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Letter to the Editors

On the relationship among 'f' texture factors for the principal planes of zirconium, hafnium and titanium alloys

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Abstract

Previous work on the relationship among f_{0002}, $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ in hexagonal materials is examined, and a single cell analysis is described that provides further insight on this subject. The analysis is extended to show the general relationship between f_{0002} and 'f' for any plane in the system. Also presented is a method for computation of $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ from inverse pole figure data. Results are consistent with results from direct pole figure data.

1. Background

The 'f' texture factor that was introduced in [1] was developed to provide a means of resolving basal pole [0 0 0 1] distributions into an effective fraction in each of the three principal directions of fabricated forms of zirconium and other hexagonal materials. Perfect alignment of the basal poles in one direction yields an 'f' value of 1.0 in that direction and zero in the other two; a value of 1/3 is obtained for all directions in a random sample. The sum in the three directions is 1.0 regardless of texture. In addition to providing a convenient, compact index to basal texture, the 'f' values may be used to account quantitatively for the texture effect in properties such as thermal expansion and irradiation growth [1,2]. The 'f' factor and other texture indices also have found widespread use for correlations and material characterization in work on other texture-dependent properties of hexagonal materials. Examples include correlations of 'f' with elastic properties in zirconium and titanium alloys [3–5] and the use of 'f' factors and related parameters in explanations of hydride orientation behavior and its effects on cracking in Zircaloy [6,7].

Kelly and Watson [8] calculated 'f' for the $\{10\bar{1}0\}$ prism planes in zirconium plate and observed that they were related to the basal plane 'f' by the relationship,

$$f_{0002} + 2f_{10\bar{1}0} = 1. \tag{1}$$

In a paper by Lewis et al. [9] on a round robin study of Zircaloy tubing, Eq. (1) was found to hold within 10% in most cases.

Bowen [4] provided insight on the relationship between basal plane 'f' values and values for the prism planes. He noted that if orthogonal axes composed of principal crystallographic directions were chosen, this would yield the relationship

$$f_{0002} + f_{10\bar{1}0} + f_{11\bar{2}0} = 1 \tag{2}$$

for any sample direction.

In his tests on a titanium alloy, Bowen noted that Eq. (2) held within ~5%, whereas deviations were as high as 10% for Eq. (1).

One purpose of this Letter is to offer a model showing that, although the titanium data conform better to Eq. (2) than to Eq. (1), $f_{10\bar{1}0}$ is analytically equal to $f_{11\bar{2}0}$ and, hence, that the expressions in Eqs. (1) and (2) are equivalent, at least analytically. This model also may be extended to create an expression showing the relationship between f_{0002} and 'f' for any plane in the hexagonal system.

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A second purpose of this letter is to present a method for the determination of $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ from inverse pole figure data. In this regard, it is noted that in the round robin study, only those laboratories that obtained direct pole figures calculated 'f' for the $\{10\bar{1}0\}$ planes.

2. Analytical model

The relationship among f_{0002}, $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ may be illustrated with Fig. 1. A single cell is depicted with the basal pole normal to the plane of the paper, which corresponds to f_{0002} equaling unity in the normal direction and zero in the longitudinal and transverse directions. Sets of three $\{10\bar{1}0\}$ and three $\{11\bar{2}0\}$ poles are represented in the plane of the paper. The contribution of each of the three $\{10\bar{1}0\}$ poles to 'f' in the longitudinal direction is 1/3 times the cosine squared of the angle between the pole and the longitudinal direction. Therefore, $f_{10\bar{1}0}$ in this direction is given by the expression,

$$f_{10\bar{1}0} = \tfrac{1}{3}(\cos^2 0° + \cos^2 60° + \cos^2 60°) = \tfrac{1}{2}. \quad (3)$$

In the transverse direction, the expression is

$$f_{10\bar{1}0} = \tfrac{1}{3}(\cos^2 90° + \cos^2 30° + \cos^2 30°) = \tfrac{1}{2}. \quad (4)$$

The same result is found for $f_{11\bar{2}0}$ since the combination of angles is the same.

