Computational Materials Science 153 (2018) 338–347

Contents lists available at ScienceDirect

Computational Materials Science

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

Deformation of metals under dynamic loading: Characterization via atomic-scale orientation mapping

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ARTICLE INFO

Keywords:
Crystallographic orientation
Texture
EBSD
Molecular dynamics

ABSTRACT

Crystallographic orientation evolution of metals under dynamic loading conditions is of considerable interest, but rarely explored in simulations at atomistic scales. Here we present a methodology for atomic-scale orientation mapping, with atomic positions as input. The rotation matrix representing the orientation of a crystallite consisting of a central atom and its nearest neighbors, and corresponding Euler angles, are calculated, which are used for orientation analysis and visualization. As application cases, we investigate orientation evolution related to grain boundary migration, deformation twinning, deformation within grain interior, partial grain rotation, and grain refinement in representative FCC, BCC and HCP metals under dynamic loading conditions including shock loading.

1. Introduction

Since deformation of a crystallite is accompanied by a change in crystallographic orientation [1], its orientation evolution during dynamic loading conditions is directly relevant. Quantitative characterization of three-dimensional (3D) microstructure is critical for understanding deformation mechanisms, and materials design and manufacturing [2]. Orientation map (OM), orientation distribution function (ODF), pole figure (PF) and inverse pole figure (IPF) are widely used to present quantitative information on texture. OM provides spatially-resolved orientation information, while ODF, PF and IPF can provide statistical (overall) information on texture. In experiments, combining quantitative optical and scanning electron microscopy with serial sectioning [3,4], yields 3D microstructures to be mapped. Focused ion-beam micromachining [5] allows for sectioning at nanometer spacing. However, these procedures are destructive and time-consuming, and inappropriate for dynamic processes [6]. Differential aperture microscopy [7,8], 3D X-ray diffraction microscopy [6,9,10] and X-ray diffraction contrast tomography [11–13] have been developed for nondestructive 3D grain orientation mapping and can be implemented for quasi-static deformation experiments, which takes several minutes to hours [14–16]. For high strain rate experiments such as shock loading, 3D orientation mapping in real time is still impractical [17].

Currently, simulation is likely the only way to achieve 3D orientation mapping for high strain rate deformation processes, including finite element analysis based on crystal plasticity finite-element models [18–22]; viscoplastic self-consistent approach [23–27]; and Monte Carlo method which is implemented in grain growth simulation considering grain boundary energy and mobility via grain boundary misorientation [28–31]. However, the simulations of orientation evolution at the atomic scale for nanocrystalline materials under dynamic loading are extremely rare. Comparing to above simulation methods, molecular dynamics (MD) simulations are ideal to simulate the high strain rate deformation processes in nanocrystalline materials [32–34]. However, the vast majority of conventional characterizations in atomistic modeling are limited to calculation of local properties of each atom in terms of local structure type, energy, stress or local lattice distortion [35–39], lacking quantitative crystallographic orientation information as offered by electron backscatter diffraction (EBSD) experiments.

At the atomic scale, different orientation mapping methods were recently developed for face-centered cubic (FCC) [40,41] and body-centered cubic (BCC) systems [42,43]. For example, polyhedral template matching (PTM) can not only classify local structures, but also identify local lattice orientations [44]. A major difference between these methods lies in color-coding which represents the orientation of a crystallite formed by an atom under consideration and its nearest neighbors, i.e., the definition of orientation vector. Here, we present a

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https://doi.org/10.1016/j.commatsci.2018.06.020
Received 7 May 2018; Received in revised form 9 June 2018; Accepted 9 June 2018
0927-0256/

methodology for atomic-scale orientation mapping and quantitative texture characterization from atomic configurations extracted from MD simulations under elevated stresses. In particular, our methodology defines orientation vector and color-coding in a way similar to EBSD-based orientation mapping widely used in experiments, and can be applied to FCC, BCC and HCP (hexagonal close-packed) systems. Texture characterization is based on Euler angles calculated for each atom (in terms of the crystallite consisting of this atom and its nearest neighbors), and quantifies ODF, PF, and IPF. Five application cases are presented for representative crystal structures, microstructures and loading conditions, including shock-induced grain boundary migration in Cu, deformation in columnar Al, grain refinement in Ta, and texture evolution in nanocrystalline Ta, as well as tensile deformation in nanocrystalline Mg with embedded nanotwins.

