithm

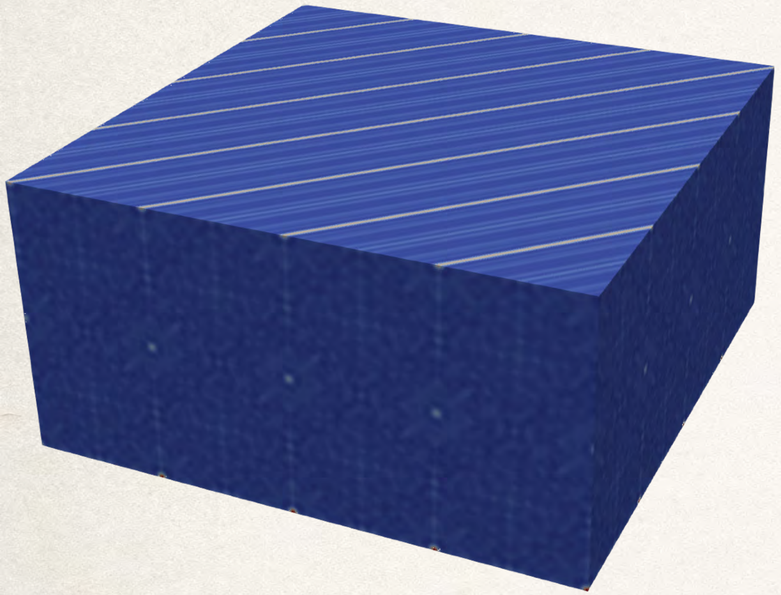


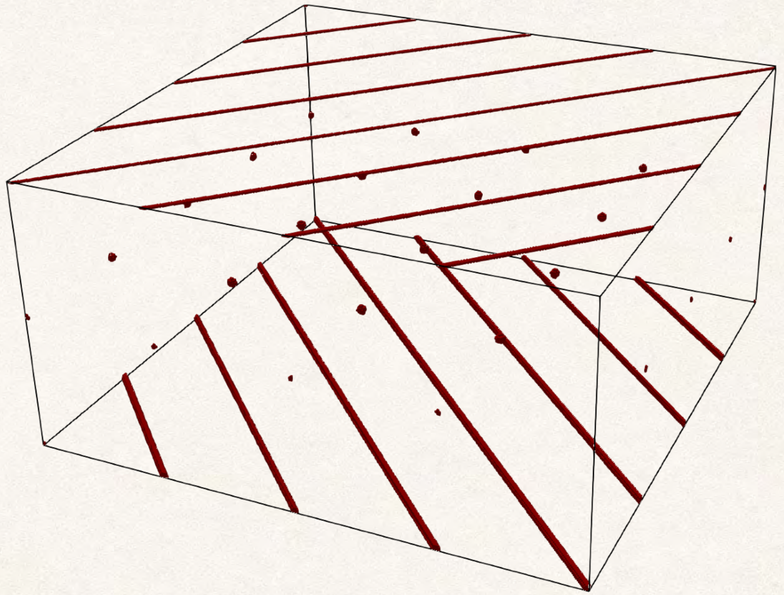


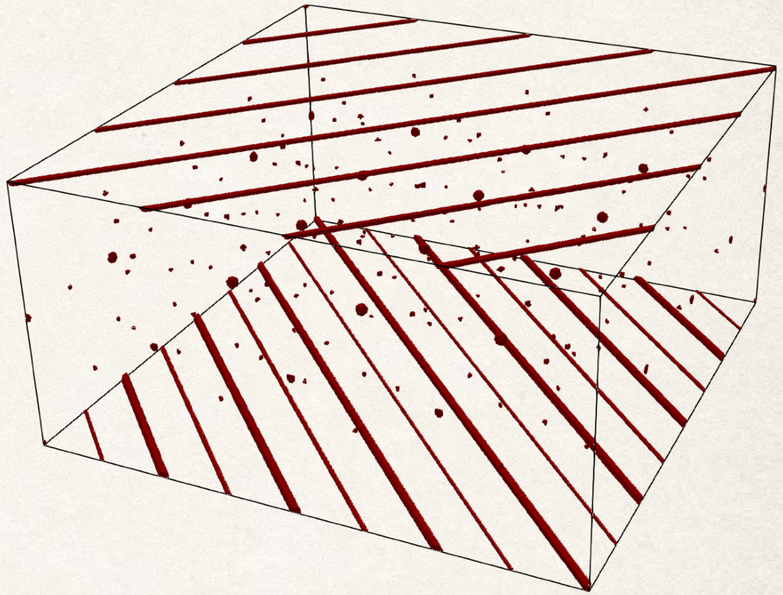


