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Computational Imaging XI

Charles A. Bouman
Ilya Pollak
Patrick J. Wolfe
Editors

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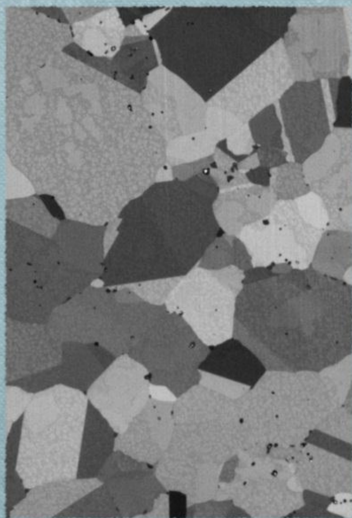

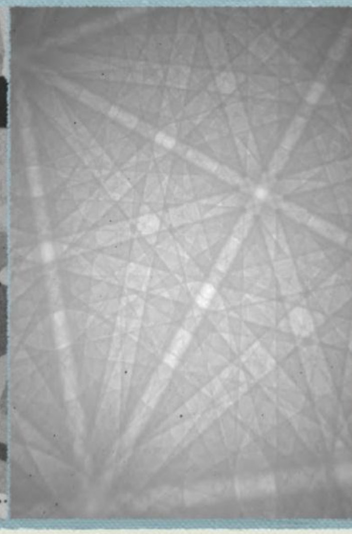

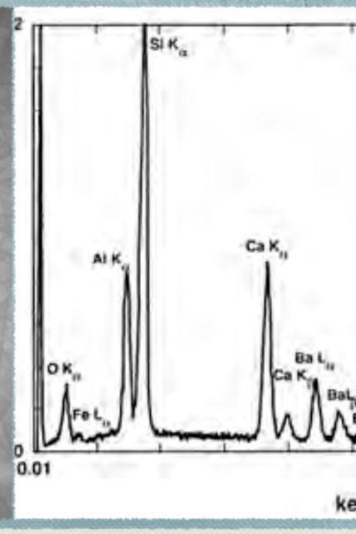

Imaging Diffraction Spectroscopy

A forward modeling approach to electron back-scatter diffraction patterns

Marc DeGraef
Carnegie Mellon University

SPIE, 2/6/13, 8657-17

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Funding Sources

- ONR ONR N00014-12-1-0075
- MURI AFOSR-FA9550-12-1-0458
- Electronic Imaging component of the ICMD program of the Materials and Manufacturing Directorate (AFRL)

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Outline

- Background on EBSD
- Geometry and special projections
- Dynamical simulations
- What's next?
- Summary

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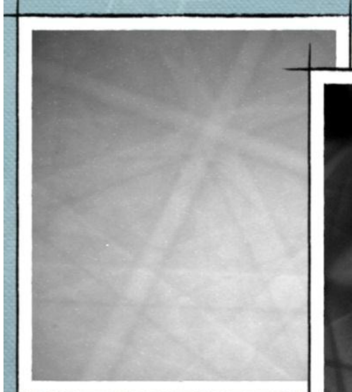
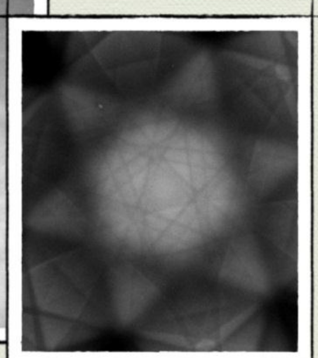
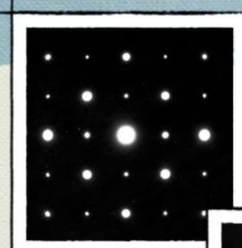
Lots of electron diffraction modalities ...



