

Volume of intersection of two balls in orientation space

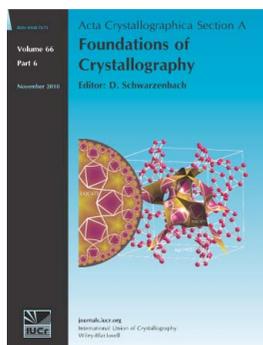
A. Morawiec

Acta Cryst. (2010). **A66**, 717–719

Copyright © International Union of Crystallography

Author(s) of this paper may load this reprint on their own web site or institutional repository provided that this cover page is retained. Republication of this article or its storage in electronic databases other than as specified above is not permitted without prior permission in writing from the IUCr.

For further information see <http://journals.iucr.org/services/authorrights.html>



Acta Crystallographica Section A: Foundations of Crystallography covers theoretical and fundamental aspects of the structure of matter. The journal is the prime forum for research in diffraction physics and the theory of crystallographic structure determination by diffraction methods using X-rays, neutrons and electrons. The structures include periodic and aperiodic crystals, and non-periodic disordered materials, and the corresponding Bragg, satellite and diffuse scattering, thermal motion and symmetry aspects. Spatial resolutions range from the subatomic domain in charge-density studies to nanodimensional imperfections such as dislocations and twin walls. The chemistry encompasses metals, alloys, and inorganic, organic and biological materials. Structure prediction and properties such as the theory of phase transformations are also covered.

Crystallography Journals **Online** is available from journals.iucr.org

Volume of intersection of two balls in orientation space

A. Morawiec

Polish Academy of Sciences, Institute of Metallurgy and Materials Science, Krakow, Poland. Correspondence e-mail: nmmorawi@cyf-kr.edu.pl

Received 6 April 2010
Accepted 2 September 2010© 2010 International Union of Crystallography
Printed in Singapore – all rights reserved

Orientations deviating from an ideal orientation by angles not exceeding a given limit constitute a ball in the metric space of orientations. Such balls arise in crystallographic computations, and in some cases intersections of the balls are of interest. This paper provides an analytical formula for calculation of the volume of the intersection of two balls from their radii and the distance between their centers. The formula is used to determine the volumes of the intersections of balls corresponding to misorientations of coincident lattices.

1. Introduction

Elements of the orthogonal group $SO(3)$ are frequently used in crystallography. They represent crystal orientations, misorientations or various rotations. Orientations, for instance, are of primary importance for analysis of crystallographic textures in polycrystalline materials. The description of textures often involves particular ideal orientations with allowance for certain tolerance. In most cases, the tolerance is given as an angle of rotation by which an orientation may differ from the ideal orientation. Formally, all orientations within such tolerance constitute a ball in the space of orientations with the center at the ideal orientation and the radius given by the limiting angle.

Such balls arise when orientations or misorientations are measured with limited accuracy. For example, in the case of popular electron-backscatter-diffraction-based orientation mappings, the accuracy of relative orientations is estimated to be about 0.5° . Similarly, one may consider balls centered at ideal orientations of texture components like 'copper', 'brass' or 'S' common in deformed face-centered cubic metals with orthorhombic sample symmetry (Bunge, 1982); the radius can be linked to the typical spread of these components, which is usually $10\text{--}15^\circ$. Balls are also used in the analysis of crystal misorientations corresponding to the coincident lattices (CSLs) of Kronberg & Wilson (1949). Their radii are ordinarily assumed to be given by the Brandon criterion, *i.e.* with Σ being the inverse of the fraction of coinciding lattice nodes, the radius equals $15^\circ/\Sigma^{1/2}$ (Ranganathan, 1966; Grimmer *et al.*, 1974; Fortes, 1983).

The balls of (mis)orientations may intersect each other. This occurs for the balls centered at the ideal orientations of conventional texture analysis: *e.g.*, if the radii exceed 10° , the ball centered at the ideal 'S' orientation intersects those centered at 'brass' and 'copper'. Intersections also occur for some balls of CSL misorientations.

When two balls intersect each other, there is a fraction of (mis)orientations that belong to both of them. The question is, how big is this fraction? In the random case, it is determined by the volume of the common part of the balls. Since the space of orientations is non-Euclidean, the volume will definitely differ from the Euclidean approximation and, knowing the exact solution, one could assess how big is the difference.

Below, this problem of the volume of the intersection of two balls is addressed. One might expect that a solution is to be found some-

where in the mathematical literature but we have not been able to locate such a publication. Therefore, a proper formula is derived. It is compared with the approximate result of the conventional Euclidean geometry. In the end, the formula is applied to intersections of balls corresponding to low- Σ cubic CSLs.

