Reconstructing Polycrystal Grain Map from 3D X-ray Diffraction Data

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Outline

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Introduction

- Many materials, natural or artificial, are found in crystalline forms (e.g., metals, ceramics, minerals, ice, bones and drugs).
- As such, crystalline structures are of basic interest to various branches of science, including materials science, physics, geophysics, chemistry, biology, pharmacy, and forensic science.
- It is the crystal structure what governs many of the physical, chemical, and mechanical properties of a crystalline material.

Grains and Orientations

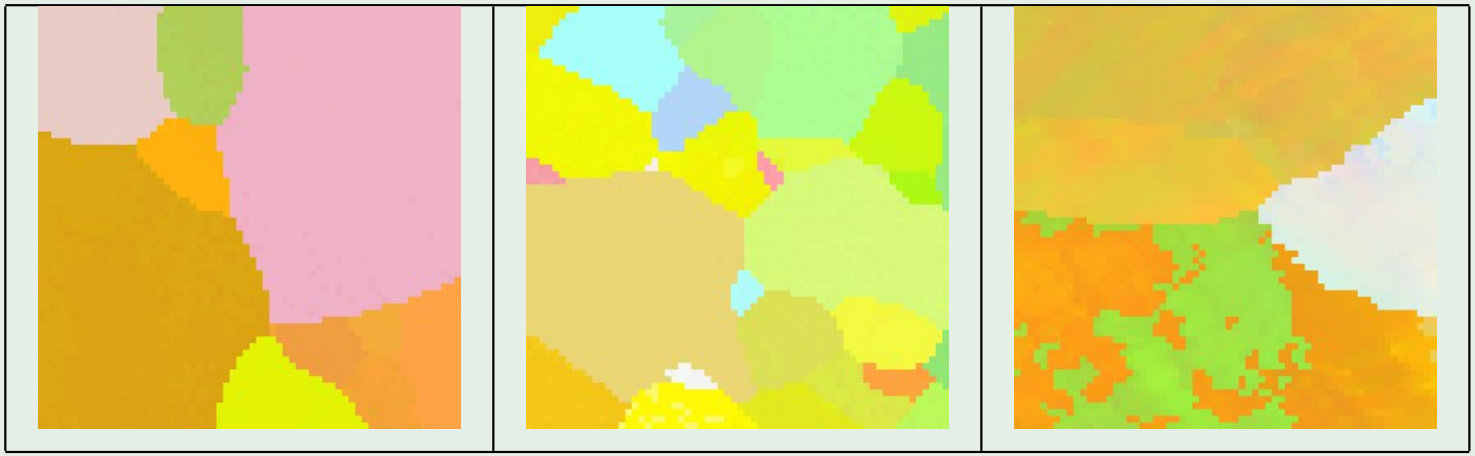
- Most crystalline materials are polycrystals, i.e., they are composed of an assemblage of crystals, called *grains* or *crystallites*.
- Each grain can be associated with one orientation which describes how that grain is oriented in 3D space (relative to a fixed coordinate system).
- Undeformed specimen: the lattice within each grain is typically near-perfect i.e. each element has nearly same orientation.
- Moderately Deformed specimen: orientations within a grain will vary within a certain orientation range around the so-called basic orientation.

What is Grain Map?

Definition

A labeling (coloring) of a polycrystalline specimen, where each grain is represented by a color according to its basic orientation.

Example



Methods to Reconstruct Grain Maps

- Surface probes such as optical and electron microscopy (EM).
  - Drawback:
    - destructive in nature.
    - rule out any study of the dynamics of the individual grains during typical processes such as annealing or deformation.
- Three-dimensional X-ray diffraction (3DXRD) microscopy
  - Developed at European Synchrotron Radiation Facility (ESRF)
  - Non destructive in nature.
  - Uses high-energy monochromatic X-rays and the physical phenomenon known as diffraction

