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Comments on an asymmetric domain for intercrystalline misorientation in cubic materials in the space of Euler angles

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Abstract. The following comments are made on a paper by Zhao & Adams [*Acta Cryst.* (1988), A44, 326–336]. An asymmetric domain for intercrystalline misorientation in cubic materials has also been published for the parametrization of rotations by a rotation vector instead of Euler angles. The former parametrization minimizes discontinuities in contrast to the latter. The value $1152/m$ of distinct equivalent rotations has not been determined correctly for a number of CSL (coincident site lattice) boundaries; the correct values are available in earlier publications.

Zhao & Adams (1988) consider in a clearly written paper two crystallites of cubic symmetry with a common interface. The relative orientation of their cubic lattices can always be described by a proper rotation. An element of the rotation group can be picked out by giving the values of three real parameters. Zhao & Adams choose Euler angles (ϕ_1, ϕ, ϕ_2) denoting a rotation by ϕ_1 about the z axis, followed by a rotation by ϕ about the new x axis and by a rotation by ϕ_2 about the new z axis. These angles may be restricted to

$$0 \le \phi_1 \le 2\pi, \quad 0 \le \phi \le \pi, \quad 0 \le \phi_2 \le 2\pi. \qquad (1)$$

Another possibility is to use 'rotation vector' parametrization, *i.e.* to give the three coordinates of a vector with direction parallel to the rotation axis and length proportional to the rotation angle θ, which may be restricted to $0 \le \theta \le \pi$. Rotations with $\theta < \pi$ are in one-to-one correspondence with points in the interior of this sphere with radius π, whereas diametrical pairs of points on its surface correspond to the same rotation with $\theta = \pi$.

The parametrization by Euler angles is more seriously non-unique for points on the surface of domain (1). As an example, the identity (0° rotation) is represented by (0, 0, 0), $(2\pi, 0, 2\pi)$, and by any $(\phi_1, 0, \phi_2)$ with $\phi_1 + \phi_2 = 2\pi$. Omission of certain points on the surface of (1) in order to make the representation unique does not eliminate the discontinuity of the representation at those points.

The cubic symmetry of the two crystal lattices and the possibility to start out from either lattice in describing their relative orientation make it possible to restrict the rotations to an asymmetric domain, the invariant measure of which is $24 \times 24 \times 2 = 1152$ times smaller than for the whole rotation group. The discontinuities of the parametrization are reflected also in the asymmetric domain. Although Zhao & Adams avoid $\phi = 0°$ by choosing a domain where $\phi \ge \arccos(1/3) \simeq 70.53°$ they cannot avoid, for instance, the fact that the identity is represented by two points, *i.e.* C and D in their Fig. 3.

Zhao & Adams (1988) do not seem to be aware that an asymmetric domain for cubic symmetry has also been defined by Grimmer (1974) whose methods were influenced by Handscomb (1958). These authors make use of the one-to-two correspondence between rotations and unit quaternions. The four parameters a, b, c, d of a unit quaternion satisfy

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$$a^2+b^2+c^2+d^2 = 1. \quad (2)$$

They are closely related to an axis angle description because $a = \cos(\theta/2)$ and b, c, d are the components of a vector of length $\sin(\theta/2)$ in the direction of the axis. The volume of the asymmetric domain is 2×1152 times smaller than the volume of the hypersurface of the unit sphere (2) in four-dimensional space. In order to visualize the domain, Grimmer (1974) and, more explicitly, Grimmer (1980) expressed it in the rotation-vector language defined above. The result is shown in Fig. 5 of Grimmer (1980).

The numbers appearing in the illustration at the bottom right of that figure are the values m of Zhao & Adams (1988). The formal definition of m in their equation (33) shows that m does not depend on the parametrization of the rotation group. For rotations describing CSL boundaries m has already been determined by Grimmer (1973). In fact, the weight W in his Table 1 satisfies $W = 48/m$. His Table 2 gives W explicitly for CSL boundaries with $49<\Sigma<59$. Similar tables have been published by Mykura (1980) for $\Sigma<102$ and by Grimmer (1984) for $\Sigma<40$.These tables are to be preferred to Table 2 in Zhao & Adams (1988), which unfortunately contains a considerable number of errors. In particular, too many boundaries are classified as $m = 1$ and as $m = 6$: only 39b should be classified as $m = 1$ and only boundaries with axis [1,1,1] should be classified as $m = 6$; all the other boundaries classified as $m = 1$ or 6 have $m = 2$.

References

GRIMMER, H. (1973). *Scr. Metall.* **7**, 1295–1300.

GRIMMER, H. (1974). *Acta Cryst.* A**30**, 685–688.

GRIMMER, H. (1980). *Acta Cryst.* A**36**, 382–389.

GRIMMER, H. (1984). *Acta Cryst.* A**40**, 108–112.

HANDSCOMB, D. C. (1958). *Can. J. Math.* **10**, 85–88.

MYKURA, H. (1980). *Grain Boundary Structure and Kinetics*, edited by R. W. BALLUFFI, pp. 445–456. Metals Park, Ohio: American Society for Metals.

ZHAO, J. & ADAMS, B. L. (1988). *Acta Cryst.* A**44**, 326–336.