Formally, we consider $SO(3)$ with the invariant measure and the balls constructed using the metric based on the rotation angles. With texture-related applications in mind, a less formal language of this particular field is used.

2. Volume of an intersection of two balls

Balls are easily defined in metric spaces, and orientations constitute such a space with the angular distance between two orientations given by the smallest rotation angle needed to transform one of them onto the other. The largest possible distance is 180° or π rad.¹ A ball of radius ω ($0 < \omega \leq \pi$) centered at a given orientation consists of all orientations with the distance to the central orientation not larger than the radius. The metric based on the angular distance implicates a measure, which is a standard reference for distributions of orientations. With this measure, the volume V of a ball of radius ω (rad) is given by the well known expression

$$V(\omega) = (\omega - \sin \omega)/\pi,$$

where the normalization was chosen so the whole space has the volume of 1, or $V(\pi) = 1$ (see, *e.g.*, Morawiec, 2004).

The formula for the volume of the intersection of two balls is more complicated but it can be derived by elementary means using the so-called Rodrigues parameters (*e.g.* Frank, 1988). For the rotation given by the parameters (r_1, r_2, r_3) , the angle of the rotation is equal to $2 \arctan[(r_1^2 + r_2^2 + r_3^2)^{1/2}]$. Moreover, the measure equals $dr_1 dr_2 dr_3 / [\pi(1 + r_1^2 + r_2^2 + r_3^2)]^2$ (Morawiec, 2004). In general, a ball in the Cartesian system with Rodrigues parameters as coordinates is bounded by axially symmetric quadric surfaces (ellipsoid, paraboloid or two-sheet hyperboloid) but if the ball is centered at $(r_1, r_2, r_3) = (0, 0, 0)$, it is simply bounded by a sphere (Fig. 1).

We start with calculating the volume of the cap bounded by the sphere $(r_1^2 + r_2^2 + r_3^2)^{1/2} = R = \tan(\omega/2)$ and the plane $r_3 = a$ (where

¹ From now on, angles related to experiments or conventions will be given in $^\circ$, whereas angles in formulas will be in rad.

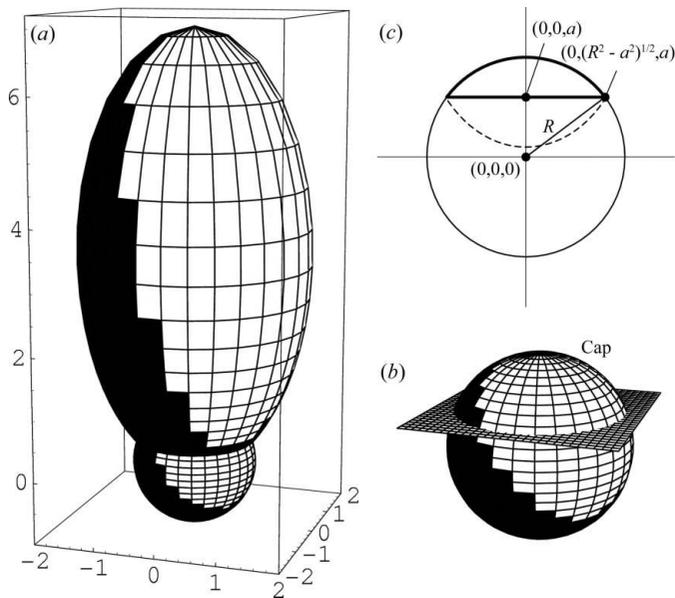


Figure 1
Intersecting orientation balls (of equal radii = $\pi/2$) shown in the Rodrigues parameterization (a), the ball centered at (0, 0, 0) with a plane cutting off a cap (b) and a schematic section through this ball (c).

$|a| < R$) by integrating the measure over the cap. The volume of the cap turns out to be

$$\left[\arctan(R) - \arctan(a) - (R - a)/(R^2 + 1) \right] / \pi.$$

One can transform the whole system by a rotation so the second ball becomes centered at (0, 0, 0) and obtain the volume of the second cap. The volume of the lens-shaped intersection of the balls is the sum of the volumes of the two caps, if the transformation does not move any points beyond the cap. In fact, this does not occur because the transformation is continuous, and in the Rodrigues coordinates, a rotation transforms a plane to a plane (Frank, 1988); in particular, the latter applies to the plane separating the caps.