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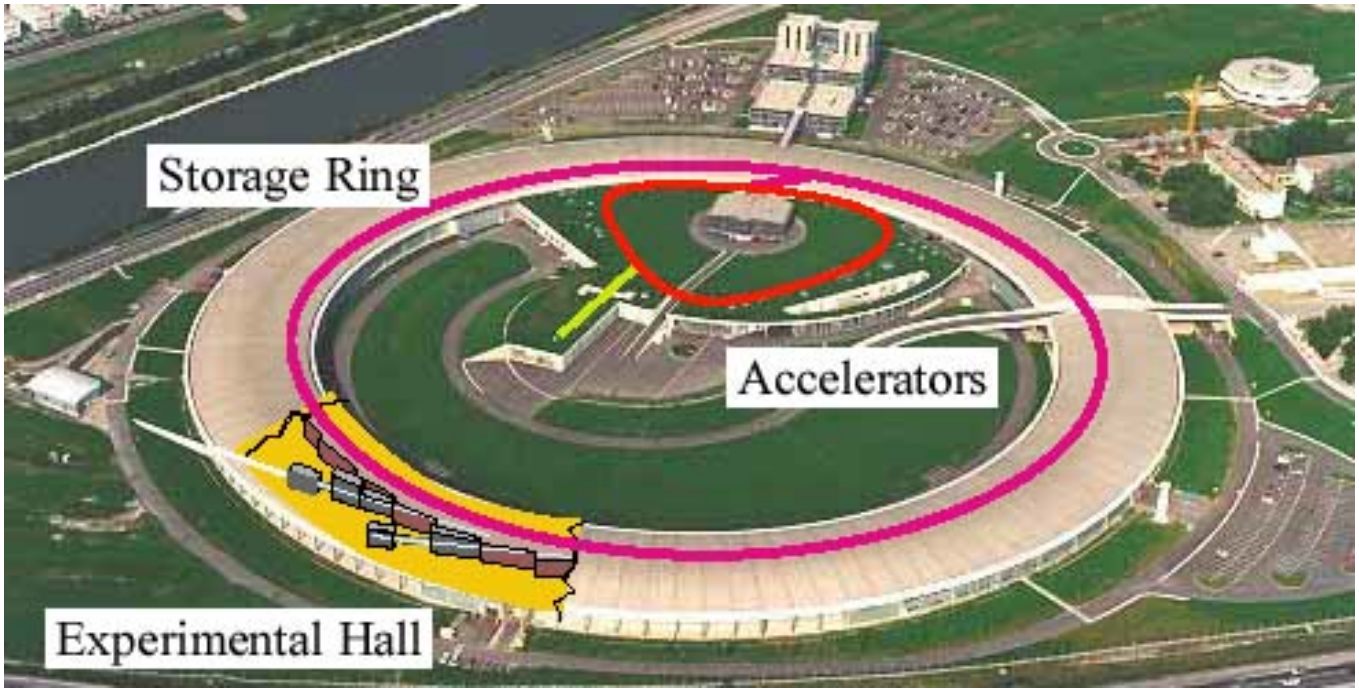
ESRF Synchrotron



- One of the three largest and most powerful synchrotrons in the world.

Outline

3DXRD

- Nondestructive imaging technique: makes dynamic studies feasible.
- Uses high-energy monochromatic X-rays and the physical phenomenon known as diffraction.
- Exceptional penetration depth (several mm's for steel and some cm's for aluminum).
- 3D reconstructions can be performed by imaging multiple cross-sections.
- It produces an image of a 2D layer of the sample in the form of diffraction patterns called projections.
- Projections are recorded by a detector plate while the sample is rotated about an axis perpendicular to the X-ray beam.

