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The Random Orientation Probability in Consecutive Inverse Pole Figure Method for Texture Determination

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A new texture determination method has been developed (Chou, Rolland, and Dicks, paper submitted to this conference), using two consecutive Inverse Pole Figures (IPFs) to determine a texture component {hkl}<uvw> in a sample: the first IPF displays the sample normal (ND) of the set of data corresponding to the mapped area in the sample; a second IPF is used to display the rolling direction (RD) of a subset of data selected from the first IPF. Conversely, the RD IPF can be used as the starting point and ND IPF is used for a subset of data selected from the first IPF.

The times random, a ratio of the measured volume fraction of a texture over the calculated random probability of this crystal orientation, is widely used to quantify the significance of a texture {hkl}<uvw> in a sample. The random probability of the crystal orientation {hkl}<uvw>, a prerequisite for the calculation of the times random, can be expressed by the product of two terms: (1) the probability p_1 of a direction [uvw] that points to RD within a tolerance angle $\Delta\theta$, multiplied by a multiplicity factor m, the number of equivalent <uvw> in the crystal; (2) the probability p_2 of a plane normal (hkl) perpendicular to [uvw] that points to ND within a tolerance angle $\Delta\theta$, multiplied by another multiplicity factor n, the number of equivalent {hkl} that is perpendicular to [uvw]. The first term mp_1 is not affected by the use of the IPF method; however, the second term np_2 needs to be modified in order to obtain the correct random probability of the crystal orientation in the new IPF texture determination approach.

For a randomly oriented vector [uvw] in space, the probability that it will fall into a cone of semi-angle $\Delta\theta$ with RD is $p_1 = (1-\cos\Delta\theta)/2$. There are m equivalent <uvw> in space and therefore the probability for any one of them to fall into the cone will be mp_1. Values of m in different crystal systems can be found in reference books, e.g. [1]. The probability of finding the second crystal direction (it is the plane normal (hkl) in this case) to be close to ND within a tolerance angle $\Delta\theta$ is given by $p_2 = \Delta\theta/\pi$. The multiplicity factor n depends on both {hkl} and <uvw> of the crystal, and will be discussed below.

Fig 1a shows a standard stereographic projection (IPF whole space) for a cubic crystal. In this example an arbitrary direction [112] has been chosen as RD (red/yellow circle). Consequently all possible planes {hkl} that are parallel to ND will be situated along the great circle that is 90° to the point of [112]. In a unit triangle IPF shown in Fig 1b, this great circle becomes a 'zigzag' track shown by the white curves. When a crystal is considered to rotate 360° about the chosen RD, the ND moves along the track and n is the number of times that the point {hkl} on the track coincide with ND. In Fig 1b, when (hkl) = (-531) is chosen, four equivalent plane normals, namely (-531), (-5-13), (-1-53) and (3-51) exist in the upper hemisphere. We thus obtain the multiplicity factor n = 8 for the {-531}<112> orientation. A circle centered at (-531) with tolerance angle 5° ($\pi/36$) is shown to have covered a part of the track displayed in red color. The accumulated angle range $\Sigma\varphi$ of the track in this circle is also shown by thick red sections along the great circle in Fig 1a. The angle range $\Sigma\varphi$ divided by 2π is used to replace np_2. In this example $\Sigma\varphi/2\pi \approx 0.22= 8\times\Delta\theta/\pi = np_2$. Complicated situations arise when tracks of (hkl) in the IPF form closely knitted networks, an example is shown in Fig 2a-c, where the [uvw] is chosen as [148]. Along the great circle a unique plane normal (-4-11 6) is found in the upper hemisphere, the “conventional” multiplicity factor n is 2 for this orientation, and when $\Delta\theta = 5°$ we have $np_2 = 2\times\Delta\theta/\pi \approx 0.055$. However, as shown in Fig 2b the 5° circle centered at (-4-11 6) will include not only the section containing the (-4-11 6) point, but also additional sections of the track: AB, CD and EF. It turns out that for the orientation {-4-11 6}<148> we have $\Sigma\varphi/2\pi = 0.194$, more than 3 times the np_2. When $\Delta\theta = 10°$ and ND is the same as in Fig 2b, more additional sections of the track are included in the circle (Fig 2c), the random probability $\Sigma\varphi/2\pi$ for {hkl} reaches 0.456, more than 4 times the np_2 (= 0.11).

