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Acta Materialia 53 (2005) 1179–1190
Acta MATERIALIA
www.actamat-journals.com

Representation of misorientations in Rodrigues–Frank space: application to the Bain, Kurdjumov–Sachs, Nishiyama–Wassermann and Pitsch orientation relationships in the Gibeon meteorite

Youliang He *, Stéphane Godet, John J. Jonas

Department of Metals and Materials Engineering, McGill University, Wong Building, 3610 University Street, Montreal, Que., Canada H3A 2B2

Received 7 July 2004; received in revised form 14 September 2004; accepted 5 November 2004
Available online 24 December 2004

Abstract

The three classical orientation relationships describing the γ-to-α transformation, namely the Bain, Kurdjumov–Sachs (K–S) and Nishiyama–Wassermann (N–W), are represented in Rodrigues–Frank (R–F) space. Two alternative reference systems are used to highlight the differences between the three types of misorientation. Some observations obtained on the Gibeon meteorite are analyzed using the two classes of reference system to reveal features of the transformation under conditions of very slow cooling. It is shown that the Bain correspondence relations are never satisfied, while the measurements fall in the full range of direction parallel conditions extending from the K–S to the N–W. The crystallographic features of the Pitsch orientation relation are presented in R–F space in Appendix A. The experimental observations conform to this type of transformation to a considerably lesser extent than to the classical K–S and N–W relations.

Keywords: Metals; Phase transformation; Misorientation; EBSD; Rodrigues–Frank space

1. Introduction

Misorientation, the crystallographic orientation difference between two individual crystallites, is an important parameter used to describe the microtexture of materials. For instance, the grain boundary texture is commonly specified in terms of a rotation about an axis common to both crystallites that brings the coordinate system of the first into coincidence with that of the other. This is the so-called angle–axis pair description and it provides significant information about the grain boundary geometry. An important example is that of coincident site lattice (CSL) boundaries, which are uniquely described by the axis and angle of misorientation between the two neighboring grains [1].

In other cases, such as phase transformations, where the misorientation between the initial phase and its transformed products is the major concern, it is more convenient to represent the misorientation between the two phases using the Rodrigues–Frank (R–F) vector, since the latter takes the lowest angle solution and integrates the four parameters (i.e. the rotation angle and the three components of the rotation axis) into a three-component vector that can be readily displayed in a three-dimensional Cartesian space (R–F space) [2]. One of the advantages of R–F parameterization is that either the specimen or the crystal axes can be chosen for reference; according to this system of representation, the rotation angle and axis are directly related to a

* Corresponding author. Tel.: +1 514 3984755x09501; fax: +1 514 3984492.
E-mail address: youliang.he@mail.mcgill.ca (Y. He).

1359-6454/$30.00
doi:10.1016/j.actamat.2004.11.021

vector drawn from the center of the space to the point representing the rotation axis.

The use of R–F space to represent orientations and misorientations is relatively new compared to that of using rotations about three successive axes, i.e. that of Euler space, and its advantages over the employment of such other spaces have been addressed by several researchers [3–5]. However, most of these investigations were focused on the representation of *orientations* in R–F space; only a few were concentrated on the representation of *misorientations* [2,6,7]. In this study, the misorientation between two crystallites, which is calculated from orientations measured by electron backscatter diffraction (EBSD) techniques, is represented as an R–F vector, taking one of the crystallites as the reference system. Specifically, the three classical correspondence relationships that describe the FCC to BCC transformation, namely the Bain [8], Kurdjumov–Sachs [9] and Nishiyama–Wassermann [10,11], are represented in this space. A second reference system is then introduced, which has certain advantages in the present case.

The variants of the three orientation relationships are derived directly from the parallelism conditions applying to the crystallographic planes and directions that define these relationships. Some recent results concerning the transformation of taenite (FCC austenite) in the Gibeon meteorite are then presented to illustrate the advantages of the use of this space. In Appendix A, the variants of the Pitsch [12] transformation relationship are also derived from the parallelism conditions. These are then represented in R–F space using the two frames of reference (austenite and Bain). Their positions on a {0 0 1} pole figure are compared with those of K–S and N–W. Some meteorite observations are then plotted in these two forms of representation (pole figure and R–F space) and the extent to which the Pitsch relation applies is evaluated.