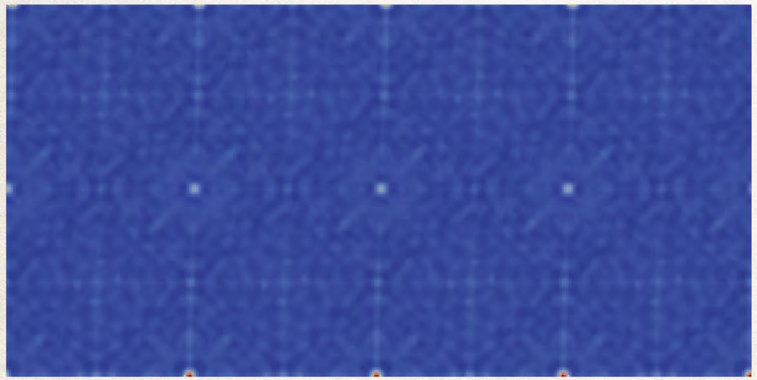


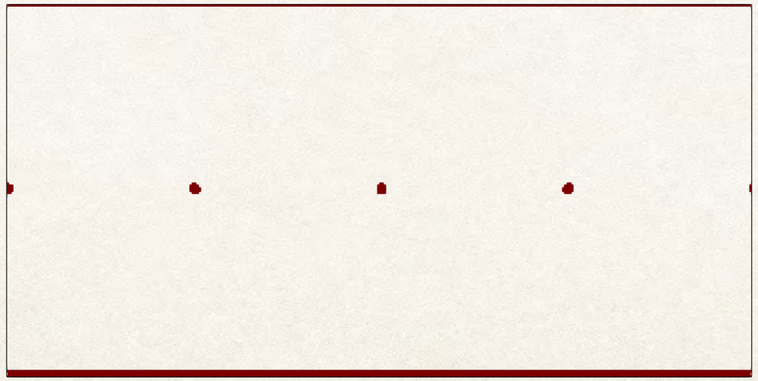
Spherical Autocorrelation (Pseudosymmetry)

