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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Table 1. *CSL boundaries for $\Sigma \le 49$ (m is the multiplicity)*

		Euler angles			Axis-angle				Euler angles			Axis-angle	
Σ	m	φ_1	ϕ	φ_2	$\langle h, k, l\rangle$	ω	Σ	m	φ_1	ϕ	φ_2	$\langle h, k, l\rangle$	ω
3	12	45·00	70·53	45·00	1, 1, 1	60·00	33*b*	2	12·34	83·04	58·73	3, 1, 1	33·56
5	8	0·00	90·00	36·86	1, 0, 0	36·86	33*c*	4	38·66	75·97	38·66	1, 1, 0	58·99
7	6	26·56	73·40	63·44	1, 1, 1	38·21	35*a*	2	16·86	80·13	60·46	2, 1, 1	34·05
9	4	26·56	83·62	26·56	1, 1, 0	38·94	35*b*	2	30·96	88·36	59·04	3, 3, 1	43·23
11	4	33·68	79·53	33·68	1, 1, 0	50·47	37*a*	8	0·00	90·00	18·92	1, 0, 0	18·92
13*a*	8	0·00	90·00	22·62	1, 0, 0	22·62	37*b*	2	12·53	85·35	40·60	3, 1, 0	43·14
13*b*	6	18·43	76·66	71·57	1, 1, 1	27·79	37*c*	6	36·87	71·08	53·13	1, 1, 1	50·57
15	2	19·65	82·33	42·27	2, 1, 0	48·19	39*a*	6	21·80	75·14	68·20	1, 1, 1	32·20
17*a*	8	0·00	90·00	28·07	1, 0, 0	28·07	39*b*	1	29·20	87·06	48·12	3, 2, 1	50·13
17*b*	4	45·00	86·63	45·00	2, 2, 1	61·92	41*a*	8	0·00	90·00	12·68	1, 0, 0	12·68
19*a*	4	18·44	86·98	18·44	1, 1, 0	26·53	41*b*	2	17·10	84·40	36·03	2, 1, 0	40·88
19*b*	6	33·69	71·59	56·31	1, 1, 1	46·83	41*c*	4	36·87	77·32	36·87	1, 1, 0	55·88
21*a*	6	14·03	79·02	75·97	1, 1, 1	21·78	43*a*	6	9·46	81·98	80·54	1, 1, 1	15·18
21*b*	2	22·83	79·02	50·91	2, 1, 1	44·41	43*b*	2	12·10	87·33	24·78	2, 1, 0	27·91
23	2	15·25	82·51	52·13	3, 1, 1	40·45	43*c*	4	45·00	80·63	45·00	3, 3, 2	60·77
25*a*	8	0·00	90·00	16·26	1, 0, 0	16·26	45*a*	2	10·30	83·62	63·44	3, 1, 1	28·62
25*b*	2	36·87	90·00	36·87	3, 3, 1	51·68	45*b*	2	26·57	83·62	63·43	2, 2, 1	36·87
27*a*	4	21·80	85·75	21·80	1, 1, 0	31·59	45*c*	2	38·66	84·90	51·34	2, 2, 1	53·13
27*b*	2	15·07	85·75	31·33	2, 1, 0	35·43	47*a*	2	26·56	87·56	63·44	3, 3, 1	37·07
29*a*	8	0·00	90·00	43·60	1, 0, 0	43·60	47*b*	2	22·71	82·67	35·39	3, 2, 0	43·66
29*b*	2	33·69	84·06	56·31	2, 2, 1	46·40	49*a*	6	30·96	72·17	59·04	1, 1, 1	43·57
31*a*	6	11·31	80·72	78·69	1, 1, 1	17·90	49*b*	2	10·62	85·32	47·49	5, 1, 1	43·57
31*b*	2	27·41	78·84	43·66	2, 1, 1	52·20	49*c*	2	30·35	75·82	49·27	3, 2, 2	49·23
33*a*	4	14·04	88·26	14·04	1, 1, 0	20·05							

