Computer Physics Communications 184 (2013) 2489–2493

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Unique visualization of multiply oriented lattice structures using a continuous wavelet transform

Zhijun Wang, Junjie Li, Yaolin Guo, Sai Tang, Jincheng Wang *

State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, PR China

ARTICLE INFO

Article history:
Received 27 November 2012
Received in revised form
9 May 2013
Accepted 17 June 2013
Available online 26 June 2013

Keywords:
Grain orientation
Wavelet transform
Phase field crystal

ABSTRACT

The application of continuous wavelet transformation in the phase field crystal model has yielded excellent results for the crystal lattice orientation and grain boundaries with different misorientation angles [H.M. Singer, I. Singer, Phys. Rev. E 74 (2006) 031103]. However, we show here that the orientation map from this simple method cannot distinguish symmetric orientations using a single convolution template. By introducing additional rotational templates, the grain orientation can be uniquely visualized in two and three dimensions.

1. Introduction

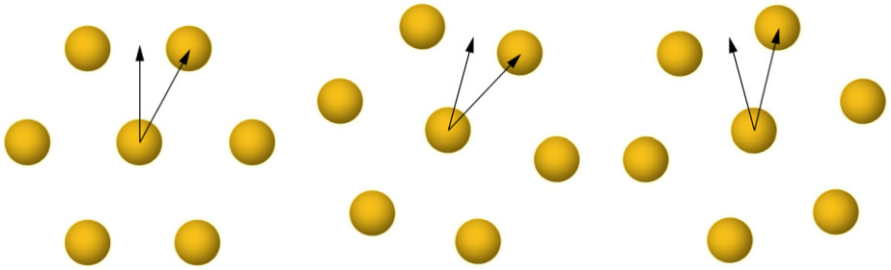
Multiply oriented lattice structures (grains) are very common in crystals and metallic materials [1]. Lattice orientation is one of the typical characteristics that determine grain boundary misorientation and hence affect material properties. Many physical phenomena are related to grain orientation, so grain orientation evolution is a hot topic in materials science. Visualization of grain orientation is crucial for multiply oriented lattice systems. Many experimental approaches have been used to reveal the grain orientation, such as electron backscattering diffraction in scanning electron microscopy [2], 3D atomic reconstruction of synchrotron diffraction data in transmission electron microscopy [3], and atomic probe tomography [4]. In atomic construction and probe tomography, atomic position data (lattice field) are detected and used to obtain an orientation map for nanocrystalline grains. In simulations, the lattice field can be obtained using approaches such as molecular dynamics [5], Monte Carlo [6] and phase field crystal (PFC) methods [7], for which the routine from the lattice field to the orientation map is the main issue.

Many methods have been used to identify the grain orientation from the lattice field. An intuitive way to identify the orientation of a unit cell is to locate the positions of all the nearest neighbors for the central atom. Although the detection principle of this method is very simple, there are great challenges in implementing it for multi-grain structures. One challenge is how to precisely find the lattice point locations before the orientation is determined. Another is how to deal with lattice points near defects. Differing from direct approaches, Fourier transformation can be used to find the grain orientation for a lattice field. In the Fourier spectral space, a lattice orientation corresponds to a spike. However, this method also has problems in treating lattice defects because the Fourier transform can introduce noise or mask spikes. A simple and efficient method is still lacking.

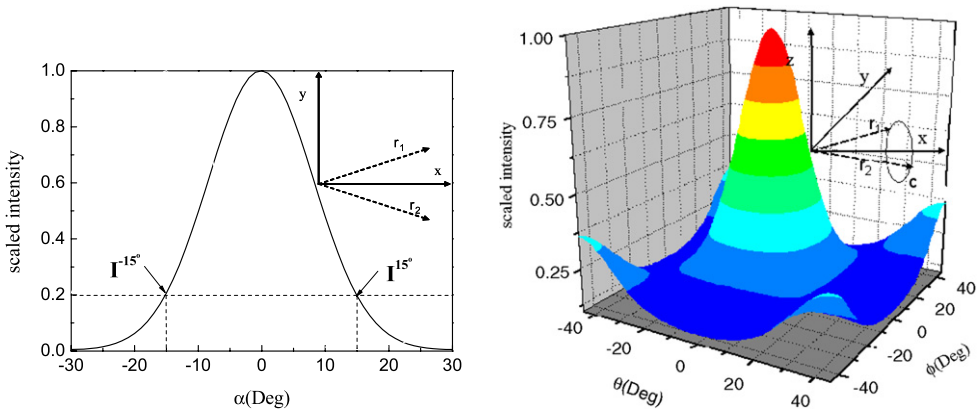
Wavelet transformation is an efficient method for extracting orientation fields from nonlinear evolution systems with multiply oriented lattice structures [8,9]. Singer and Singer extended this method to a much simpler arithmetic to reveal the orientation field in polycrystalline materials [10]. It has been proposed that the 2D continuous wavelet transform they developed can be used to visualize large-scale atomistic results. However, a bug exists for orientation detection using a continuous wavelet transform with a single template. Fig. 1 illustrates this bug in the 2D and 3D cases. The hexagonal close-packed (hcp) pattern shown in 2D in Fig. 1(a) has six-fold rotation symmetry. Fig. 1(b) and (c) show patterns rotated by 15° to the left and right, respectively. The rotational symmetry of the crystal lattice makes it impossible to identify the orientation symmetric with respect to the axis according to the continuous wavelet transform method, as shown in Fig. 1(d). Although the patterns in Fig. 1(b) and (c) have different orientations and the grain boundary is symmetric, the continuous wavelet transform with Fig. 1(a) as a convolution template yields the same convolution results. The 3D case is more complicated,