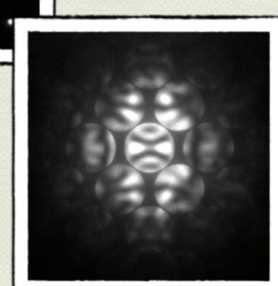
EBSD



ECP



SADP



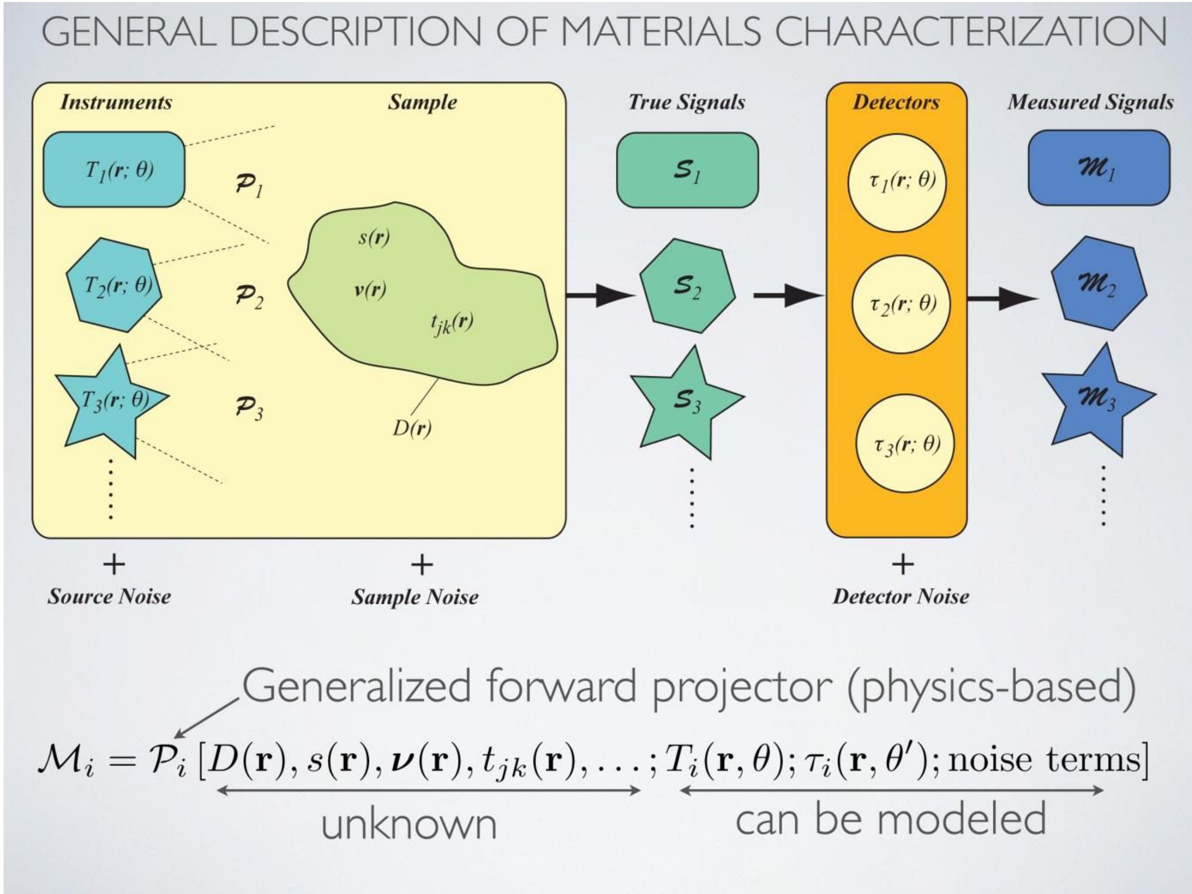
CBED

Scanning

Transmission

There's only one theory that underlies all of these modalities ...

x Wednesday, February 13, 13 4



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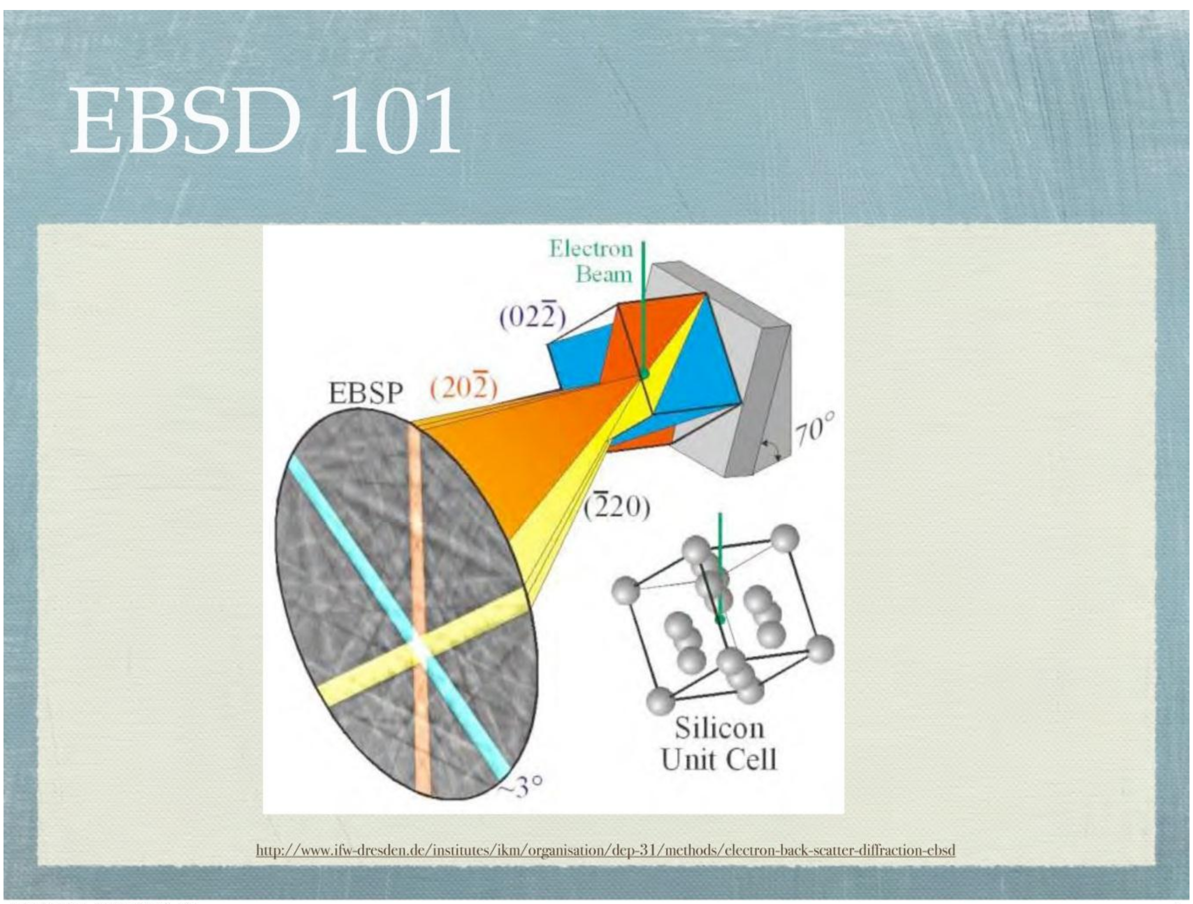