These results show that rotation about the basal pole has no effect on 'f' for the $\{10\bar{1}0\}$ and $\{11\bar{2}0\}$ planes. Since the poles of these planes lie in the plane of the paper, 'f' in the normal direction is zero for each. Thus,

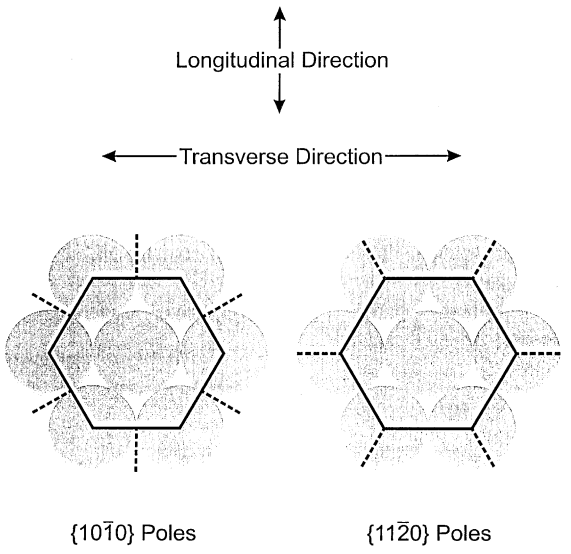

Fig. 1. Single cell model showing the $\{10\bar{1}0\}$ and $\{11\bar{2}0\}$ poles.

the sum of 'f' for the (0002), $\{10\bar{1}0\}$ and $\{11\bar{2}0\}$ planes is unity, as also shown earlier by Bowen and, therefore,

$$f_{10\bar{1}0} = f_{11\bar{2}0} = \frac{1 - f_{0002}}{2} \quad (5)$$

for any reference direction.

This reasoning may be extended to evaluate 'f' for any plane in the hexagonal system. Consider a sample with the fraction of basal poles in each of the three principal directions represented by the three basal 'f' factors, f_N, f_T and f_L. The 'f' factor for an $\{hkil\}$ set of poles in one of the reference directions will be the sum of the contributions of the cell fraction in that direction and the two perpendicular directions. The contribution from the former, say the N direction, is equal to $f_N \cos^2 \phi$, where ϕ is the angle between the N direction and the poles of the $\{hkil\}$ planes, a single value in this direction. The contributions from the perpendicular directions are given by the expressions,

$$\tfrac{1}{3} f_T(\cos^2 \phi_{1T} + \cos^2 \phi_{2T} + \cos^2 \phi_{3T})$$

and

$$\tfrac{1}{3} f_L(\cos^2 \phi_{1L} + \cos^2 \phi_{2L} + \cos^2 \phi_{3L}),$$

where the ϕs in these cases refer to the angles between the three poles in the $\{hkil\}$ set and the N direction for the cell fractions in the T and L directions. Adding the three contributions, after observing that the two quantities in parentheses are equal, as in Eqs. (3) and (4), and applying the fact that the sum of the squares of the three direction cosines for each of the poles is unity, gives the following expression for the N direction:

$$f_{hkil} = f_N \cos^2 \phi_N + \tfrac{1}{2}(1 - \cos^2 \phi_N)(f_T + f_L).$$

Substituting $(1 - f_N)$ for $(f_T + f_L)$ and dropping the N subscript yields the following relationship for f_{hkil} in any reference direction:

$$f_{hkil} = \tfrac{1}{2}[f_{0002}(3\cos^2 \phi - 1) + \sin^2 \phi], \quad (6)$$

where f_{0002} is the value in the reference direction and ϕ is the angle between the $\{hkil\}$ pole and the basal pole.

For $\phi = 90°$, Eq. (6) reduces to Eq. (5), showing that the latter is applicable to all $\{hki0\}$ planes. Also, a combination of Eqs. (6) and (5) permits the evaluation of 'f' for any $\{hkil\}$ plane from the 'f' value for any of the three principal planes.

