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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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Accurate computation of the rotation matrices.

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Abstract

A new recurrence relation between the reduced matrices of the irreducible representations of the rotation group is proposed, which permits their accurate computation for high orders of the representation.

This work was motivated by the appearance of numerical divergences during the computation of the fast rotation function (Crowther, 1972). The origin of this behaviour was found to be the numerical instability of the recurrence relation used to compute the rotation matrices, for moderately high angular momenta and a wide range of angles. Overflows were in fact detected for expansions involving spherical harmonics of order $j \geq 74$.

In an irreducible representation of the rotation group of dimension $2j+1$, the rotation parameterized by the Euler angles (α, β, γ) is represented by the matrix (Brink & Satchler, 1975)

$$D^j_{mn}(\alpha, \beta, \gamma) = d^j_{mn}(\beta) \exp -i(m\alpha + n\gamma). \quad (1)$$

The reduced matrices d^j_{mn} are determined by means of the 'triangular' relationship (Altmann & Bradley, 1963)

$$\begin{aligned}&[(j-m)(j+m+1)]^{1/2} d^j_{m,n}(\beta)\\ &\quad + [(j-n+1)(j+n)]^{1/2} d^j_{m+1,n-1}(\beta)\\ &\quad + (m-n+1) \cot(\beta/2) d^j_{m+1,n}(\beta), \quad (2)\end{aligned}$$

starting from the analytical expression

$$\begin{aligned}d^j_{mj}(\beta) &= (2j)!/[(j+m)!(j-m)!]^{1/2}\\ &\quad \times \sin(\beta/2)^{j-m} \cos(\beta/2)^{j+m}. \quad (3)\end{aligned}$$

Only the elements with $-n \leq m \leq n$, $n \geq 0$ have to be evaluated. According to (2) and (3), $(j-n+1)$, $(j-n+2)/2$ elements are necessary to determine d^j_{mn}. The number of operations grows as j^2 for small values of n, and the propagation of errors causes the observed divergences.

The unitarity of the representation implies the following orthogonality condition for the reduced matrices:

$$\sum_{n=-j}^{j} d^j_{m,n}(\beta) d^j_{m',n}(\beta) - \delta_{m,m'} = 0, \quad -j \leq m, m' \leq j. \quad (4)$$

Therefore, the magnitude of the errors produced by the numerical calculation may be described by computing the maximum, when m and m' are varied, of the absolute value of the left-hand member of (4), for given j and β. This is shown in Fig. 1, for $j \leq 60$, which are the values used in the standard program of Crowther. Although big enough, such errors do not produce overflows in most computers and are seldom detected.

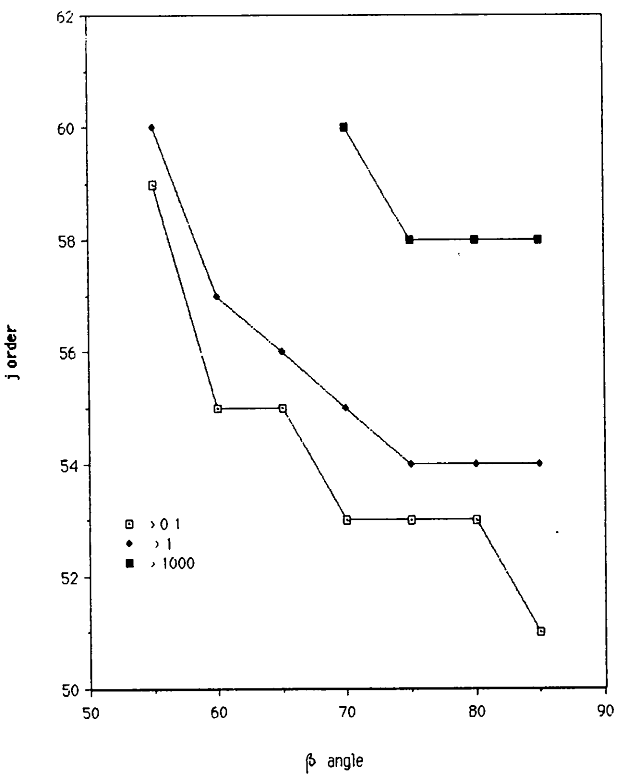

Fig. 1. Contour levels of the maximal deviation from the orthogonality conditions, of the reduced matrices $d^j(\beta)$, computed with the recurrence relation (2).