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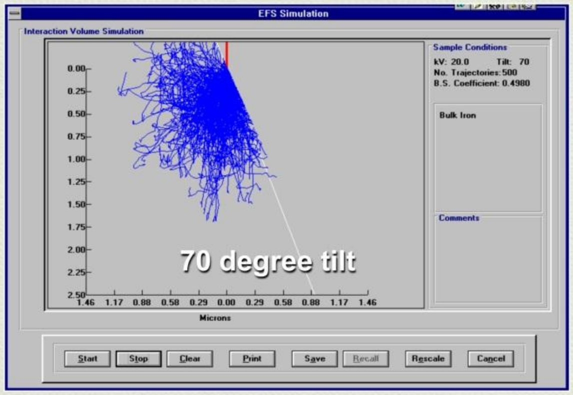
Complicating factor

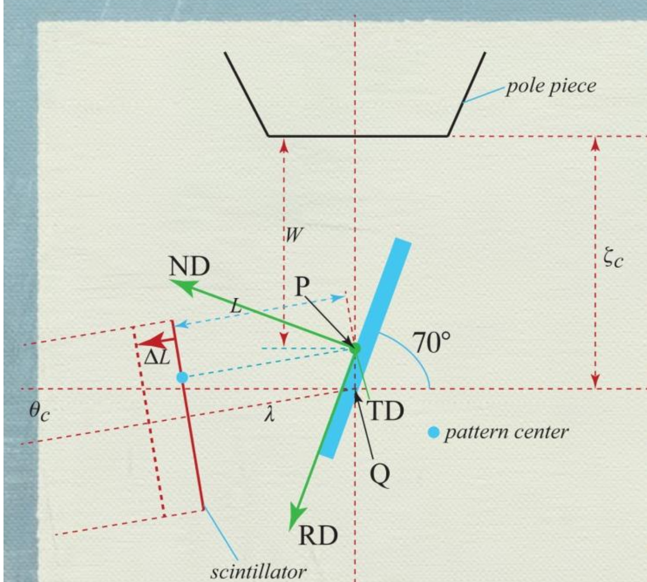
- the back-scattered electrons arise from a range of locartions and depths inside the sample (stochastic process).



The electrons that escape from the surface undergo interactions with the crystal lattice while they approach the exit surface. These interactions are deterministic, not stochastic

ELECTRON BACK-SCATTER DIFFRACTION

as an example of a forward modeling approach



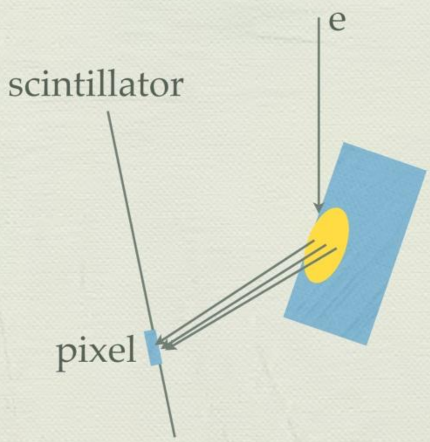
Diffraction process consists of 3 steps:

- beam-sample interaction
- diffracted beam - scintillator interaction
- scintillator - CCD transfer

Our simulation approach follows this separation by computing ALL possible EBSD patterns first, and then interpolating from this “master pattern” to determine a given pattern on the scintillator.

Ongoing work supported by ONR-N00014-12-1-0075

ELECTRON BACK-SCATTER DIFFRACTION



For a given scintillator pixel, BSEs originate at a range of depths inside the sample.

Therefore, the signal in single pixel will correspond to an integration over the depth in the sample.

$$\mathcal{P}(\mathbf{k}) = \sum_i \frac{Z_i^2 DW_i}{z_0} \int_0^{z_0} \mathrm{d}z\, |\Psi_{\mathbf{k}}(\mathbf{r}_i)|^2$$

Z_i = atomic number
DW_i = Debye-Waller factor
$\mathbf{r}_i$ = atom coordinates
$\mathbf{k}$ = electron wave vector

ELECTRON BACK-SCATTER DIFFRACTION

Schroedinger equation +
Bloch wave ansatz $\Psi(\mathbf{r}) = \sum_j \alpha^{(j)} \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} e^{2\pi \mathrm{i}(\mathbf{k}^{(j)}+\mathbf{g})\cdot\mathbf{r}}$

leads to complex non-symmetric eigenvalue problem

$$\mathcal{P}(\mathbf{k}_0) = \sum_{\mathbf{g}} \sum_{\mathbf{h}} S_{\mathbf{gh}} L_{\mathbf{gh}},$$

$$S_{\mathbf{gh}} \equiv \sum_n \sum_{i \in \mathcal{S}_n} Z_n^2\, e^{-M_{\mathbf{h}-\mathbf{g}}^{(n)}}\, e^{2\pi \mathrm{i}(\mathbf{h}-\mathbf{g})\cdot\mathbf{r}_i};$$