2. Methodology

In this section, we present the methodology for atomic-scale orientation mapping and texture analysis, which are based on the orientation analysis of a crystallite containing an atom under consideration and its nearest neighbors. We use "crystallite" and "atom" (which anchors the crystallite) interchangeably unless stated otherwise.

Given a crystal structure, we find the nearest neighbors of each atom within the nearest neighbor distance, which is obtained from the radial distribution function [45]

$$g(r)=\frac{1}{\rho_0}\frac{\langle n(r)\rangle}{4\pi r^2\Delta r}, \tag{1}$$

where $\langle n(r)\rangle$ is the average number of atoms in a shell of thickness Δr at distance r from an atom under consideration, and ρ_0 is atom density. The value of r at the valley between the first and second peaks of $g(r)$ is considered as the average nearest neighbor distance. A crystallite is defined by a central atom under consideration and the nearest neighbors, and used for subsequent orientation analysis.

The implementation of atom-scale orientation mapping and texture analysis consists of three steps. (i) Calculate the direction vectors of three crystallographic axes ($\boldsymbol{a}_i$) for each crystallite to obtain an orthogonal rotation matrix, $\mathbf{R}$. (ii) For each crystallite k, compute its orientation mapping vector $\boldsymbol{q}_{\mathrm{om},k}$ and Euler angles from the rotation matrix. (iii) Visualize the orientation mapping by coloring each atoms with orientation mapping vector as RGB scheme, and calculate the orientation distribution functions from the Euler angles.

2.1. Rotation matrix

The orientation of a crystal with respect to a reference coordinate system is represented by a three-dimensional orthogonal rotation matrix, $\mathbf{R}$ [1,46]. Once the rotation matrix is calculated, orientation mapping vectors $\boldsymbol{q}_{\mathrm{om},k}$ and Euler angles can be computed from the rotation matrix, and then the orientation maps and orientation distribution functions can be obtained. A similar way to determine rotation matrix was used previously by Song and Hoyt [47]. In their work, grain misorientation or interphase boundaries are quantitatively identified by the rotation axis and the rotation angle between grains deduced from a rotation matrix. However, orientation mapping vectors and Euler angles, which can be used for visualizing orientations of individual grains and statistical analysis of orientations, are largely lacking in literature.

For cubic systems, $\mathbf{R}$ is defined as the misorientation between three crystallographic axes ($\boldsymbol{a}_1$: $[1\,0\,0]_\mathrm{c}$, $\boldsymbol{a}_2$: $[0\,1\,0]_\mathrm{c}$, and $\boldsymbol{a}_3$: $[0\,0\,1]_\mathrm{c}$), and those of the sample coordinate system, i.e., rolling (RD: $[100]_\mathrm{s}$), transverse (TD: $[0\,1\,0]_\mathrm{s}$), and normal (ND: $[0\,0\,1]_\mathrm{s}$) directions (Fig. 1).

