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Combining 2D synchrosqueezed wave packet transform with optimization for crystal image analysis

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ABSTRACT

We develop a variational optimization method for crystal analysis in atomic resolution images, which uses information from a 2D synchrosqueezed transform (SST) as input. The synchrosqueezed transform is applied to extract initial information from atomic crystal images: crystal defects, rotations and the gradient of elastic deformation. The deformation gradient estimate is then improved outside the identified defect region via a variational approach, to obtain more robust results agreeing better with the physical constraints. The variational model is optimized by a nonlinear projected conjugate gradient method. Both examples of images from computer simulations and imaging experiments are analyzed, with results demonstrating the effectiveness of the proposed method.

1. Introduction

Defects, like dislocations, grain boundaries, and vacancies, play a fundamental role in polycrystalline materials. They greatly change the material behavior from a perfect crystal and affect the macroscopic properties of the materials. Analysis of images arising from atomistic simulations or imaging of polycrystalline materials hence becomes very important to characterize and help understand the defects and their effects on crystalline materials. While the defect analysis is traditionally done by visual inspection, the large amount of data made available due to advances in imaging and simulation techniques creates a need of efficient computer-assisted or automated analysis.

Crystal deformation at the atomic scale is another important quantity that characterizes polycrystalline materials. When the deformation, denoted by ψ, is well-defined, the tensor field $F = \nabla\psi$ describes the local crystal strain; the polar decomposition of F at each point gives grain rotations; the curl of F provides information about defects and the well-known Burgers vector that represents the magnitude and direction of the lattice distortion resulting from a dislocation. Since it is almost impossible to estimate the deformation manually, the development of computer-aided analysis becomes important.

For crystalline materials, defects are physical domains of the materials such that it is not possible to identify a smooth crystal deformation $\phi = \psi^{-1}$ that maps the atomic configuration back to a perfect lattice. In other words, the deformation gradient $G = \nabla\phi = F^{-1}$ is irregular and has nonzero curl at the defect location. In the opposite case, when a smooth deformation map does exist, the affine transform given by the gradient of the map, $G = \nabla\phi$, transforms the image locally to an

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undistorted lattice of atoms. Therefore, for a defect-free region of the material, G is a gradient field and thus is curl-free: curl $G = 0$. Crystal image analysis hence requires the detection of the defect regions and preferably also the estimation of the local elastic deformation G away from the defects.

In recent years several variational image processing methods for crystal analysis have emerged. The most basic versions just segment the crystal image into several crystal grains and identify their orientation, using clever formulations as convex optimization in 2D (Boerdgen et al., 2010; Strekalovskiy and Cremers, 2011) or efficient, sophisticated optimization algorithms for 3D images (Elsey and Wirth, 2014b). Berkels et al. (2008) additionally determine a full deformation field ψ via nonlinear optimization, while defects and local crystal distortion G are identified in Elsey and Wirth (2014a).

If accurate atom positions can easily be extracted from the image (or if the data stems from atomistic simulations) such that the input data consists of a discrete list of atom positions, then the local lattice orientation and deformation as well as defects can be obtained efficiently by identifying the nearest neighbors of each atom (Stukowski and Albe, 2010a,b; Begau et al., 2012).

Another efficient approach is the crystal image analysis via 2D synchrosqueezed transforms (SSTs) in Yang et al. (2014). The SST was originally proposed in Daubechies and Maes (1996), rigorously analyzed in Daubechies et al. (2011); Thakur and Wu (2011) and Yang (2015), and extended to 2D in Yang and Ying (2013, 2014b). It is proved that the 2D SST can accurately estimate the local wave vector of a nonlinear wave-like image. Inspired by the fact that a deformed atomic crystal grain can be considered as a superposition of several nonlinear wave-like components, Yang et al. (2014) propose an efficient crystal image analysis method based on a 2D band-limited SST. In particular, tracking the irregularity of the synchrosqueezed energy can identify defects, and the deformation gradient G can be obtained by a linear system generated with local wave vector estimations. A recent paper (Yang and Ying, 2014a) on the robustness of SSTs supports the application of this analysis method to noisy crystal images. The idea of exploiting the local periodic structure in the Fourier domain to extract a deformation gradient has also been considered in Hÿtch et al. (1998) in the crystal imaging literature.

Our work here is a variational approach based on the information obtained from a band-limited 2D synchrosqueezed wave packet transform following Yang et al. (2014). In this paper, we use this information as input to a variational optimization in order to improve the robustness of the analysis and, importantly, to make the results better agree with the physical nature of defects.

2. Variational method to retrieve deformation gradients

Let us fix a perfect, unstrained crystal with a fixed orientation as our reference lattice. Let $\Omega \subset \mathbb{R}^2$ be the domain of the image. Our objective is to find at each $x \in \Omega$ the local strain or deformation gradient $G(x) \in \mathbb{R}^{2\times 2}$ of a (locally defined) deformation ϕ which deforms a defect-free neighborhood of x into the reference lattice. (Note that since the image corresponds to a deformed crystal state, x should be understood as an Eulerian coordinate.) In other words, we seek the affine map defined by $G(x)$ which maps the local atom arrangement to the reference lattice. This is however impossible around defects. In particular, while curl $G = 0$ in the elastic region, in the defect region, curl G is not zero, and the integral of curl G over a neighborhood of the defect such as a dislocation should match the defect's Burgers vector (Elsey and Wirth, 2014b).

Assume that the defect region is given by $\Omega_d \subset \Omega$ and the curl of G is given by b, consistent with the Burgers vectors and with curl $G = 0$ on $\Omega\backslash\Omega_d$. We expect the displacement field to minimize the elastic energy of the system outside the defect region, since the system under imaging is in a quasistatic state. Given G_0 a rough guess of the deformation gradient, this motivates the energy minimization

$$\begin{aligned} \min_{G} \quad & \int_{\Omega\backslash\Omega_d} |G - G_0|^2 + W(G)\,\mathrm{d}x \\ \text{s. t.} \quad & \operatorname{curl} G = b, \end{aligned} \tag{1}$$

where $|\cdot|$ denotes the Frobenius norm of a matrix, $|A| = (\mathrm{tr}(A^{\mathrm{T}}A))^{1/2}$, and W is the elastic stored energy density.

Since our reference lattice represents the undeformed equilibrium state of the crystal and the atom configuration in the image is produced by the (local) deformation ϕ^{-1}, the stored elastic energy can be expressed in the standard Lagrangian form as the integral over the reference domain $\phi(\Omega\backslash\Omega_d)$ of an elastic energy density w that depends on $\nabla(\phi^{-1}) = G^{-1}\circ\phi^{-1}$,

$$\int_{\phi(\Omega\backslash\Omega_d)} w(G^{-1}\circ\phi^{-1}(y))\,\mathrm{d}y.$$

Here, w satisfies the standard conditions coming from first principles, i.e. w is frame indifferent, $w(A) = 0$ for $A \in SO(2)$, $w(A) > 0$ else, and $w(A) = \infty$ if $\det A \le 0$. After a change of variables the elastic energy turns into

$$\int_{\Omega\backslash\Omega_d} W(G)\,\mathrm{d}x$$

for $W(G) = w(G^{-1})\det G$, where it is easy to see that W has the same above properties as w. For w (or equivalently W) one can use a material-specific, possibly anisotropic energy density. To be specific, since our numerical examples are all concerned with a triangular lattice exhibiting isotropic elastic behavior, we here simply restrict ourselves to the following