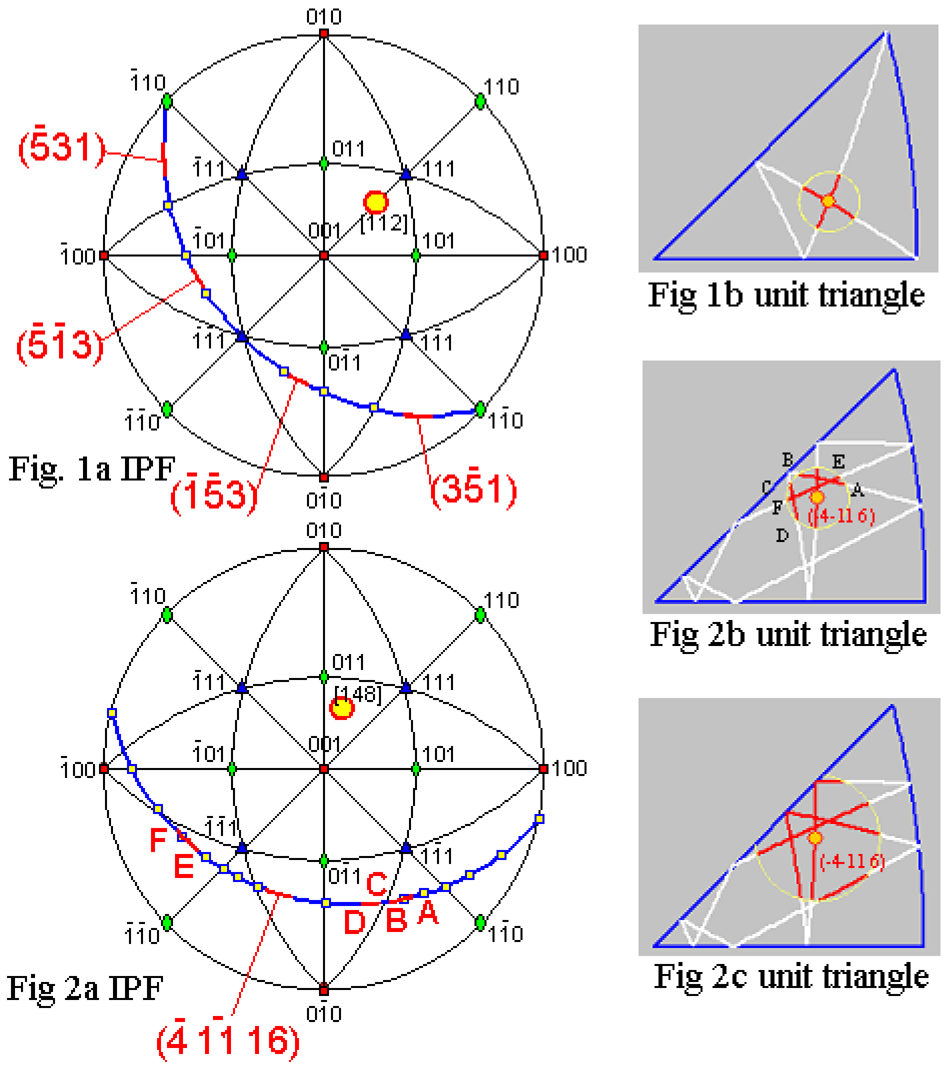

Fig. 1a IPF

Fig 1b unit triangle

Fig 2b unit triangle

Fig 2a IPF

Fig 2c unit triangle

A new calculation method for the random probability of a crystal orientation has been developed. This method is also useful for the correct choice of the tolerance angle in the texture determination.

[1] International Tables for Crystallography, Vol. A, (1996), Ed. T. Hahn.

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