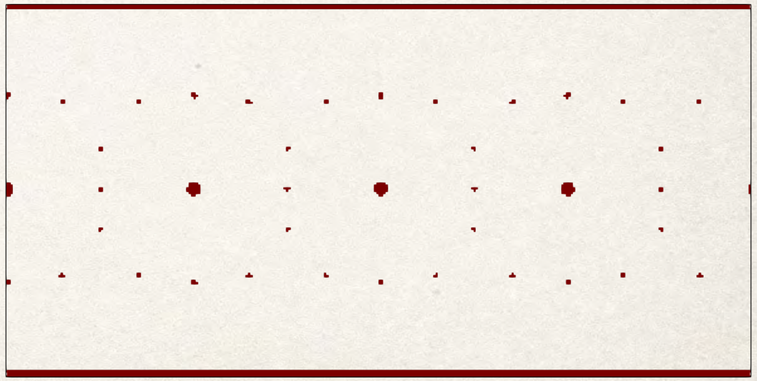










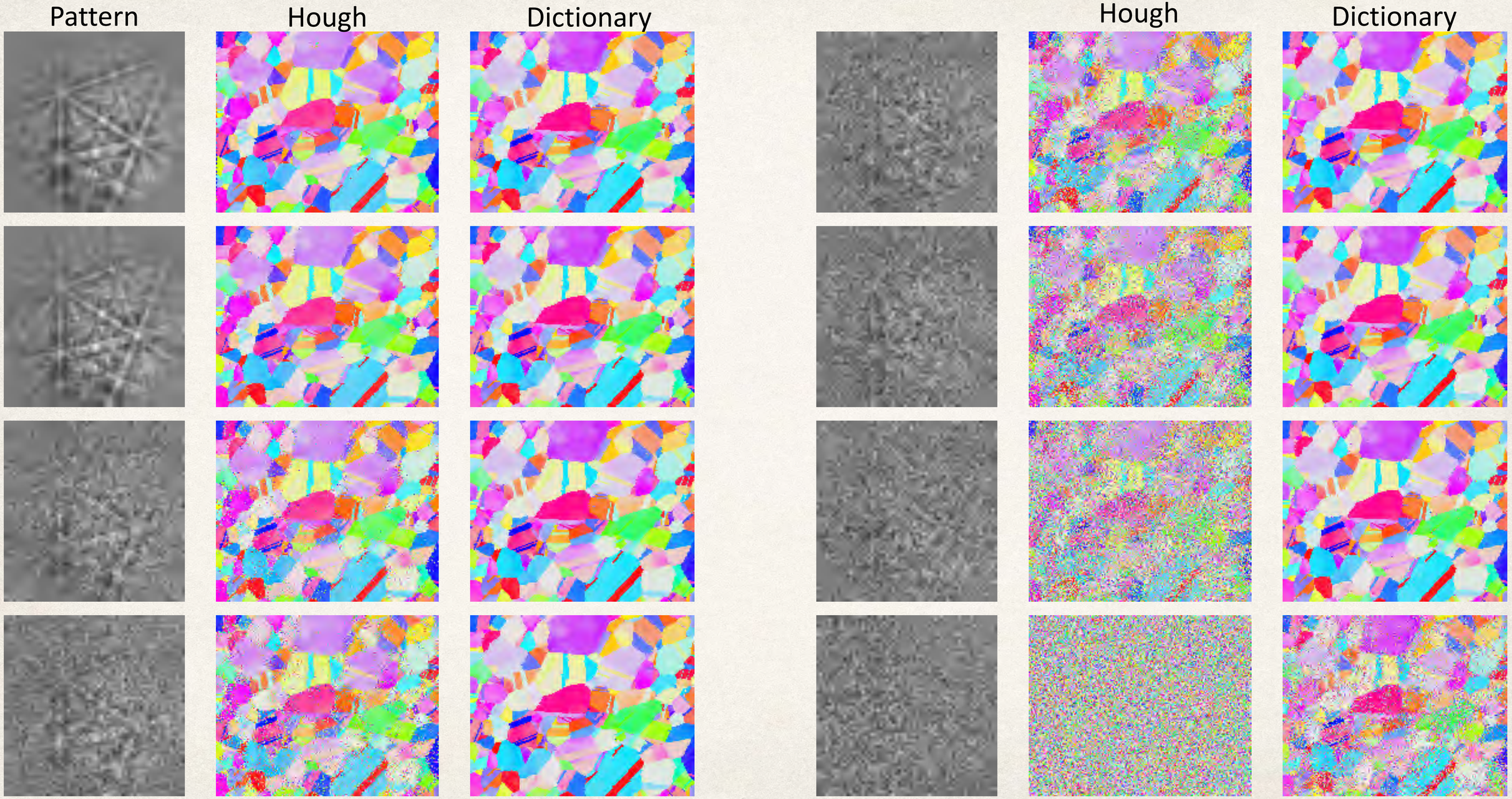


Autocorrelation (Nickel)