3. Inverse pole figure method for $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$

A method for $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ determinations from the intensities in 2θ X-ray diffractometer scans is de-

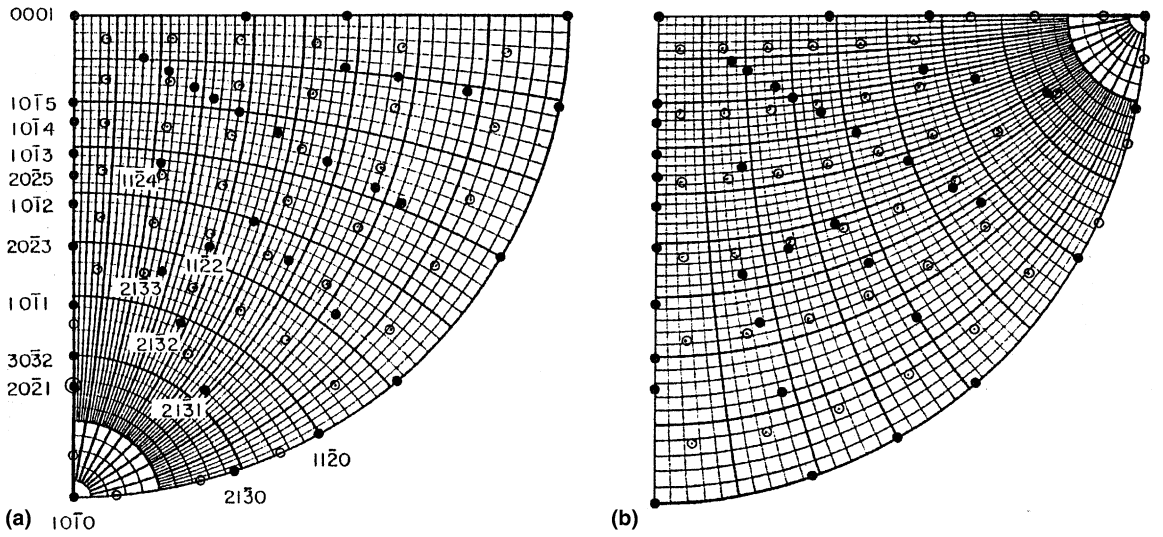

Fig. 2. Standard projection of zirconium showing the poles of the diffraction planes (closed symbols) and the locations (open symbols) used for determination of the average density along arcs of constant tilt from the $(10\bar{1}0)$ pole (a), and the $\{11\bar{2}0\}(\bar{1}2\bar{1}0)$ pole (b). This projection also is applicable to titanium and hafnium.

scribed, and data that were reported in [1] are used to evaluate the method and to substantiate Eqs. (1), (2) and (5).

As shown in Fig. 2, a full quadrant standard projection for zirconium ($c/a = 1.59$) was constructed by twice rolling over the 30° sector containing the identified diffraction planes. This operation was performed on Wulff nets so that the intensity (pole density) could be determined as a function of the angle of tilt from the $(10\bar{1}0)$ pole (Fig. 2(a)) and the $\{11\bar{2}0\}$ $(\bar{1}2\bar{1}0)$ pole (Fig. 2(b)). Because the c/a ratios of titanium and hafnium are also 1.59, the projection in Fig. 2 is applicable also to these materials.

The intensities at the locations indicated by the open symbols were estimated from the intensities of the surrounding diffraction points. These values were then used in a summation procedure that was described in [1] to evaluate the following equation for 'f' in a reference direction:

$$f = \frac{\int_0^{\pi/2} I_\phi \sin\phi \cos^2\phi \, d\phi}{\int_0^{\pi/2} I_\phi \sin\phi \, d\phi}, \tag{7}$$

where I_ϕ is the average intensity at an angle of tilt, ϕ, from a reference direction. For I_ϕ evaluation in the present calculations, the open symbols were located along 90° arcs at 10° intervals of ϕ from 5° to 85°. Along the arcs from 35° to 85°, the symbols are located at the center of six 15° segments of arc and were averaged to obtain I_ϕ. At lower angles, either the two terminal values or these along with a value at 45° were used. In the latter case, the intensity at 45° was used twice to obtain the correct average for the two 45° segments. Piece-wise linear curves of intensity versus location along the three boundaries of the pole figure were used to estimate the density at the open points on or near the boundaries.