2. Misorientation and Rodrigues–Frank space

Here, the orientation matrices for two crystallites **A** and **B** are $\mathbf{M}_A$ and $\mathbf{M}_B$, respectively. Then the *misorientation* matrix $\mathbf{M}_{AB}$ relating these crystallites, arbitrarily taking crystallite **A** as the reference system, can be written as

$$\mathbf{M}_{AB} = \mathbf{M}_B \mathbf{M}_A^{-1}. \quad (1)$$

This matrix defines a rotation that transforms the coordinate system of the reference crystallite into coincidence with that of the other crystallite. [1] The angle–axis form associated with this misorientation matrix can then be calculated as: $\theta = \arccos(\frac{1}{2}[\mathrm{Tr}(\mathbf{M}_{AB}) - 1])$ and $[u, v, w] = [m_{23} - m_{32}, m_{31} - m_{13}, m_{12} - m_{21}]$ [13], where $\mathrm{Tr}(\mathbf{M}_{AB})$ is the trace of matrix $\mathbf{M}_{AB}$ and m_{ij} $(i, j = 1, 2, 3)$ are the elements of $\mathbf{M}_{AB}$.

The four parameters can be further reduced to three using the Rodrigues formula: $\mathbf{R} = \tan\frac{\theta}{2}[u, v, w]$ [14], which defines the three components $(\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3)$ of the R–F vector. Each misorientation is now represented as an R–F vector or more specifically as the endpoint of the vector in R–F space. To avoid the singularity associated with the R–F vector approaching infinity when the rotation angle θ reaches its upper limit π, the space is reduced to a finite subspace called the *fundamental zone* by utilizing the minimum angle–axis pair representation or *disorientation*. The latter is obtained by taking the crystal symmetry into account, i.e. employing the 24 symmetry operations for cubic crystals [4,7].

The fundamental zone of R–F space for cubic symmetry is reproduced here in Fig. 1 since most of the discussion that follows about the four transformation relationships will be presented in this subspace. Some authors have reduced the fundamental zone even further by considering only 1/48 of this space [7]. However, this approach is not satisfactory for the present study since, as will be evident in what follows, both the signs and orders of the components of the rotation axis are of importance.

The three points A, B and C illustrated in the diagram typify the centers of the octahedral (A) and triangular (B) faces of the fundamental zone, while the vertices of the triangles are characterized by C. There are 6, 8 and 24, respectively, such points in the fundamental zone. It should be emphasized that it is a prop-

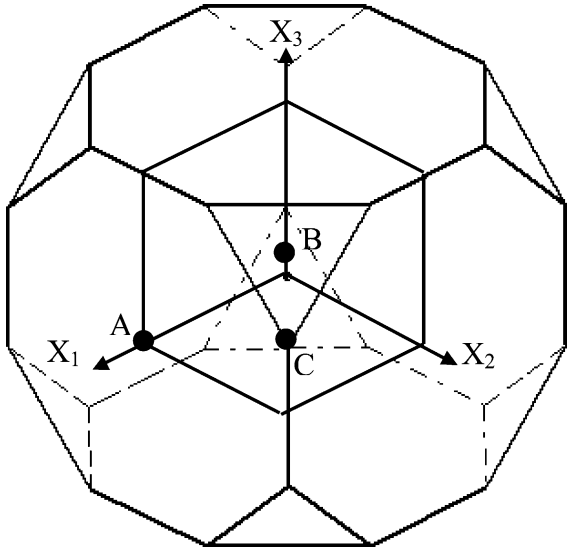

Fig. 1. Fundamental zone of R–F space for cubic symmetry. The three illustrated points correspond to the following angle–axis pairs: A: 45° [1 0 0], B: 60° [1 1 1] and C: 62.8° $[1\,1\,(\sqrt{2}-1)]$.

[1] It should be noted that the matrices used here are associated with the coordinate frame transformations that are often cited in material science rather than the body rotations usually employed in other fields. Moreover, the transformation is always expressed as a conversion of the reference coordinate system into that of the product.