$$L_{\mathbf{gh}} \equiv \sum_j \sum_k C_{\mathbf{g}}^{(j)*} \alpha^{(j)*} \mathcal{I}_{jk} \alpha^{(k)} C_{\mathbf{h}}^{(k)}.$$

eigenvectors

eigenvalues

$$\alpha_{jk} = q^{(j)} + q^{(k)};$$
$$\beta_{jk} = \gamma^{(j)} - \gamma^{(k)}.$$

$$\mathcal{I}_{jj} = \frac{1 - e^{-4\pi q^{(j)} z_0}}{4\pi q^{(j)} z_0};$$

$$\mathcal{I}_{jk} = \frac{1 - e^{-2\pi(\alpha_{jk} + \mathrm{i}\beta_{jk}) z_0}}{2\pi(\alpha_{jk} + \mathrm{i}\beta_{jk}) z_0} \qquad (j \neq k);$$

adjustable parameter

- Each detector pixel corresponds to a different exit beam direction, so first we compute all possible exit beam directions (accounting for crystal and diffraction symmetry), and then we sample this set via interpolation.
- This produces a pattern at the scintillator, which is then further adjusted to account for: orientational modulation of back-scatter yield, scintillator detective quantum efficiency, Poisson electron detection noise, fiber or lens coupling optics, CCD point spread function, and CCD binning mode.

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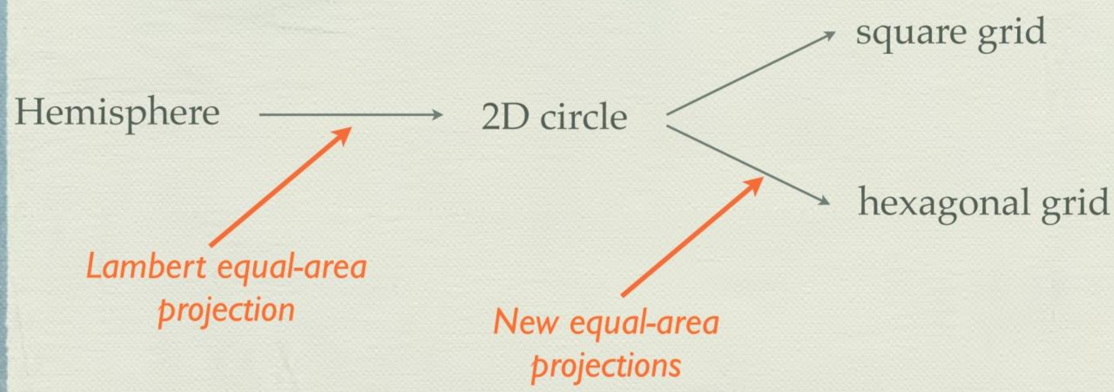
ELECTRON BACK-SCATTER DIFFRACTION

Sampling process: compute BSE yield for all possible electron wave vectors, which results in numerical values on a (hemi)-sphere.

For efficient storage and easy interpolation, project the hemisphere on a square or hexagonal 2D grid using an equal-area projection.



D. Rosca, *New uniform grids on the sphere*, Astronomy & Astrophysics, **520**, A63 (2010)

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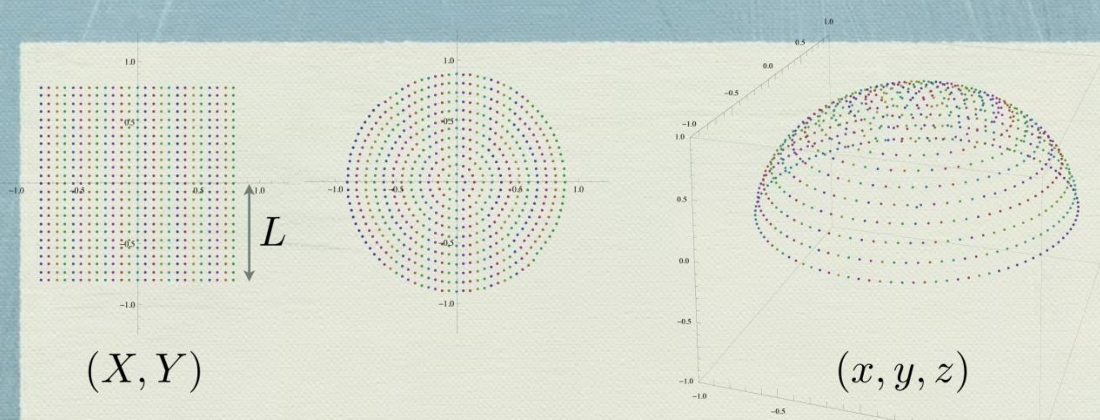
ELECTRON BACK-SCATTER DIFFRACTION