Table 2. *Classification of multiplicity m for all cubic–cubic misorientations using quaternion representation*

m	a	b	c	d	Conditions
48	1	0	0	0	
16	1	$\sqrt{2}-1$	0	0	
12	1	1/3	1/3	1/3	
8	1	$\sqrt{2}-1$	$\sqrt{2}-1$	$3-2\sqrt{2}$	
	1	b	0	0	$\sqrt{2}-1>b>0.$
6	1	b	b	b	$1/3>b>0.$
4	1	b	b	0	$\sqrt{2}-1\ge b>0.$
	1	b	$(1-b)/2$	$(1-b)/2$	$\sqrt{2}-1\ge b>1/3.$
	1	b	b	$1-2b$	$\sqrt{2}-1>b>1/3.$
2	1	b	c	0	$\sqrt{2}-1\ge b>c>0.$
	1	b	c	c	$\sqrt{2}-1\ge b>c>0,\ 1>b+2c.$
	1	b	b	d	$\sqrt{2}-1\ge b>d>0,\ 1>2b+d.$
	1	b	c	$1-b-c$	$\sqrt{2}-1\ge b>c>1-b-c.$
	1	$\sqrt{2}-1$	c	$(\sqrt{2}-1)c$	$\sqrt{2}-1>c>0.$
1	All others				

$\Sigma 29b$, $35b$, $45b$, $45c$, $47a$ should be classified as $m=2$ because they lie upon the *ABD* plane (but not upon the edges) of Fig. 4 in the paper. Boundaries $\Sigma 23$, $27b$, $35a$, $37b$, $47b$, $49b$ were erroneously classified as $m=1$ because the authors had difficulties in analyzing points on the curved surface *ABD*. It is confirmed now that every misorientation point on the surface *ACD* should be classified as $m=2$; the inverse g^{-1} for all points on this curved surface can be shown to be equivalent to g under relation (44) of the paper. For the convenience of future usage, we have produced two tables in the following which classify the multiplicities m of all cubic–cubic misorientations in Euler angle and quaternion representations. A cubic–cubic misorientation corresponds to an interior point of an asymmetric domain or one or two points on its surface. The multiplicity m of a misorientation satisfies $m=1$ if the misorientation is represented by an interior point and $m\ge 1$ otherwise.

For quaternions $[a, b, c, d]$, the following is chosen as the definition of an asymmetric domain:

$$b\ge c\ge d\ge 0,\quad a\ge(\sqrt{2}+1)b,\quad a\ge b+c+d$$

Using normalization $a=1$, instead of the usual $a^2+b^2+c^2+d^2=1$, we have classified all points of multiplicity in Table 2.

In Fig. 1, multiplicities associated with points are indicated at the locations of the points and those associated with lines and planes are indicated by an oval and by a cross, respectively. For example, point *A* is represented by quaternion $[1, 0, 0, 0]$ and has multiplicity 48; line *BE* is represented by quaternions of the form $[1, \sqrt{2}-1, c, (\sqrt{2}-1)c]$ and associated with multiplicity 2. Plane *EBF* is described by quaternions of the form $[1, b, b, d]$ and associated with multiplicity 2. Points on the surface *BCEF* related as $[1, \sqrt{2}-1, c, d]$ and $[1, \sqrt{2}-1, (c+d)/\sqrt{2}, (c-d)/\sqrt{2}]$ represent physically equivalent misorientations; all other points on the surface of the asymmetric domain represent distinct misorientations. Notice that $m=1$ if $c>d>0$ and $d\ne(\sqrt{2}-1)c$ in $[1, \sqrt{2}-1, c, d]$.

For Euler angle representation, an asymmetric domain is defined by the following relations: $0\le\cos\phi\le\sin\varphi_1\sin\varphi_2/(1+\cos\varphi_1\cos\varphi_2)$ and $0\le\varphi_1\le\varphi_2\le\pi/2-\varphi_1$, $\arccos(1/3)\le\phi\le\pi/2$. Table 3 gives all multiplicities in this space.