Thus, the volume of the intersection is obtained by adding the volumes of the caps. With two balls and two caps, the quantities R , a and ω are equipped with indices, so R_i , a_i and $\omega_i = 2 \arctan(R_i)$ correspond to the i th ball ($i = 1, 2$). The distance ϑ between the centers of the balls is equal to the sum of the distances of the centers to the plane separating the caps, *i.e.* $\vartheta = 2 \arctan a_1 + 2 \arctan a_2$. Moreover, the angular distance between the points (0, 0, a_1) and (0, ($R_1^2 - a_1^2$)^{1/2}, a_1) is the same as the distance between (0, 0, a_2) and (0, ($R_2^2 - a_2^2$)^{1/2}, a_2) (see Fig. 1c). Hence, using the formula for composition of rotations in Rodrigues parameterization (*e.g.* Frank, 1988), one gets $(R_1^2 - a_1^2)/(1 + a_1^2) = (R_2^2 - a_2^2)/(1 + a_2^2)$. Based on these two relationships, a_1 and a_2 are eliminated. In effect, the volume v of the intersection of the balls can be expressed *via* their radii ω_i and the distance ϑ between their centers,

$$v(\omega_1, \omega_2, \vartheta) = \frac{V(\omega_1) + V(\omega_2)}{2} - \frac{1}{\pi} \times \left[\frac{\vartheta}{2} + \left(\cos^2 \frac{\omega_1}{2} + \cos^2 \frac{\omega_2}{2} \right) \cot \frac{\vartheta}{2} - 2 \cos \frac{\omega_1}{2} \cos \frac{\omega_2}{2} \csc \frac{\vartheta}{2} \right], \quad (1)$$

where $0 \leq \omega_1, \omega_2, \vartheta \leq \pi$. This formula is applicable if $|\omega_1 - \omega_2| \leq \vartheta \leq \omega_1 + \omega_2$; otherwise, the smaller ball is completely

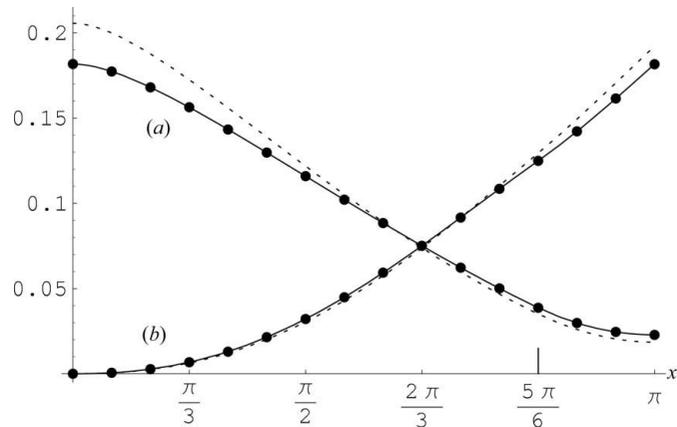


Figure 2
The functions $v(2\pi/3, \pi/2, x)$ (a) and $v(\pi/2, x, 2\pi/3)$ (b) for x in the range $(\pi/6, \pi)$. The continuous curves are based on equations (1) and (3); the mark on the abscissa (at $x = 5\pi/6$) separates domains of applicability of these equations. The dots have been obtained numerically by counting randomly generated orientations falling into ball intersections. For each point, the total number of generated orientations was 10^6 . The dashed lines represent volumes calculated using Euclidean approximation with two lens-shaped parts included for $x > 5\pi/6$.

contained in the larger one, or there is no intersection. Moreover, there must occur

$$\vartheta + \omega_1 + \omega_2 \leq 2\pi. \quad (2)$$

If this condition is not satisfied, the total intersection consists of two lens-shaped parts. The volume of one part is given by equation (1), whereas the volume of the other part can be obtained by using equation (1) with ϑ replaced by $2\pi - \vartheta$. The sum of these two volumes, *i.e.* the total volume of the intersection in the case when $\vartheta + \omega_1 + \omega_2 \geq 2\pi$, is

$$v(\omega_1, \omega_2, \vartheta) = V(\omega_1) + V(\omega_2) + \frac{4}{\pi} \cos \frac{\omega_1}{2} \cos \frac{\omega_2}{2} \csc \frac{\vartheta}{2} - 1. \quad (3)$$

Example cuts through the function $v(\omega_1, \omega_2, \vartheta)$ are shown in Fig. 2.

The above expressions can be partly tested by considering the limiting cases like externally tangent balls ($\vartheta = \omega_1 + \omega_2$), internally tangent balls ($\vartheta = |\omega_1 - \omega_2|$) or vanishing ω_1 . As expected, for $\vartheta = \omega_1 + \omega_2$ and $\vartheta = |\omega_1 - \omega_2|$, the function $v(\omega_1, \omega_2, \vartheta)$ equals 0 and $\min[V(\omega_1), V(\omega_2)]$, respectively, and $\lim_{\omega_i \rightarrow 0} v(\omega_1, \omega_2, \vartheta) = 0$.