Uniform equal-area mappings



$$(x,y,z) = \left(c(X)\cos\frac{Y\pi}{4X}, c(X)\sin\frac{Y\pi}{4X}, 1-\frac{2X^2}{\pi}\right) \quad 0 < |Y| \le |X| \le L;$$

$$(x,y,z) = \left(c(Y)\sin\frac{X\pi}{4Y}, c(Y)\cos\frac{X\pi}{4Y}, 1-\frac{2Y^2}{\pi}\right) \quad 0 < |X| \le |Y| \le L,$$

$$L = \frac{\pi}{\sqrt{2}}$$

where

$$c(p) = \frac{2p}{\pi}\sqrt{\pi - p^2}.$$

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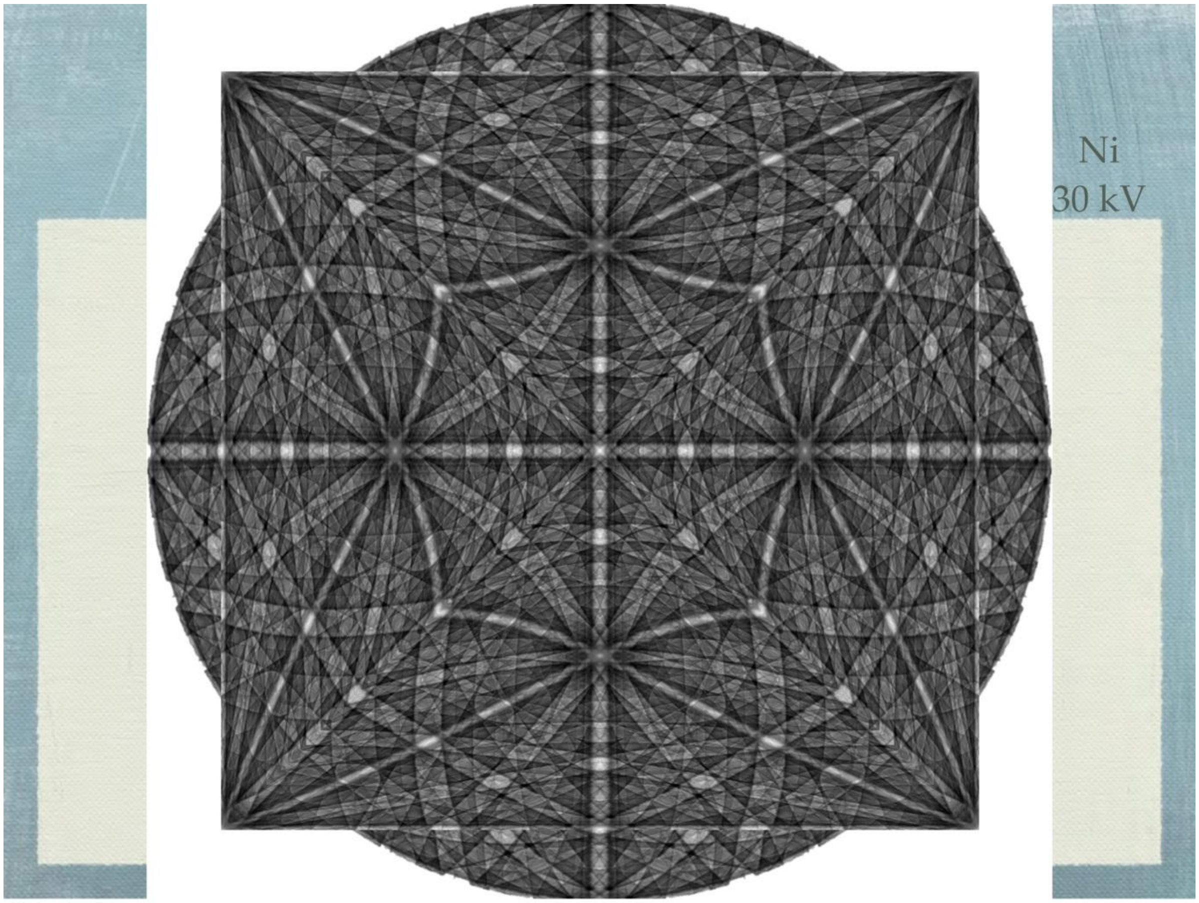
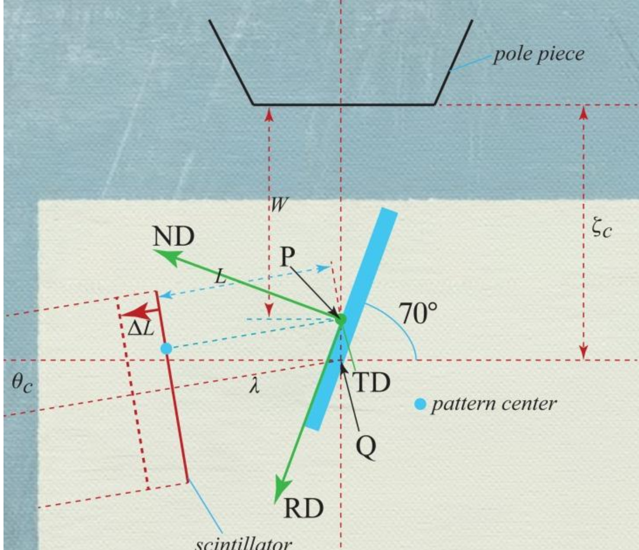




$L = 15,250\,\mu$m
$\sigma = 70°$
scintillator pixel $49.375\,\mu$m
640×480 pixels
pattern center $(3.37, 113.45)$