Highest →Symmetry

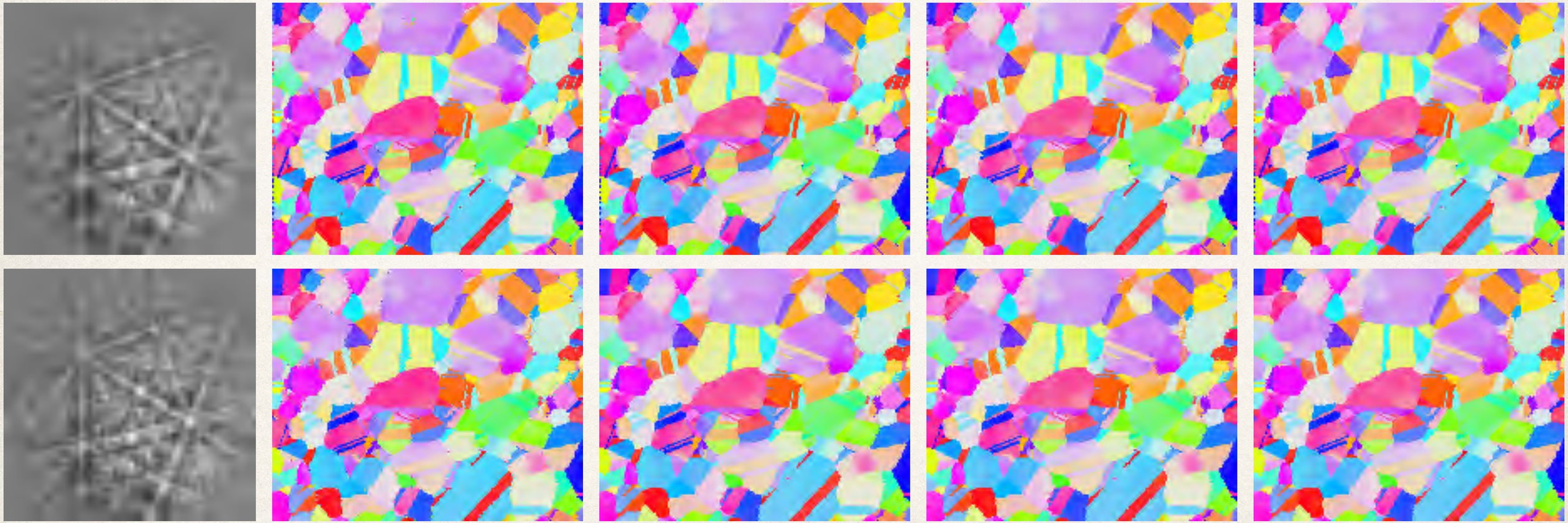
Next Highest →Pseudosymmetry

$O(n^8) \rightarrow \quad n^3 \ln(n)$



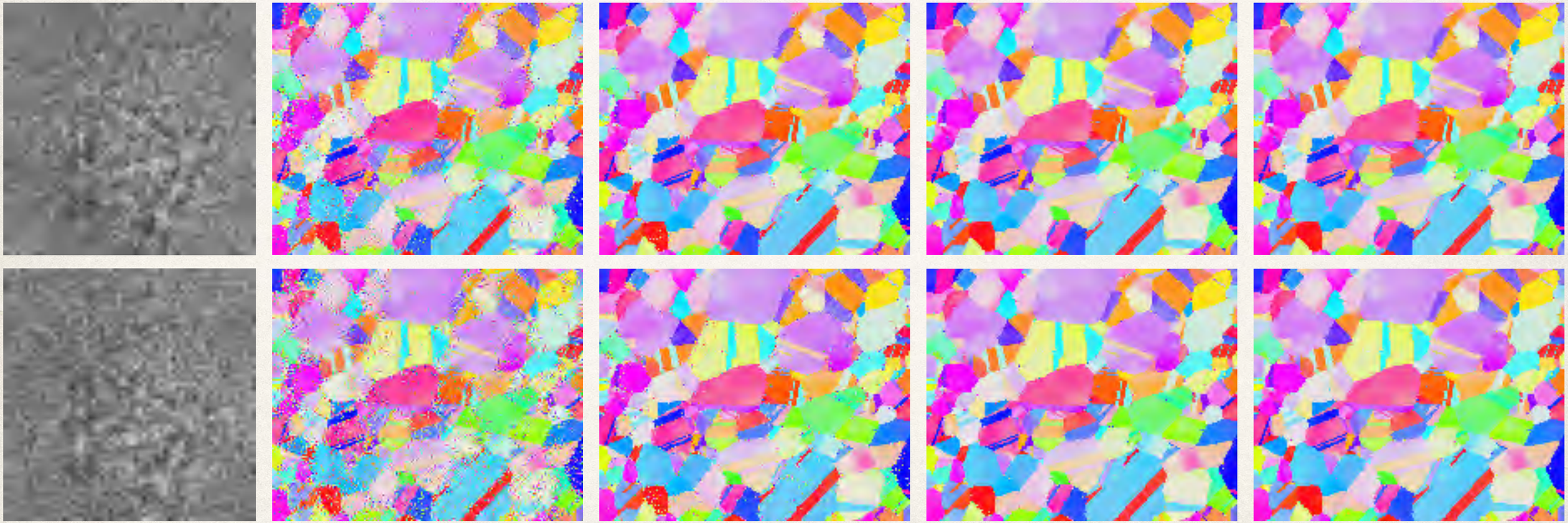
Data courtesy of Stuart Wright

First Pattern | Hough Indexing | Bandwidth = 53 | Bandwidth = 63 | Bandwidth = 74