3DXRD Experimental Setup

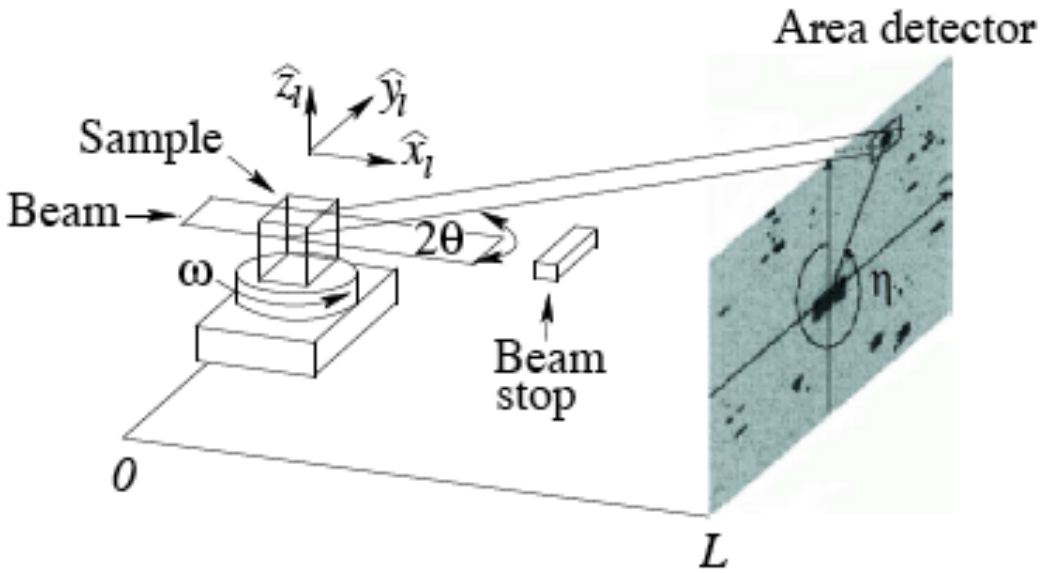


Figure: Sketch of the 3DXRD experimental setup. The Bragg angle 2θ, the rotation angle ω and the azimuthal angle η are indicated for a part of the grain that gives rise to diffraction. The laboratory coordinate system is given as $(\hat{x}_l, \hat{y}_l, \hat{z}_l)$.

Projection Geometry

- For every image pixel (x, y) its coordinates in laboratory coordinates are (x_l, y_l, z_l).
- For a given point (x_l, y_l, z_l) of the grain, we can compute the associated diffraction point on the detector (L, y_{det}, z_{det}) as

$$\begin{aligned} x_l &= x\cos(\omega) - y\sin(\omega) \\ y_l &= x\sin(\omega) + y\cos(\omega) \\ y_{det} &= -(L - x_l)\tan(2\theta)\sin(\eta) + y_l \\ z_{det} &= (L - x_l)\tan(2\theta)\cos(\eta) + z_l \end{aligned} \tag{1}$$

Representation of Grains and Orientations

- Let the total number of locations in the $2D$ area of interest (sample layer) be I.
- We assign to each location $i (1 \leq i \leq I)$ both a grain label, $f(i)$, and an orientation, $o(i)$.
- Grains are labeled by $l \in \{1, 2, 3, \ldots, n\}$, where n, the total number of grains, is assumed to be known *a priori*.
- Orientations can be represented in various ways, most common are representations in Euler angles, Rodrigues vectors and unit quaternions. These representations describe rotations in 3D-space.
- Quaternion representation was used.

Quaternion

Definition

Unit quaternions is a 4-tuple of the form

$$\boldsymbol{q} = (a, b, c, d) = (\cos(\varphi/2), \boldsymbol{n}\sin(\varphi/2))$$

where the 3D unit vector $\boldsymbol{n}$ and the real scalar φ are the axis and angle of rotation, respectively.

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Single Grain Reconstruction

- Lets consider the subproblem of reconstructing a single grain (with known orientation o and grain label l) and no deformation.
- If we consider the whole image then at every pixel (x, y) , it either belongs to grain l or not.
- Let $\rho_0 = (l, o)$ be the assignment corresponding to the grain.
- Let $\rho(x, y)$ be the density of the intersection between the grain and the illuminated layer.
- For all pixels except those at the boundary, we expect either $\rho_{ij} = \rho_0$ or $\rho_0 = 0$.
- The pixelated values are listed in the one-dimensional array X.
- For each reflected ray, r, the normalized intensities are saved in array b^r.

Single Grain Reconstruction

There is a linear relationship between density and intensity and it can be derived from equation (1). For each reflection, r , we may write

$$A^r X = b^r \tag{2}$$

where A^r comprises the information on geometry (equation 1). Next we pile the A^r values for all the reflection into a block matrix A and define the compound array b as follows:

$$A = \begin{pmatrix} A^1 \\ A^2 \\ \vdots \end{pmatrix} \qquad b = \begin{pmatrix} b^1 \\ b^2 \\ \vdots \end{pmatrix} \tag{3}$$

Single Grain Reconstruction

Hence we have the following equation for the reconstruction of single grain:

$$AX = b \tag{4}$$

where A is a matrix of integers of size $I \times I$, b is a matrix of integers (since intensities on detector are integer values) of size $I \times 1$, X is a- vector of unknowns of size $I \times 1$.
NOTE: Here I is the number of pixels in the 2D area of interest in sample and it is a variable chosen based upon the application.

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NP-Complete Problem

We have the following:

- A is a matrix of integers of size $I \times I$.
- b is a matrix of integers of size $I \times 1$.
- X is a vector of size $I \times 1$.
- Each element of X is either 0 or ρ_0, where ρ_0 is a constant.
- $X = \frac{1}{\rho_0} x$, where x is a 0-1 vector. We can ignore ρ_0 for the purpose of solving the equations.
- Now problem reduces to $Ax = b$, where A and b are as defined above and x is a 0-1 vector.
- This is an integer programming problem.