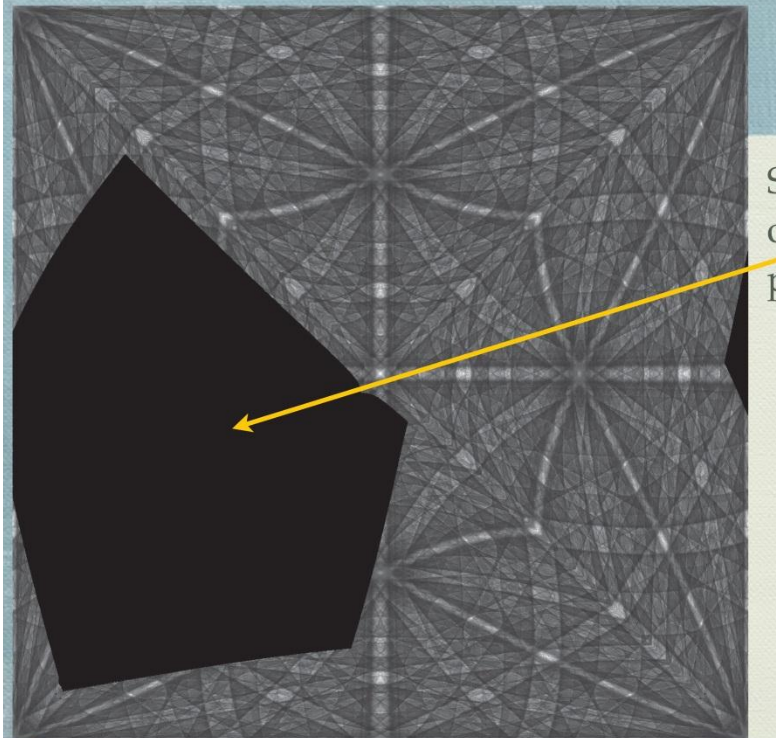
[parameters for Megna Shah's data set (AFRL/WPAFB)]

The direction cosines of a screen pixel $(x_s, y_s, 0)$ in the (RD,TD,ND) reference frame are given by:

$$\hat{\mathbf{r}}_g(x_s, y_s) = \frac{1}{\rho_s}\left[(y_{pc} - y_s)\cos\alpha + L\sin\alpha, x_{pc} - x_s, -(y_{pc} - y_s)\sin\alpha + L\cos\alpha\right].$$

Insert these in the modified Lambert projection to determine the corresponding BSE yield using standard bilinear interpolation on the square map.

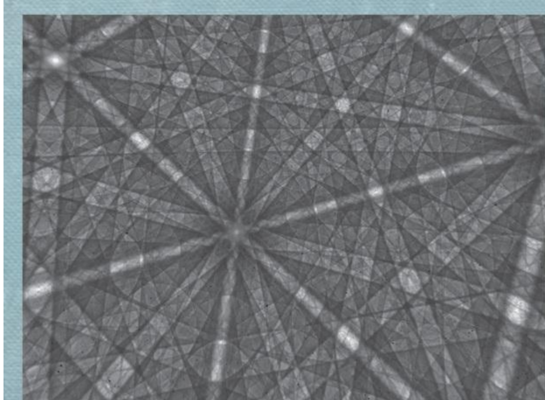
ELECTRON BACK-SCATTER DIFFRACTION

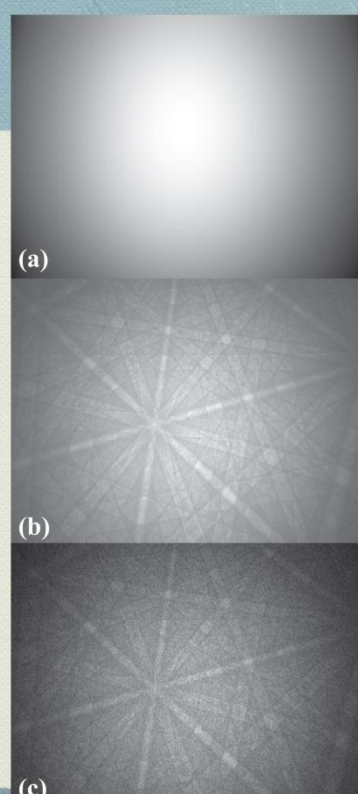


Scintillator mapped onto modified Lambert projection.

$$(\varphi_1, \Phi, \varphi_2) = (27°, 75°, 310°)$$

ELECTRON BACK-SCATTER DIFFRACTION





background intensity profile by averaging experimental patterns

EBSD pattern with background included

Poisson noise added

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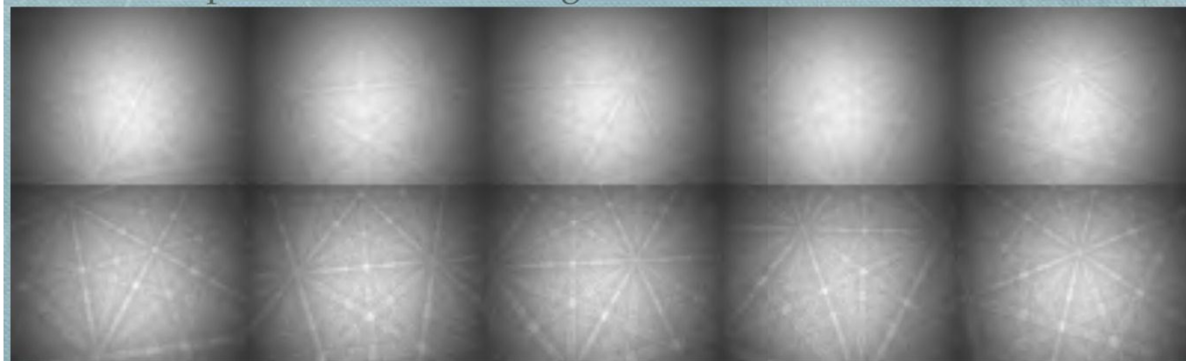
ELECTRON BACK-SCATTER DIFFRACTION

Experimental, 8x binning



Simulated

Simulation speed: about 10 patterns per second on single 3GHz processor

Problem: background intensity model does not contain any physics ...