For small ω , one has $8\pi^2 V(\omega) \simeq 4\pi\omega^3/3$ – the expression for the volume of a ball in the Euclidean geometry. Similarly, the first term of the Maclaurin series of $8\pi^2 v(\omega_1, \omega_2, \vartheta)$ with respect to ϑ, ω_1 and ω_2 is equal to the volume of intersection of two balls in the Euclidean geometry. From the practical viewpoint, the exact expression for v differs significantly from the Euclidean approximation only if both balls are large. This means that the Euclidean approximation can be used in many crystallographic applications.

3. Intersections of balls corresponding to CSLs

Let us consider the intersections of balls corresponding to low- Σ CSLs in the cubic case. For Σ up to 33, there are ten cases in which balls corresponding to different Σ intersect each other. They are listed in Table 1. For instance, the misorientations of $\Sigma 1$ and $\Sigma 25a$ are separated by the distance of 16.26° , and the Brandon radii are 15 and 3° , respectively. The volume of the intersection of the two balls constitutes 18.02% of the volume of the ball linked to $\Sigma 25a$. In order to calculate the total volumes of CSL misorientations, crystal symmetry needs to be taken into account. Because of symmetry, a ball

Table 1
CSLs with intersecting balls.

The radii of the balls are based on the Brandon criterion. The last column (v/V_2) shows the percentage of the volume of the smaller ball contained in the other ball.

| Σ_1 | Σ_2 | ϑ (°) | v/V_2 (%) |
|------------|------------|-----------------|-------------|
| 1 | 25a | 16.26 | 18.02 |
| 5 | 17a | 8.80 | 8.19 |
| 5 | 29a | 6.73 | 41.59 |
| 7 | 19b | 8.61 | 0.95 |
| 9 | 27a | 7.36 | 1.56 |
| 13a | 17a | 5.45 | 14.93 |
| 13a | 25a | 6.36 | 2.97 |
| 13b | 21a | 6.01 | 7.41 |
| 19a | 27a | 5.06 | 7.32 |
| 21a | 31a | 3.89 | 21.47 |

has symmetrically equivalent copies. The number of copies is determined by the symmetry and the multiplicity (Matthies *et al.*, 1987; Field, 1995) of the ball center. For instance, in the considered case, the number of $\Sigma 25a$ balls is six times larger than the number of balls corresponding to $\Sigma 1$, and – consequently – each ball of $\Sigma 1$ intersects six distinct balls of $\Sigma 25a$.

Symmetrically equivalent balls of the same Σ may also partly overlap. In the cubic case, this occurs for $\Sigma 17b$ and $\Sigma 29a$. The distance between the nearest $\Sigma 17b$ misorientations is 6.74° , and the

overlapping of two balls constitutes 0.78% of the volume of one ball. For $\Sigma 29a$, these numbers are 2.79° and 31.07%, respectively.

The presence of the intersections has an impact on the overall percentage of CSL misorientations among random misorientations (*cf.* Warrington & Boon, 1975; Morawiec *et al.*, 1993). Detailed analysis of this subject is beyond the scope of this note.

References

- Bunge, H. J. (1982). *Texture Analysis in Materials Science*. London: Butterworths.
- Field, D. P. (1995). *Scr. Metall. Mater.* **32**, 67–70.
- Fortes, M. A. (1983). *Acta Cryst.* **A39**, 351–357.
- Frank, F. C. (1988). *Metall. Trans. A*, **19**, 403–408.
- Grimmer, H., Bollmann, W. & Warrington, D. H. (1974). *Acta Cryst.* **A30**, 197–207.
- Kronberg, M. L. & Wilson, F. H. (1949). *Trans. Met. Soc. AIME*, **185**, 501–514.
- Matthies, S., Vinel, G. W. & Helming, K. (1987). *Standard Distributions in Texture Analysis*. Berlin: Akademie-Verlag.
- Morawiec, A. (2004). *Orientations and Rotations. Computations in Crystallographic Textures*. Berlin: Springer.
- Morawiec, A., Szpunar, J. A. & Hinz, D. C. (1993). *Acta Metall. Mater.* **41**, 2825–2832.
- Ranganathan, S. (1966). *Acta Cryst.* **21**, 197–199.
- Warrington, D. H. & Boon, M. (1975). *Acta Metall.* **23**, 599–607.