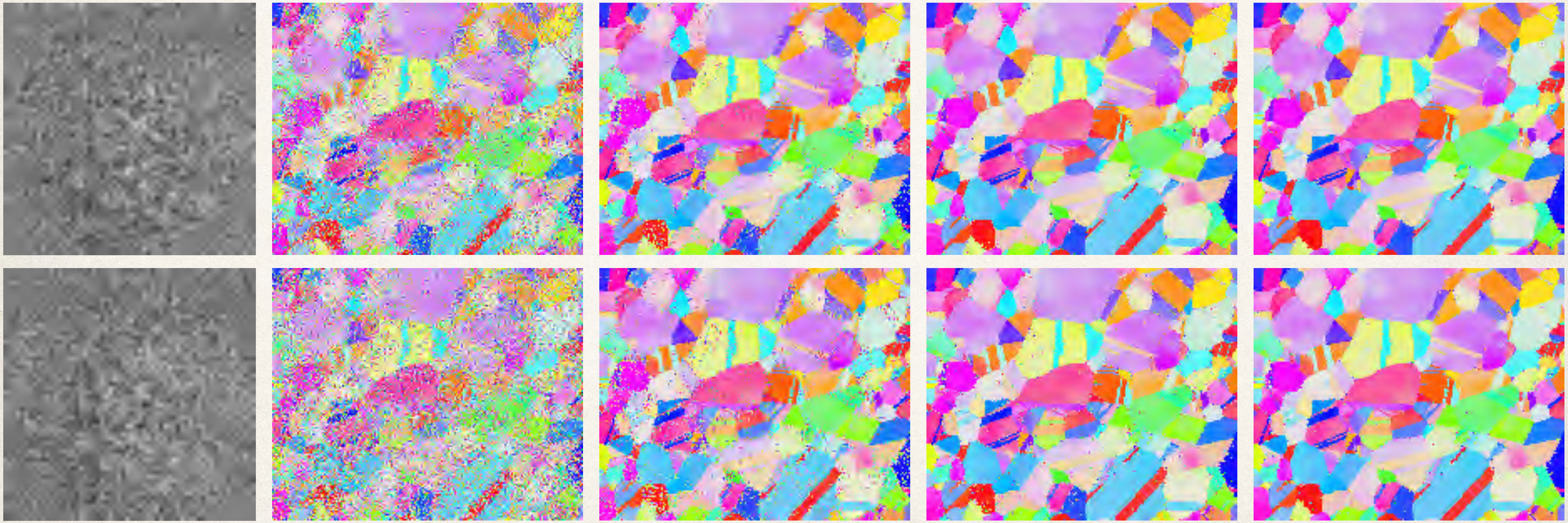
Data courtesy of Stuart Wright

First Pattern | Hough Indexing | Bandwidth = 53 | Bandwidth = 63 | Bandwidth = 74



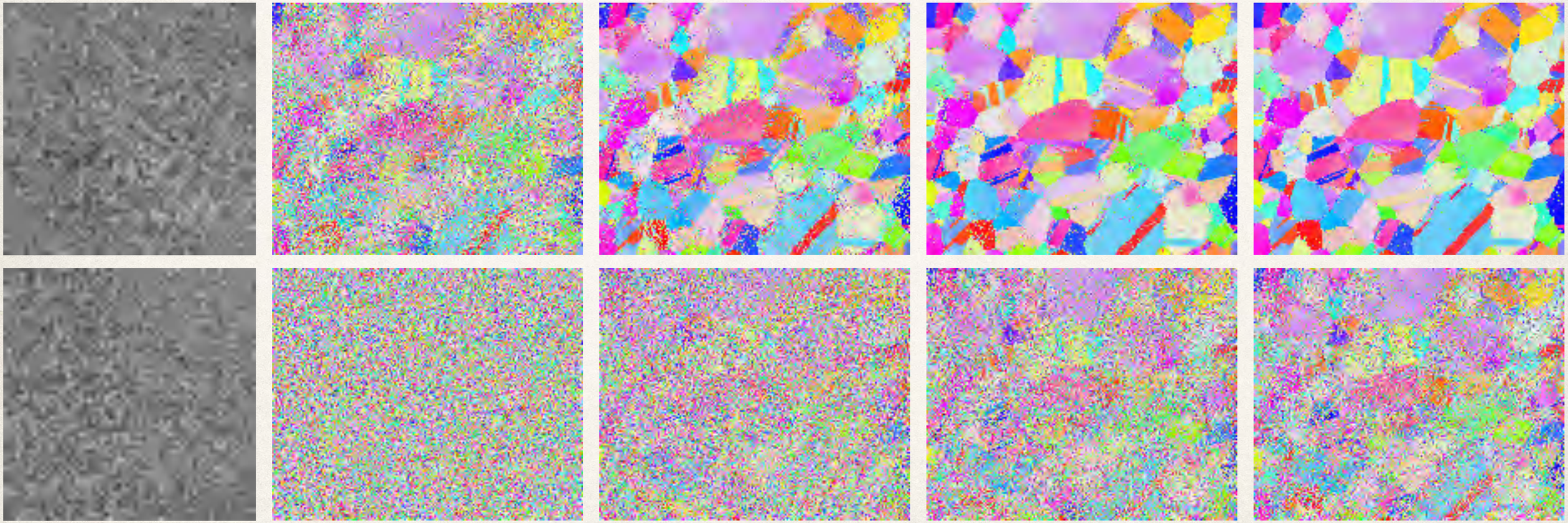
Data courtesy of Stuart Wright

First Pattern | Hough Indexing | Bandwidth = 53 | Bandwidth = 63 | Bandwidth = 74