ELECTRON BACK-SCATTER DIFFRACTION

- the real problem: there is no easy way to combine the essentially stochastic nature of electron back-scattering with dynamical elastic scattering theory...

Monte Carlo

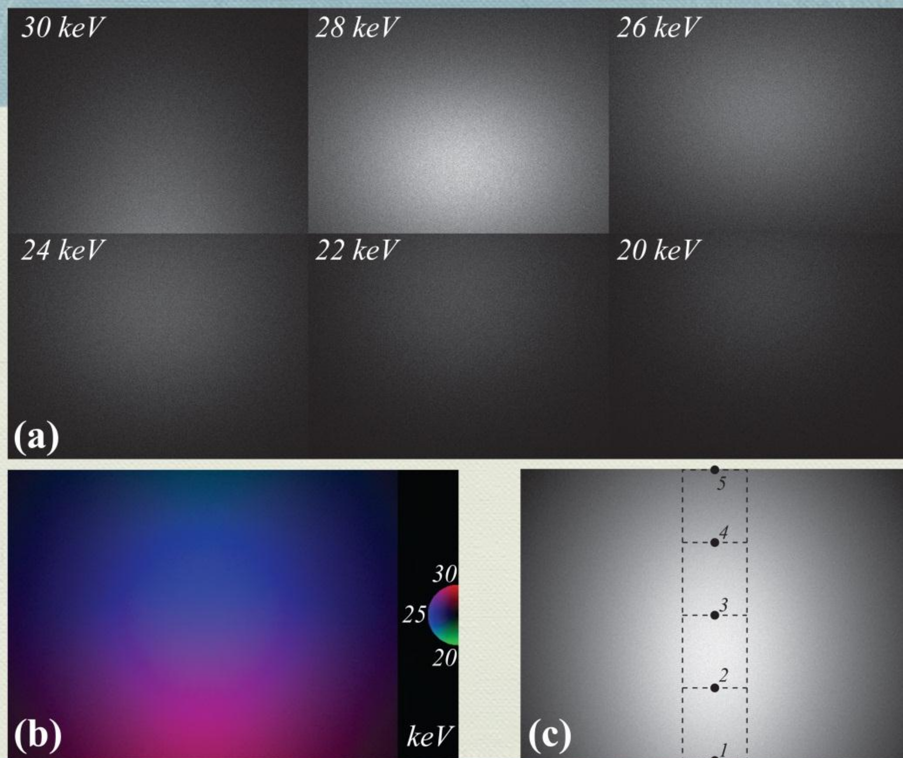
Schroedinger Equation

MC can be used to study the depth distribution of BSE events, as well as the energy distribution...

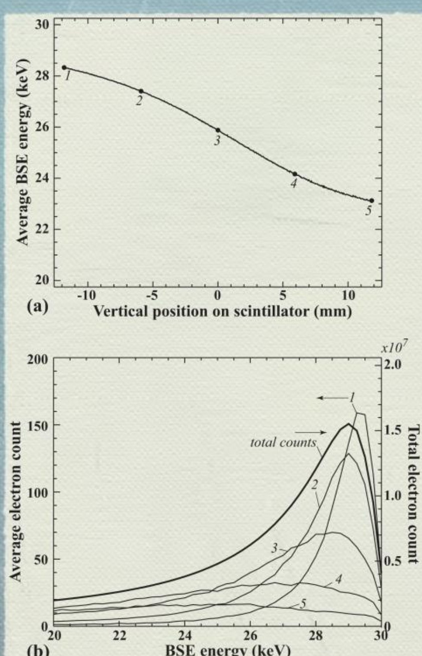
We have implemented a basic MC model to study depth and energy distributions for a specific geometry.

ELECTRON BACK-SCATTER DIFFRACTION

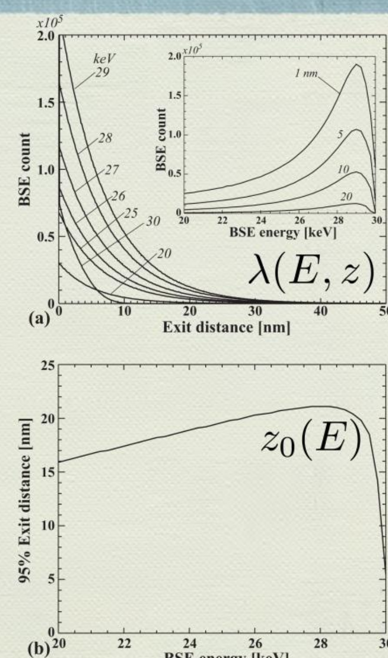
1 billion incident electrons, 30 kV; 48% reach scintillator



ELECTRON BACK-SCATTER DIFFRACTION



These curves can be used as weight factors for dynamical simulations ...



