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Comments on "Bounds to Texture Components in Superposed Crystallographic Textures," by Jacob L. Jones

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In a recent paper, Jones[1] suggests to revisit the use of the concept of "superposed crystallographic textures." This introduction is motivated by the calculation, for a textured sample with a given randomly oriented volume fraction, of the maximum pole density value of the textured component from the minimum and maximum values of the "superposed" ODF. In particular, the author wants to address the following:

(1) reintroduction of the concept of multi-component superposed ODFs, specifically for textures comprising a random component,

(2) demonstration that the volume fraction bounds of a randomly-oriented texture component can be quantified from the superposed ODF without forcing the textured component to conform to a predetermined function,

(3) quantification of the pole density intensity bounds of the textured component from the intensities in the superposed ODF, and

(4) illustration of one application of these developed formalisms.

Unfortunately, the author's point (1) is apparently raised by a misinterpretation of previous papers by Virnish *et al.*[2] and Lücke *et al.*[3] What Jones calls "superposed ODF" is in fact the representation of an ODF (or $f(g)$) by the superposition of functions, which is currently used in quantitative texture analysis. This is misleading as for a single-phase material there is no necessity to introduce several ODFs, particularly because of the definition itself of the ODF:

$$\frac{\mathrm{d}V(g)}{V} = \frac{1}{8\pi^2} f(g)\,\mathrm{d}g$$

which is bound to 100% of the material volume. This, as a first consequence, implies that $f(g)$ is normalized to $8\pi^2$, and not to 2π as denoted by Eq. (5) of the manuscript. The former normalization factor comes from the integration of $f(g)$ over the three Euler angles that define the orientation of a crystallite, $g = \{\alpha,\beta,\gamma\}$, in the orientation space. The 2π factor and Eq. (5) are for the pole figure normalization (and not for $f(g)$).

Unfortunately, point (2) undergoes the previous misinterpretation. As $f(g)$ is a density, one has to integrate over a given orientation range Δg to obtain a volume ratio. For a random sample, $f(g) = 1$ m.r.d. whatever g, and then the integral over all gs gives $8\pi^2$, meaning $\Delta V/V = 100\%$. For a sample containing a random part $1-x$ (e.g., 20% of the volume), then x is the volume associated with the textured part (80%), whatever its distribution shape, and Jones' Eq. (3) should read:

$$1 = \frac{1}{8\pi^2}\int_g f'(g)\,\mathrm{d}g = \frac{x}{8\pi^2}\int_g f_1(g)\,\mathrm{d}g + \frac{1-x}{8\pi^2}\int_g f_2(g)\,\mathrm{d}g$$

then

$$\frac{1}{8\pi^2}\int_g f'(g)\,\mathrm{d}g = \frac{x}{8\pi^2}\int_g f_1(g)\,\mathrm{d}g + 1 - x$$

which is a quite different equation that does not allow a reasoning on only one g value like in Jones's Eq. (9). These equations are not forcing any predetermined function for $f(g)$, and give rise to distribution densities different from the one illustrated in Jones's Fig. 1,[1] which is a pole figure. One has to understand here that a pole figure point depends on several g values of $f(g)$ as the fundamental equation of texture analysis that relates pole figures and the ODF[4] implies an integral of $f(g)$ on a given path. Then, the modification of a single pole figure as proposed in Fig. 1 and related equations is false, because it does not include the modifications of all the other pole figures linked by $f(g)$.

We agree with the author that "the maximum bound for x [max(x)] is 1, yielding a random fraction component ($1-x$) of 0" for a two-component texture in which one is a random part. This specific case for x stands for a fully textured volume with $f_1(g)$ as the crystallite distribution. However, the author then conludes that "the minimum bound of x [min(x)] can be solved from Eq. (6) using the minimum value of the superposed ODF, min(f')." This cannot be true if one wants the material's volume retained at 100%. The minimum x value for the textured component is $\min(x) = 0$, meaning a perfectly randomly oriented sample, with $1-x = 1$. Consequently, unless the author's ideas have not been illustrated correctly, Jones's developments and discussion are no longer valid.

References

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