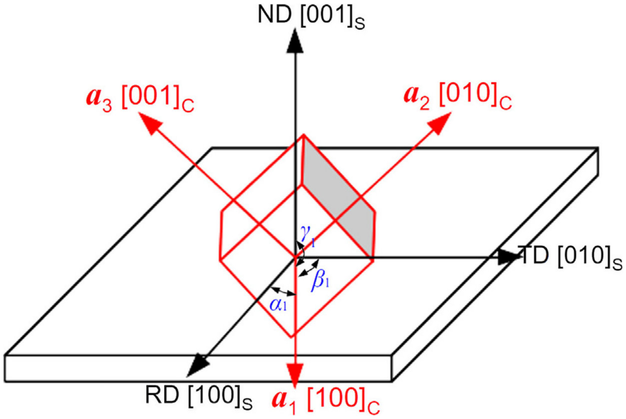

Fig. 1. Definition of crystal and sample coordinate systems for cubic crystals, denoted with subscripts c and s, respectively. The crystal coordinate system axes (red) are $\boldsymbol{a}_1$: $[1\,0\,0]_\mathrm{c}$, $\boldsymbol{a}_2$: $[0\,1\,0]_\mathrm{c}$, and $\boldsymbol{a}_3$: $[0\,0\,1]_\mathrm{c}$, and the sample or reference system axes are (black) RD ($[1\,0\,0]_\mathrm{s}$), TD ($[0\,1\,0]_\mathrm{s}$), and ND ($[0\,0\,1]_\mathrm{s}$). α_i, β_i, and γ_i are defined as the direction angles between $\boldsymbol{a}_i$ and RD, TD, and ND, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Here α_i, β_i, and γ_i (i = 1, 2, and 3) are defined as direction angles between $\boldsymbol{a}_i$ and RD, TD, and ND, respectively, and the rotation matrix, $\mathbf{R}$, is expressed alternatively in terms of direction cosines as

$$\mathbf{R}=\begin{pmatrix}\cos\alpha_1 & \cos\beta_1 & \cos\gamma_1\\ \cos\alpha_2 & \cos\beta_2 & \cos\gamma_2\\ \cos\alpha_3 & \cos\beta_3 & \cos\gamma_3\end{pmatrix}, \tag{2}$$

and

$$\begin{aligned}\cos\alpha_i&=\mathrm{RD}\cdot\hat{\boldsymbol{a}}_i,\\ \cos\beta_i&=\mathrm{TD}\cdot\hat{\boldsymbol{a}}_i,\\ \cos\gamma_i&=\mathrm{ND}\cdot\hat{\boldsymbol{a}}_i,\end{aligned} \tag{3}$$

where $\hat{\boldsymbol{a}}_i$ is the unit vector of $\boldsymbol{a}_i$.

For HCP crystals, the hexagonal crystal coordinate system is transformed to the orthogonal coordinate system, and the three crystallographic axes in the orthogonal coordinate system, $\boldsymbol{a}_1$: $[1\,0\,0]_\mathrm{c}$, $\boldsymbol{a}_2$: $[0\,1\,0]_\mathrm{c}$, and $\boldsymbol{a}_3$: $[0\,0\,1]_\mathrm{c}$, correspond to $[2\,\bar{1}\,\bar{1}\,0]_\mathrm{c}$, $[0\,1\,\bar{1}\,0]_\mathrm{c}$, and $[0\,0\,0\,1]_\mathrm{c}$ directions in the hexagonal system, respectively. Then the orthogonal rotation matrix $\mathbf{R}$ for HCP crystals can be obtained from Eqs. (2) and (3).

2.2. Crystallographic orientation

In order to calculate rotation matrix at the atomic scale, a key step is to determine crystallographic orientation of a crystallite formed by an atom under consideration and in crystals. This process depends on crystal lattice system. FCC, BCC and HCP are three most common crystal systems with different stacking sequences, atomic packing factors, coordination numbers (n_{CN}), and symmetry (Fig. 2(a)–(c)), and are thus considered here. An atom under consideration and its nearest neighbors form a crystallite. The crystal orientation of this crystallite is obtained via analyzing the directions between the central atom and its nearest neighbors.

For a perfect FCC lattice, we define a set of 12 vectors pointing from the central atom to its 12 nearest neighbors, i.e., the $\langle 1\,1\,0\rangle$ direction vectors [41]. Among the 12 vectors, the vector forming the smallest angle with $[1\,0\,1]_\mathrm{s}$ is defined as $[1\,0\,1]_\mathrm{c}$. We then choose the vector which