ELECTRON BACK-SCATTER DIFFRACTION

Merging Monte Carlo and dynamical computations:

$$\mathcal{P}(\mathbf{k}_0) = \sum_{\mathbf{g}} \sum_{\mathbf{h}} S_{\mathbf{gh}} L_{\mathbf{gh}},$$

$$S_{\mathbf{gh}} \equiv \sum_{n} \sum_{i \in \mathcal{S}_n} Z_n^2 \, e^{-M^{(n)}_{\mathbf{h}-\mathbf{g}}} \, e^{2\pi \mathrm{i}(\mathbf{h}-\mathbf{g})\cdot \mathbf{r}_i};$$

$$L_{\mathbf{gh}} \equiv \sum_{j} \sum_{k} C^{(j)*}_{\mathbf{g}} \alpha^{(j)*} \mathcal{I}_{jk} \alpha^{(k)} C^{(k)}_{\mathbf{h}}.$$

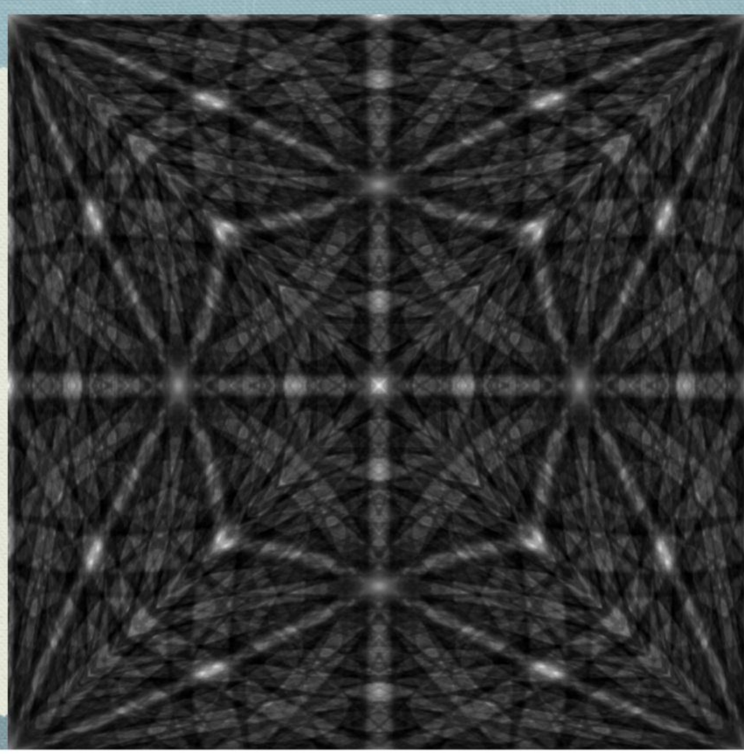
$$\mathcal{I}_{jk} = \frac{1}{z_0} \int_0^{z_0} e^{-2\pi(\alpha_{jk} + \mathrm{i}\beta_{jk})} \, \mathrm{d}z$$

$$\mathcal{I}_{jk} = \frac{1}{z_0(E)} \int_0^{z_0(E)} \lambda(E, z) e^{-2\pi(\alpha_{jk} + \mathrm{i}\beta_{jk})} \, \mathrm{d}z$$

from MC

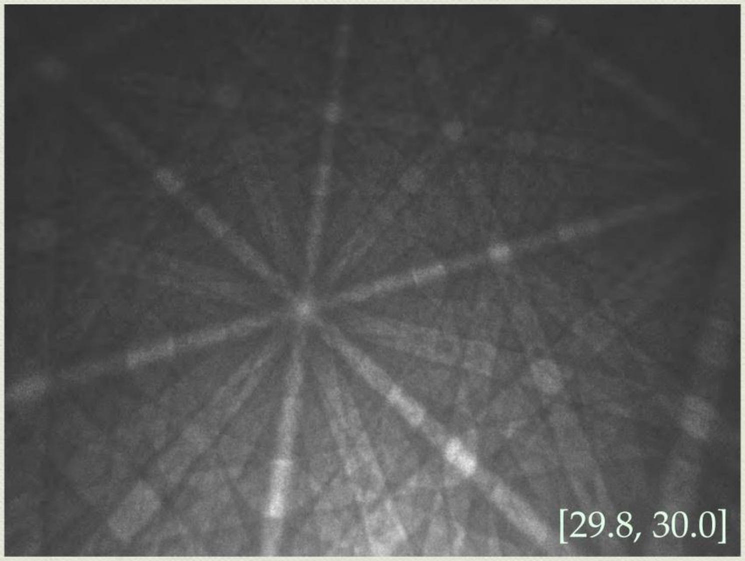
ELECTRON BACK-SCATTER DIFFRACTION

Energy-dependent master EBSD pattern for Ni [15 - 30 keV]



EBSD with E-dependence

IN100, Euler angles (146.38°, 19.63°, 172.87°)



What's next?

- improve realism of MC simulations by using different models for stopping power; currently we use a continuous stopping power model, which is probably not fully realistic, so the actual output of the MC model could change quite a bit in the future ...
- current energy-weighted dynamical EBSD simulations provide electron count at the scintillator.
- to get from scintillator to CCD, we need to know the point spread function of the camera
  - we are currently measuring this function for a number of camera systems
- include detector noise, both at the scintillator and the CCD stage (Poisson counting statistics), as well as binning, and proper brightness/contrast scaling

Conclusions

- We have successfully merged Monte Carlo simulations with dynamical electron channeling simulations, to obtain a new algorithm for EBSD patterns.
- Ongoing work will lead to better understanding of EBSD camera systems as well as realistic simulated patterns.
- A similar approach (physics-based, exploring all steps in the pattern formation process) will need to be applied to all other imaging/diffraction/spectroscopy modalities; several of these are currently ongoing.