A Short Introduction to Tomographic Grain Map Reconstruction

Andreas Alpers,
Center for Fundamental Research: 'Metal Structures in Four Dimensions,'
Risø-DTU, Technical University of Denmark, DK-4000 Roskilde, Denmark,
aal@imm.dtu.dk

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Abstract

Recent X-ray techniques allow for the first time to image small crystals – known as *grains* – deep inside of polycrystalline materials. This is of interest in materials science. Two important techniques are based on tomography principles related to discrete tomography. We give a short introduction to the basic reconstruction problems arising in this context. The focus is on revealing the mathematical structure and the relationship to discrete tomography by abstracting from the experimental setup details. Concepts are explained for readers with no background in diffraction theory.

1 Introduction

Many materials – in particular most metals, ceramics and alloys – are *polycrystalline materials*, which means that they are comprised of a set of small crystals. These small crystals, typically $10 - 100\,\mu\text{m}$ in diameter, are known as *grains*. Each grain is characterized by its center of mass, shape and internal lattice structure. The geometric features of the grains within the 3-dimensional complex determine most of the material's physical, chemical and mechanical properties. It is therefore not surprising that the study of grain complexes is of central importance in materials science. Studies, for example, on crack corrosion [11], responses to stress [9, 17], and grain growth phenomena [25, 20], require techniques to probe grain complexes deep inside of bulk materials. Only recently, three experimental techniques have emerged that allow such imaging of millimeter-to-centimeter thick samples. These techniques are known as *3-dimensional X-ray diffraction* (3DXRD) [22], *diffraction contrast tomography* (DCT) [16], and *differential-aperture X-ray microscopy* (DAXM) [13]. While the techniques utilize very penetrating high-energetic X-rays as produced by third-generation synchrotrons, are they yet based on different physical principles. 3DXRD and DCT are based on tomography principles. In Section 3 we focus on a very basic reconstruction problem in 3DXRD and DCT that assumes a maximum amount of prior knowledge. The reconstruction problems in the relevant literature are generalizations of this basic problem, and they are related to discrete tomography. We aim at highlighting this relationship in an abstract sense by hiding most of the underlying physics and experimental setup details. Pointers to the literature on 3DXRD, DCT, and DAXM are given in Section 5.

2 A General Reconstruction Problem

A crystal is, generally speaking, a 3-dimensional repetition of some unit of atoms or molecules. This unit is known as *unit cell*, the repeating structure is a *lattice structure*. An *undeformed grain* is a finite crystal, in our context three aspects are relevant: (1) its center of mass, (2) its shape, and (3) its internal

lattice structure. The lattice structure of such an undeformed grain, labeled by a suitable number g, can be described by specifying a set $B_g \subseteq \mathbb{R}^3$ of three basis vectors that generate the lattice. Say, we define an interval $I^3 = I \times I \times I \subseteq \mathbb{R}^3$ as region of interest that describes the positions in our sample. We define the *shape function* $s_g : I^3 \to \{0, 1\}$ to be the function whose support is the set of positions in the sample occupied by grain g; a position is occupied by grain g if the nearest atom belongs to grain g. That support is what we commonly refer to as the *shape* of grain g, the center of mass can be immediately derived from it.

We remark that we just introduced a 'continuous' and a 'discrete' concept, which should not be confused: shapes can be assumed to be compact sets, lattices are discrete structures, see Figure 1(a). This distinction is fundamental in the diffraction process that we describe in Section 3. *What* appears on the detector is, roughly speaking, determined by the shapes – *where* it appears is determined by the lattice structures.

Say, the sample contains ℓ grains labeled by numbers $1, \ldots, \ell$. The *continuous grain map* $f : \mathbb{R}^3 \to \{1, \ldots, \ell\}$ is defined by

$$f(\mathbf{x}) = g \Leftrightarrow s_g(\mathbf{x}) = 1.$$

We can assume that positions in real-world samples are occupied by at exactly one undeformed grain, and thus f is well-defined. By restricting the domain of f to a finite subset $D \subseteq I^3$ we obtain the *discrete grain map* (associated to D), which we denote by f_D. The idea is, of course, that while f models physical reality, computer reconstructions can only yield approximations f_D to f.