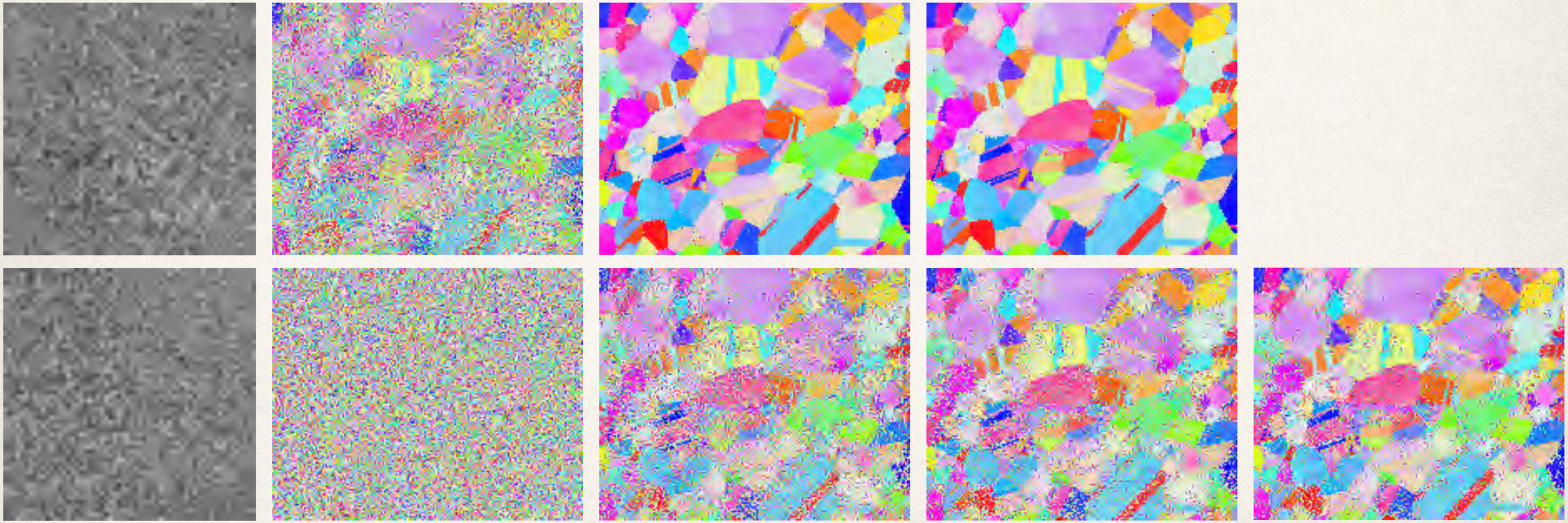
Data courtesy of Stuart Wright

First Pattern | Hough Indexing | Bandwidth = 53 | Bandwidth = 63 | Bandwidth = 74



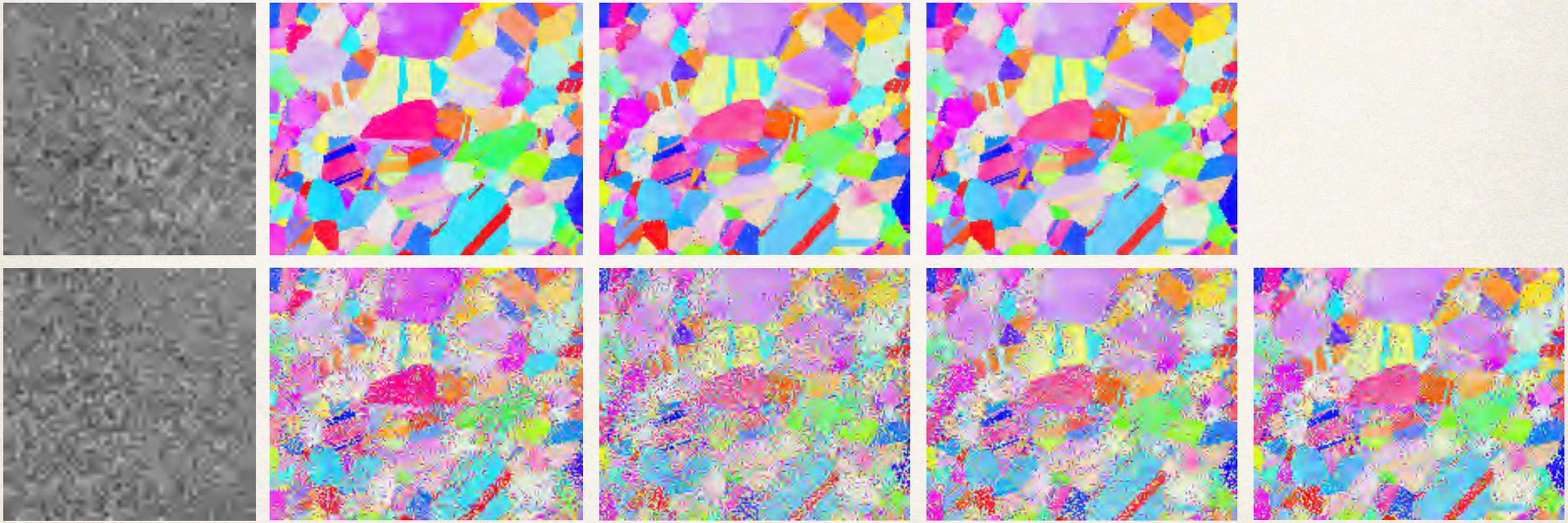
Data courtesy of Stuart Wright

First Pattern | Hough Indexing | Bandwidth = 88 | Bandwidth = 113 | Bandwidth = 158



Data courtesy of Stuart Wright

First Pattern | Dictionary Indexing | Bandwidth = 88 | Bandwidth = 113 | Bandwidth = 158