4. Results and discussion

Results of $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ calculations by the described inverse pole figure method for the principal directions in a swaged rod and a rolled plate of Zircaloy-4 are listed in the fourth and fifth columns of Table 1. Values of f_{0002} that were reported in [1] are given in the second column. The remaining columns help to evaluate the proposed equality of $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ and how well the data are fitted by Eqs. (1), (2) and (5).

The largest difference between the experimental values of $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ was 0.013 and the average absolute difference was 0.009, or 2.6%. Average absolute deviations of the measured values of $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$ from those calculated with Eq. (5) were 0.008 and 0.007, respectively, an agreement within 2.4%.

A comparison of Eqs. (1) and (2) is provided by the last two columns. Eq. (2) was closer to unity than was Eq. (1) in four of the five cases, and while the largest deviation from unity occurred in Eq. (2), the average absolute deviation was only 1.2% compared to 1.6% for Eq. (1). Although these deviations from unity are lower than those found by Bowen in direct pole figure measurements on a titanium alloy, they are consistent with his observation that Eq. (2) gave a better fit than Eq. (1). This is to be expected generally because Eq. (2) relies on more experi-

Table 1
Summary of results for Zircaloy-4

	f_{0002} [1]	$\frac{1}{2}(1-f_{0002})$ Eq. (5)	$f_{10\bar{1}0}$	$f_{11\bar{2}0}$	$f_{10\bar{1}0}-f_{11\bar{2}0}$	$f_{0002}+2f_{10\bar{1}0}$ Eq. (1)	$f_{0002}+f_{10\bar{1}0}+f_{11\bar{2}0}$ Eq. (2)
Rod							
Longitudinal	0.051	0.475	0.486	0.496	−0.010	1.023	1.033
Radial	0.488	0.256	0.264	0.260	0.004	1.016	1.012
f_L+2f_R	1.027	0.987	1.014	1.016			
Plate							
Longitudinal	0.083	0.459	0.447	0.460	−0.013	0.977	0.990
Transverse	0.329	0.336	0.328	0.341	−0.013	0.985	0.998
Normal	0.549	0.226	0.223	0.229	−0.006	0.995	1.001
$f_L+f_T+f_N$	0.961	1.021	0.998	1.030			

mental data than does Eq. (1). Thus, if data are available for both the $(10\bar{1}0)$ and $(11\bar{2}0)$ planes, but not (0002), then Eq. (2) is preferred for determination of f_{0002}. If data are available for only one of the prism planes or for the basal plane only, then Eq. (5) is acceptable for computation of 'f' for the other two planes. Eq. (6) is likewise acceptable for any plane in the system. Verification of Eq. (6) was accomplished by comparison of the value of $f_{11\bar{2}4}$ computed for the radial direction in the Zircaloy-4 rod with a value calculated with an inverse pole figure procedure similar in principle to that described for $f_{10\bar{1}0}$ and $f_{11\bar{2}0}$. The values were 0.398 and 0.406, respectively.

5. Conclusions

1. Values of $f_{(10\bar{1}0)}$ and $f_{(11\bar{2}0)}$ can be calculated accurately by the inverse pole figure method.
2. The equality of $f_{(10\bar{1}0)}$ and $f_{(11\bar{2}0)}$, indicated analytically, is confirmed.
3. The analytically derived fixed relationship among the 'f' values for the three principal planes, Eq. (5), is verified by the data.
4. Computation of 'f' for any one of the three principal planes is sufficient for evaluation of the other two, or for any plane through the use of Eq. (6).

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