A very relevant and general problem in 3DXRD and DCT is to reconstruct $B_1, \ldots, B_\ell$ and approximations f_D of f from X-ray diffraction data. This is known in the literature as *grain and orientation map reconstruction problem for undeformed grains*.

Grains are usually in an undeformed state. A deformation of the sample, however, causes deformations of the grains. This means that their lattice structure is deformed and cannot be described anymore by a single set B_g, further details can be found in [3]. Since we discuss in the following only the undeformed case, we will from now on use the term *grain* synonymously for undeformed grains.

3 A Basic Reconstruction Problem

We now consider a more restricted version of the *grain and orientation map reconstruction problem* mentioned above. The first restriction is that we assume $B_1, \ldots, B_\ell$ to be known. This is in many cases a plausible assumption, because $B_1, \ldots, B_\ell$ can be obtained by diffraction data preprocessing with so-called *indexing methods* [14]. The second restriction is that we consider only a 2-dimensional layer in the sample, i.e., we consider f to be restricted to the domain $I_a = I \times I \times \{a\}$ for a given $a \in I$. This is a natural restriction in the 3DXRD setting, since it is possible to restrict the X-ray beam to illuminate a single layer. Thus, the basic reconstruction problem of this section is to reconstruct approximations f_D of f – which are restricted to I_a – from X-ray diffraction data. To ease notations we consider for the rest of this section f and f_D to be functions on I_a.

We now need to say a bit more about the experimental setting and the diffraction process. Figure 1(b) serves as an illustration. The 3DXRD detector that records the diffracted intensities is a planar detector, and we can think of the covered area as a 2-dimensional interval contained in an affine plane, the *detector plane*. We avoid discussions about absolute values of diffraction intensities by assuming that intensities are normalized. The X-ray beam illuminating the layer in the sample can be interpreted as a collection of parallel 1-dimensional X-rays that impinge on the sample layer under a common angle θ. Now, only two phenomena can occur: either the X-ray diffracts at the surface under the same angle θ, or it does not diffract at all (this is an oversimplification of the underlying physical processes, see [29], but the general phenomena are accurately described). Diffraction occurs only in favorable conditions that depend on the X-ray's wavelength and its relative position with respect to the lattice structure of the grain on which it impinges. A mathematically precise statement of this condition is the *Bragg law*, see [29, 12].

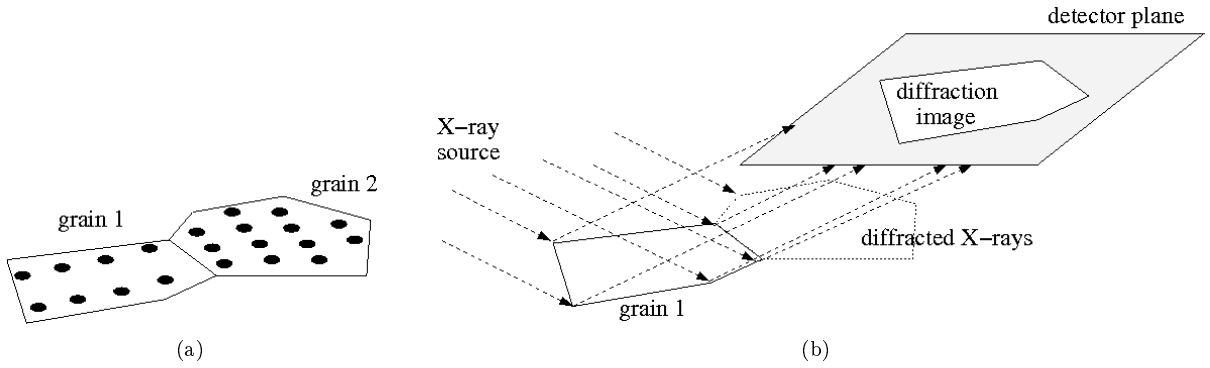

Figure 1: Schematic illustration of grains and diffraction. (a) A sample layer containing 2 grains with different lattice structures. The shapes are indicated by the polygons, the lattices by the dots – real grains contain considerably more unit cells. (b) Diffraction from a layer, assuming that only grain 1 is in diffraction condition. An affine image of its shape is recorded on the detector. The detector plane need not be parallel to the sample plane.