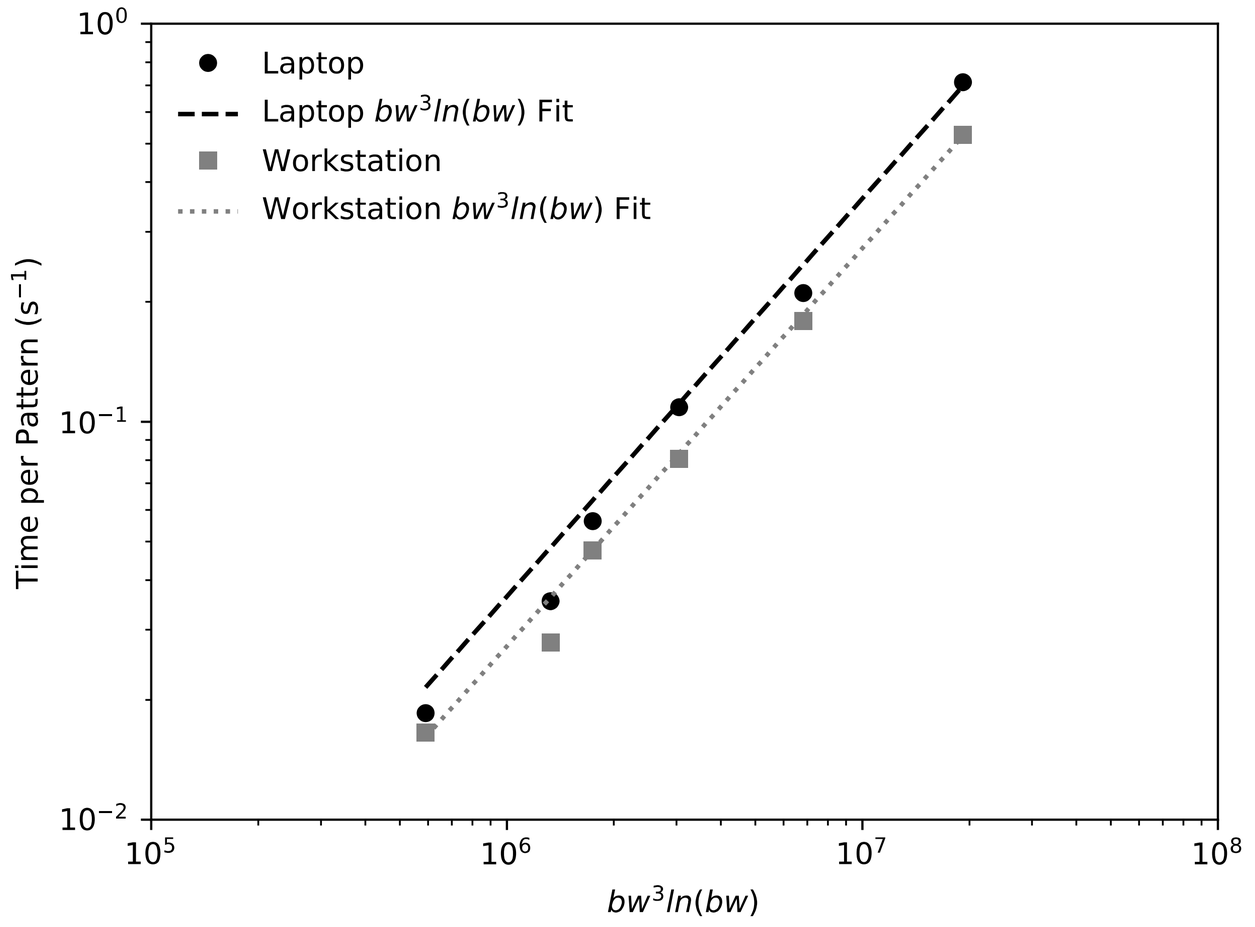
Data courtesy of Stuart Wright

EMSphInx

EM (Sp)herical (H)armonics (In)de(x)ing

$$b = \frac{1}{2}\left(1 + 3^p 5^q 7^r 11^s\right)$$

	Laptop (4 cores)		Workstation (24 cores)	
Band Width	Pat/s	Wall time	Pat/s	Wall time
53	216	2:10	1450	19.4
68	113	4:08	860	32.6
74	71.1	6:35	506	55.5
88	36.8	12:44	298	1:34
113	19.0	24:39	134	3:30
158	5.61	1:23:25	45.6	10:16



Dictionary Indexing (Workstation + GPU)
Indexing : 172 pat/s (2:36)
With Refinement: 149 pat/s (3:09)

28,000 Patterns

Summary

- Dictionary indexing is significantly more robust than Hough indexing and has been successfully used in heavily deformed materials and for low signal-to-noise data sets. Execution time increases with decreasing crystal symmetry.