0-1 Integer Programming Problem

Definition

INSTANCE: Integer matrix A and integer vector b.
QUESTION: Does $\exists$ a 0-1 vector x such that $Ax \leq b$?

- Classical problem in combinatorial optimization.
- NP-complete in general.
- 3-SAT $\Rightarrow$ 0-1 Integer Programming.

Proof of NP-Completeness

- It is easy to see that, given the value of x, it is easy to varify its correctness in deterministic polynomial time. Hence this problem is in the set NP.
- Instance of 3-SAT
  - Variables :$U = \{u_1, u_2, u_3, \ldots, u_n\}$
  - Clauses: $C = \{c_1, c_2, c_3, \ldots, c_m\}$ such that $|c_i|$ for $1 \leq i \leq m$.
- We have to construct an instance of 0-1 Integer programming.
- Boolean to arithmatic: (+) means true and (-) means false.
- Let 0 denote false and 1 denote true.
- Place OR's between the variables.
- $+x_1 + x_2 - x_3$ now means that

$$x_1 \text{ is true, or } x_2 \text{ is true, or } x_3 \text{ is false.}$$

Proof of NP-Completeness

Expressions	Values							
x_1	0	0	0	0	1	1	1	1
x_2	0	0	1	1	0	0	1	1
x_3	0	1	0	1	0	1	0	1
$+x_1 + x_2 + x_3$	0	1	1	2	1	2	2	3
$+x_1 + x_2 - x_3$	0	-1	1	0	1	0	2	1
$+x_1 - x_2 - x_3$	0	-1	-1	-2	1	0	0	-1
$-x_1 - x_2 - x_3$	0	-1	-1	-2	-1	-2	-2	-3

Proof of NP-Completeness

- Points to remember for each expression row
  - Each has exactly one column of minimum value.
  - This column corresponds to a nonsatisfying truth assignment.
  - Every other column satisfies the expression.
  - All other columnms have higher values.
- Construction of matrix $A = [a_{i,j}]_{m \times n}$:
  - n columns corresponding to variables in U.
  - m rows corresponding to clauses in C.
  - $a_{i,j} = \begin{cases} 1 & \text{if } u_j \in c_i \\ -1 & \text{if } \overline{u_j} \in c_i \\ 0 & \textit{otherwise} \end{cases}$

Proof of NP-Completeness

The vector $b = [b_i]_{n\times 1}$ is merely made up of the appropriate minimum values plus one from the chart, where the elements are defined as follows:

$$b_i = 1 - (\text{the number of complemented variables in } c_i)$$

Proof of NP-Completeness

($\Rightarrow$) Assume that 3-SAT is satisfiable and let $t : U \rightarrow \{T, F\}$ be the satisfying truth assignment for C, where T means true and F means false. We can construct matrix A and vector b as described in the above construction. Let us construct a vector $x = [x_i]_{n \times 1}$ such that

$$x_i = \begin{cases} 1 & \text{if } t(u_i) = T \\ 0 & \text{if } t(u_i) = F \end{cases}$$

Now if we multiply A and x then we will get a vector of size n where element i (corresponding to clause c_i) is of the form $\pm x_{i_1} \pm x_{i_2} \pm x_{i_3}$ which is always less than b_i because of the choice of b_i as described above. Hence x is a solution to the 0-1 Integer Programming problem.

Proof of NP-Completeness

($\Leftarrow$) Assume that there does exists a 0-1 valued vector x such that $Ax \leq b$. Now construct the truth assignment t of 3-SAT as follows:

$$t(u_i) = \begin{cases} T & \text{if } x_i = 1 \\ F & \text{if } x_i = 0 \end{cases}$$

The construction of A and b will force that each clause is satisfied. If not, then one of the values of the vector Ax will be greater that the corresponding value in vector b which will contradict the assumption that $Ax \leq b$. Hence t is the satisfying assignment for 3-SAT.

Hence, 3-SAT and 0-1 Integer Programming are equivalent problems. Since 3-SAT is known to be NP-Complete, 0-1 Integer programming must be NP-Complete.

Outline

Summary

- Crystalline substances are made up of grains governs many of the physical, chemical, and mechanical properties.
- 3DXRD is a technique which uses high energy monochrmatic X-rays and phenomena known as diffraction to determine the grain map of a polycrystal.
- Subproblem of reconstructing a single grain (with known orientation) leads to 0-1 Integer Programming problem.
- 0-1 Integer programming is a NP-complete problem.
- Reconstruction of grain maps is NP-Complete.

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