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The following 'linear' recurrence relation,

$$[(j-n+1)(j+m)]^{1/2}d^j_{m,n-1}(\beta) + [(j+n+1)(j-n)]^{1/2}d^j_{m,n+1}(\beta) + 2(m-n\cos\beta)\sin^{-1}(\beta)d^j_{m,n}(\beta)=0, \quad (5)$$

proved to be remarkably stable, the starting point being (3) and (formally) $d^j_{m,j+1}(\beta)=0$. It can be verified by direct replacement of the explicit expressions of the $d^j_{m,n}$ given by Brink & Satchler (1975). Since the type and number of operations are almost the same as in (2), and taking into account the results of Fig. 1, it can be estimated that troubles may begin for j of the order of 1000. The formula was tested for $j \leq 250$, and the deviation from the orthogonality conditions was less than 10^{-10}. All the computations were performed in double precision on the IBM 3090 of CIRCE, Orsay.

The author thanks Pascalou Rigolet for drawing his attention to this problem.

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Discussion of the representation of intercrystalline misorientation in cubic materials.

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Abstract

Salient features of various parameterizations of cubic-cubic misorientation are discussed. It is proposed that the quaternion representation of rotations, as a pair of antipodal points on the surface of a four-dimensional sphere, encompasses the most desirable properties of other proposed representations, *viz* rectilinearity, a closed form for the composition of successive rotations, and an equivalence between the Euclidean measure on its parameter space and the invariant measure in the space of rotations. The classification of cubic-cubic misorientations according to group multiplicity is described in Euler angle and quaternion representations. A correspondence between coincidence site lattice (CSL) boundaries ($\Sigma \leq 49$), Euler angles and axis-angle parameters is given.

The following pertains to the recent paper of Zhao & Adams (1988), entitled *Definition of an Asymmetric Domain for Intercrystalline Misorientation in Cubic Materials in the Space of Euler Angles*, and subsequent comments of Grimmer (1989). It is clear that the Euler angle representation of misorientation suffers from a number of disadvantages as discussed by Altmann (1986), Frank (1988), Grimmer (1989), and others. However, quantitative descriptions of orientation and misorientation distribution functions have usually been expressed in Fourier series using generalized spherical harmonics (Bunge, 1982); and these are defined in terms of Euler angles (Gelfand, Minlos & Shapiro, 1963). In their calculation of the misorientation distribution function (MDF) in copper, for example, Pospiech, Sztwiertnia & Haessner (1986) used the space of Euler angles for computation, and later transformed to the axis-angle parameters. Comparable orthogonal basis functions for axis-angle, quaternion, Rodrigues or other parameterizations have not yet been defined, even though they would be valuable. The work of Zhao & Adams (1988) was motivated by the pressing need to represent continuous functions, in the smallest physically distinctive domain of cubic-cubic misorientation, given the necessity of using Euler angles. The definition of an asymmetric domain significantly reduces computation time and increases the clarity of representation.

The quaternion representation described in the comments by Grimmer has some significant advantages. This representation, due to Handscomb (1958), defines rotation by a pair of antipodal points on the hypersurface of a unit sphere in four-dimensional space. [Note that this is not the quaternion parameter Q of Frank (1988), which is obtained from Handscomb's quaternion by omitting its fourth component.] Handscomb shows in his concise paper that his representation has the following properties. It has the rectilinearity property of Frank's mapping (ii). In fact Handscomb obtains the semi-regular truncated cube by considering the quaternions corresponding to minimum angle descriptions of misorientations between cubic crystals. It also has the property that the result of two successive rotations can be calculated as easily as in Frank's mapping (iii). Finally it has the property that the Euclidean measure on its parameter space corresponds to an invariant measure in the space of rotations as in Frank's mapping (iv). In summary, it combines the advantages of Frank's mappings (ii)-(iv) at the price of using four dimensions instead of three. Conversely, the price of going to three dimensions is that at most one of the three desired properties can be maintained.

Table 2 of the previous paper by Zhao & Adams contains some errors as noted by Grimmer. Table 1 of this comment is a corrected table. It is correct that only boundaries with rotation axis [1, 1, 1] should be classified as $m=6$. This statement is in good agreement with the analysis presented in section 3 of the paper (Zhao & Adams, 1988). Boundaries

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