Table 3. *Classification of multiplicity m for all cubic–cubic misorientations using Euler angles*

m	φ_1	ϕ	φ_2	Conditions and comments
48	0	$\pi/2$	0	
	0	$\pi/2$	$\pi/2$	$(0, \pi/2, 0)$ and $(0, \pi/2, \pi/2)$ are equivalent
16	0	$\pi/2$	$\pi/4$	
12	$\pi/4$	arccos (1/3)	$\pi/4$	
8	$\pi/4$	$\pi/2$	$\pi/4$	
	0	$\pi/2$	φ_2	$0<\varphi_2<\pi/2,\ \varphi_2\neq\pi/4$
6	φ	ϕ	$\pi/2-\varphi$	$\cos\phi=\sin 2\varphi/(2+\sin 2\varphi),\ 0<\varphi<\pi/4$
4	φ	ϕ	φ	$\cos\phi=\sin^2\varphi/(1+\cos^2\varphi),\ 0<\varphi<\pi/4,$
	$\pi/4$	ϕ	$\pi/4$	$\arccos(1/3)<\phi<\pi/2$
2	φ_1	ϕ	φ_2	$\cos\phi=\sin\varphi_1\sin\varphi_2/(1+\cos\varphi_1\cos\varphi_2),$ $0<\varphi_1<\varphi_2<\pi/2-\varphi_1$
	φ_1	$\pi/2$	$\pi/4$	$0<\varphi_1<\pi/4$
	φ	ϕ	φ	$0<\varphi<\pi/4,\ 0\leq\cos\phi<\sin^2\varphi/(1+\cos^2\varphi)$
	φ	ϕ	$\pi/2-\varphi$	$0<\varphi<\pi/4,\ 0\leq\cos\phi<\sin 2\varphi/(2+\sin 2\varphi)$
1	all others			

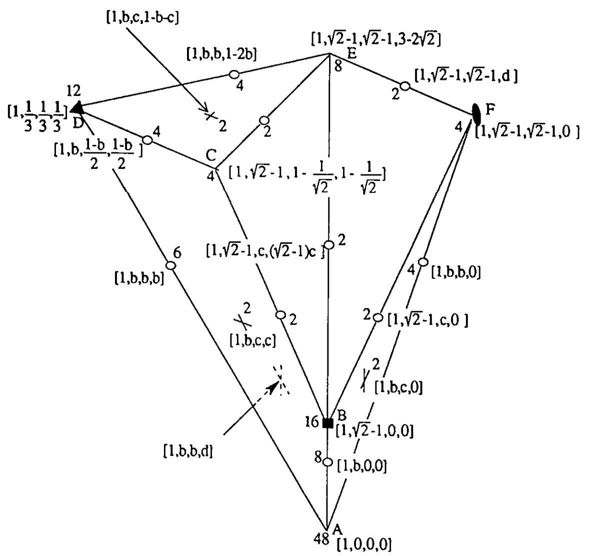

Fig. 1. Graphical representation of Table 2.

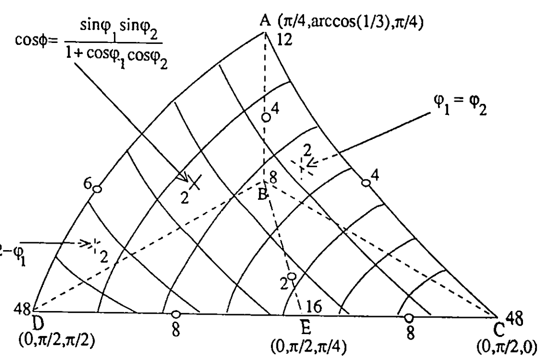

Fig. 2. Graphical representation of Table 3.

The content of Table 3 is illustrated in Fig. 2 which shows the surface of the asymmetric domain.

Again multiplicities associated with lines (curves) are indicated by ovals, and surfaces by crosses. For example, point E has coordinates $(0, \pi/2, \pi/4)$ in the Euler space and possesses multiplicity 16. Curve AD has multiplicity 6 and the curved surface ACD is associated with multiplicity 2. Points on the surface BCD related as $(\varphi_1, \pi/2, \varphi_2)$ and $(\varphi_1, \pi/2, \pi/2-\varphi_2)$ represent physically equivalent misorientations;* all other points on the surface of the asymmetric domain represent distinct misorientations. Notice that $m=1$ if $0<\varphi_1<\varphi_2<\pi/2-\varphi_1$ and $\varphi_2\neq\pi/4$ in $(\varphi_1, \pi/2, \varphi_2)$.

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* An example is $\Sigma 25b$ which is represented by the point (36·87°, 90°, 36·87°) on BC and by (36·87°, 90°, 53·13°) on BD of Fig. 2.

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