* Corresponding author. Tel.: +86 29 88460650; fax: +86 29 88491484.
E-mail address: jchwang@nwpu.edu.cn (J. Wang).

0010-4655/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cpc.2013.06.018



(a) Hexagonal lattice. (b) Lattice rotated by 15°. (c) Lattice rotated by −15°.



(d) Symmetric orientation in a 2D hexagonal lattice. (e) Symmetric orientation in a 3D bcc lattice.

Fig. 1. (Color online) Illustration of symmetric orientations with the same convolution values for wavelet transformation with a single convolution template.

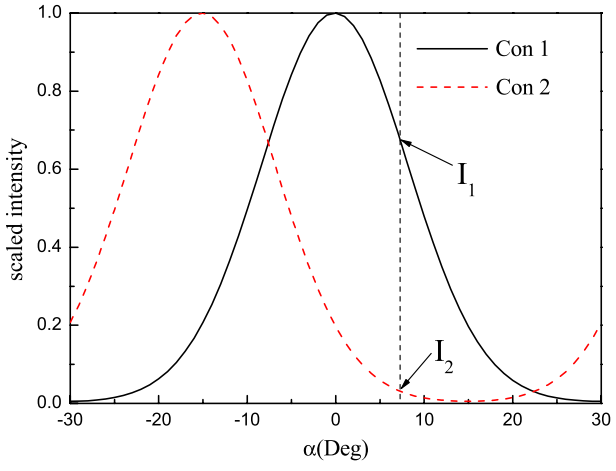


Fig. 2. (Color online) Scaled intensity profile for wavelet transformation with two convolution templates for different lattice orientations in 2D hexagonal structures.

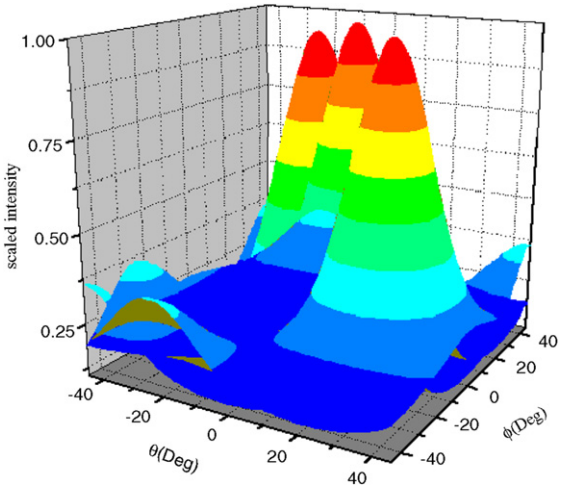


Fig. 3. (Color online) Scaled intensity profile for a wavelet transform with multiple convolution templates for a 3D bcc structure.

since orientations $[x, y, z]$ with constant x and $y^2 + z^2$ cannot be distinguished. The scaled intensity for the wavelet transform method for different lattice orientations in a body-centered cubic (bcc) structure is shown in Fig. 1(e). The scaled intensity curve has four-fold rotational symmetry and there are local maxima in the four corners. Fig. 1(e) shows that the symmetric orientation may have the same convolution value in 3D. Thus, the continuous wavelet transform method cannot distinguish the symmetric lattice orientation with only one convolution template. Therefore, the method is not suitable for analyzing orientation distributions. In this brief report, we overcome this problem by introducing additional rotated templates in the continuous wavelet transform method to uniquely determine the lattice orientation.

2. Method with multiple convolution templates

Here we use the PFC model to illustrate the method. The PFC model can resolve the atomic lattice structure of spatially periodic systems. The dimensionless free energy functional in the PFC model [7] is

$$F = \int dr \left(\frac{\rho}{2}[\varepsilon + (1 + \nabla^2)^2]\rho + \frac{\rho^4}{4} \right), \tag{1}$$

where ρ is the atomic density field period in the solid and ε is a dimensionless parameter related to supersaturation. The time-dependent density evolution equation is derived from the functional derivative using the Cahn–Hilliard formalism,

$$\partial\rho/\partial t = \nabla^2[\varepsilon + (1 + \nabla^2)^2\rho + \rho^3]. \tag{2}$$