Tutorial : 10.1007/s40192-019-00137-4

- Spherical cross correlation is nearly mathematically equivalent to dictionary indexing but is much faster; execution time is nearly independent of the crystal symmetry.

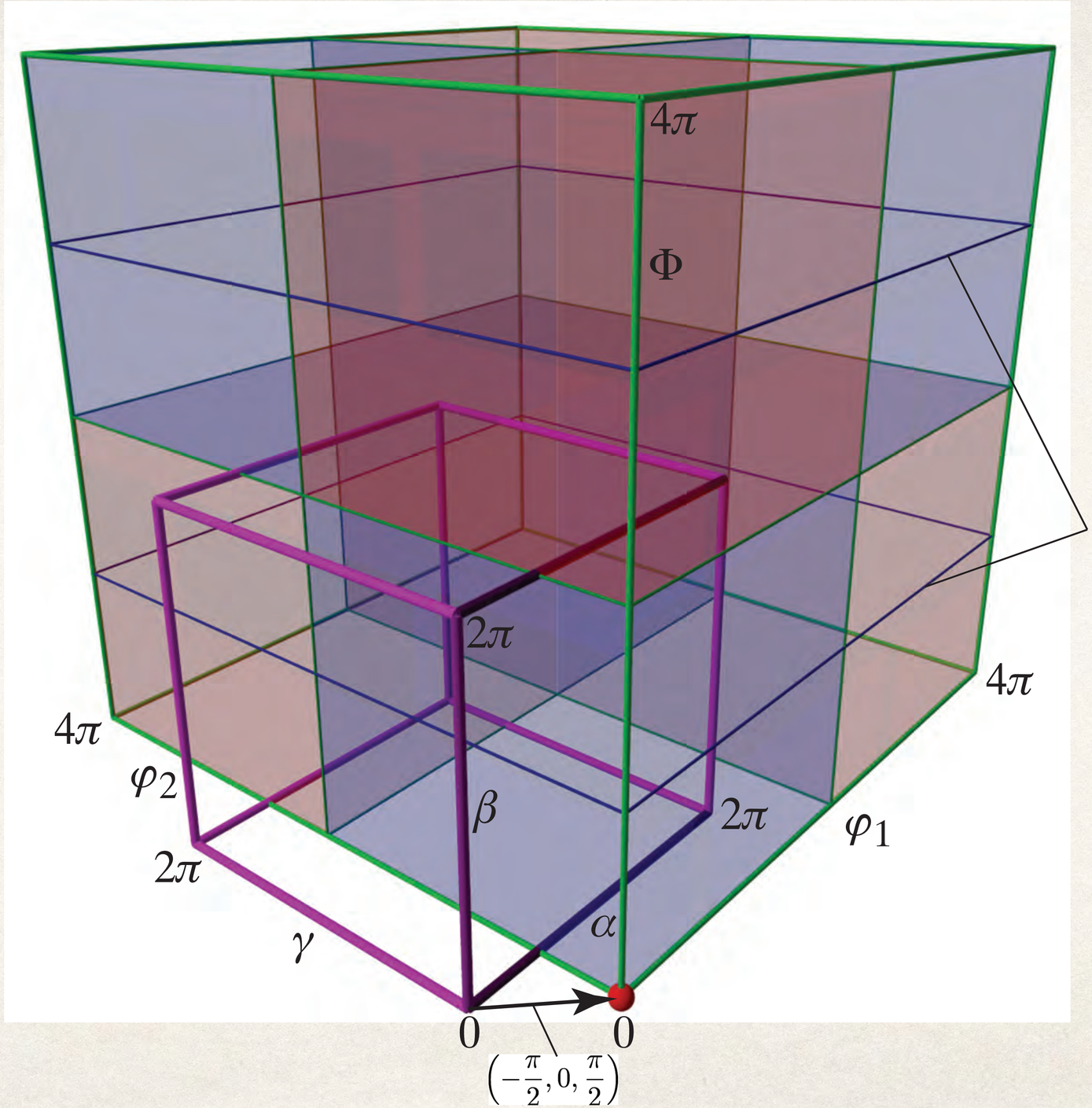
- Pseudosymmetry can be predicted by means of a master pattern auto-correlation

- Real time forward model based indexing is possible

EMSphInx will be made available under a non-commercial open-source license as part of the EMsoft 4.3 release (this Summer).

http://vbff.materials.cmu.edu/EMsoft

Questions ?


4π
Φ
2π
4π
4π
φ_2
β
2π
φ_1
2π
γ
α
0
0
$\left(-\frac{\pi}{2}, 0, \frac{\pi}{2}\right)$
diagonal glide planes

$$dV = \sin\Phi \, d\varphi_1 \, d\Phi \, d\varphi_2$$

Euler angles are degenerate when Phi=0