Now, consider the paths of the parallel X-rays diffracting at a certain grain g. As a geometrical object we can think of it as a Minkowski sum of the support of s_g and the ray describing the diffraction direction. Let M denote this geometrical object. Clearly, diffracted intensities can only be recorded if the (affine) detector plane and M have a non-empty intersection; additionally, the diffraction direction must be non-parallel to the detector plane.

Diffracted intensities are thus recorded at the points where the (affine) detector plane and M intersect. The set of intersection points defines a so-called *diffraction spot*. It is not too hard to see that the support of s_g and such a planar slice of M are related by an affine transformation. In other words, the diffraction spots produced by a single grain g are affine images of its shape. However, the affine transformation involved may vary from diffraction spot to diffraction spot.

In the 3DXRD setting, the sample is rotated around a vector perpendicular to the sample layer. In this way one can obtain different, typically $4 - 8$, affine images of each grain. The affine images can be interpreted as projections of the grain shapes. But tomography comes also into play at another place: diffraction spots may overlap – in this case diffraction intensities sum up.

We summarize the basic reconstruction problem as follows: we want to reconstruct approximations f_D of f from a set of (possibly) overlapping diffraction spots, which are affine images of grain shapes. This problem is known in the literature as *2-dimensional grain map reconstruction problem for undeformed grains*. The papers [23, 5, 18, 1, 2] present algorithms for solving this reconstruction problem – the methods in [1, 2] are based on the Gibbs prior framework in discrete tomography.

4 Relationship to Discrete Tomography

How does the *2-dimensional grain map reconstruction problem for undeformed grains* relate to discrete tomography? We have seen that it certainly is a tomography problem. However, there are three major discrete aspects:

1. The range of f is finite, thus discrete. Continuous reconstruction methods, such as the *algebraic reconstruction technique* (ART) [6], do not always produce satisfying results. It should be noted, however, that the domain of f is not discrete – we are interested in reconstructing shapes and not images at atomic resolution.

2. The number of projections is given by the number of diffraction spots per grain, which is usually around $4-8$. However, prior knowledge about grain shapes is available.

3. The diffraction spots appear at positions on the detector depending on the grain's lattice structure. In our previous discussion we assumed that the lattice structure is known, but if this is not the case then this discrete aspect becomes relevant.

The reconstruction problem is – in some sense – *semi-discrete*, because the domain of f is naturally non-discrete. The problem therefore falls in-between the areas of traditional computerized tomography and discrete tomography with QUANTITEM [26].

5 Literature Overview

We conclude with a brief survey of the existing literature on methods for grain map reconstruction. As mentioned in the introduction, three experimental techniques can be found in the literature: (1) *3-dimensional X-ray diffraction* (3DXRD), (2) *diffraction contrast tomography* (DCT), and (3) *differential-aperture X-ray microscope* (DAXM).

Table 1 lists the relevant literature categorized according to the experimental technique and reconstruction algorithm. The table's last column indicates the capability of the corresponding method to reconstruct deformed grains ('+' indicating capability, '−' incapability).

Experimental Technique	**Algorithm**	**References**	**Deformed Grains**
3DXRD	ART	[23, 5, 18]	−
	DT	[1, 2]	−
	DT	[24, 12, 3]	+
	Pure MC	[28, 27]	+
DCT	ART	[16, 10, 15]	−
DAXM	Other	[13]	+

Table 1: Grain mapping techniques and algorithms.

While the non-tomography technique DAXM deploys a special purpose algorithm, one can group the other algorithms into three classes: (1) *algebraic reconstruction techniques* (ART), as discussed in [6], (2) *discrete tomography algorithms* (DT) using Gibbs priors, as discussed in [7, 8], and (3) a pure Monte Carlo technique, as discussed in [28].

For a more general discussion of the topics touched upon in this paper we refer to the following books and surveys: [22, 21] for 3DXRD; [29, 4] for basics on diffraction physics; [19, 6] for computerized tomography and ART; and [7, 8] for discrete tomography.

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