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Characterization of microstructural anisotropy in orthotropic materials using a second rank tensor

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A second rank symmetric tensor which describes the degree of orientation in orthotropic materials is presented and shown to reflect accurately patterns of experimental data. The use of this tensor to describe microstructural anisotropy is compared to currently accepted methods and is found to be more useful and accurate in experimental studies. A method for determining the anisotropy tensor in a material is given, based on measurements on any three mutually perpendicular planes, and the fundamental restriction of this method to orthotropic materials is discussed. Experimentally determined anisotropy tensors in five specimens of cancellous bone from five different human bones are given.

1. Introduction

The degree of microstructural orientation in a material is a fundamental quantity of wide interest to those studying mechanical properties of both natural and man-made materials. Orientation level measurements in various materials including human cancellous bone, forged metal parts, multiphase composites, foamed materials, and wood have been attempted. These measurements are valuable in applications such as the design of materials with specific properties, monitoring of material manufacturing processes, and investigations of adaptive remodelling in mammalian bone tissue.

A large subset of anisotropic materials, orthotropic materials exhibit symmetry about three mutually perpendicular planes. Materials such as wood, cold-rolled steel, and human bone are essentially orthotropic, and orthotropy includes the presence of planes of isotropy or full isotropy as degenerate cases.

Structure–material property relationships in natural and man-made materials are currently limited since a description of material anisotropy which can be easily incorporated into relationships is lacking. Thus, most investigations into properties of multiphase materials based on microstructure (e.g., using the self-consistent method or the differential computation method – see Cleary *et al.* [1]) use as models for included particles the two special cases of thin plates and spheres. A method by which fully three-dimensional information on the relative orientation levels and the principal directions of material orientation can be put into tensorial form* is described herein.

"Stereology", or the generalization of planar structure measurements to three dimensions, is a common technique in materials science, and the classical text by Underwood [2] reviews the subject in detail. It is now well established, for example, that in any plane through a multiphase material, the fraction of area which cuts through a particular phase is equal to the fraction of volume which that phase occupies. Other measurements of interest to materials scientists, such as the size distribution of particles of a given phase, are addressed by Underwood. Our main concern here is the degree of overall anisotropy in the material, and it is this topic which we will first review in detail.

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2. Current techniques for orientation level measurement

Orientation level measurements in anisotropic materials typically utilize planar sections through a specimen of material which are polished and viewed microscopically. An array of parallel lines is superimposed on the sample and the number of intersections between these lines and microstructurally important features (e.g., grain/phase boundaries) are counted for a great many orientations of the line array. Various automations of this procedure facilitate the process. Stereology concatenates these planar measurements to provide three-dimensional information on the material orientation. An advance over current stereologic techniques for orientation level measurement is reported herein.

2.1. Saltykov's method for partially oriented structures

Saltykov [3], as a tool for studying grain shape in metals, developed a method for quantifying orientation in orthotropic materials which was based on measurements of the surface area of grain (or phase) boundaries per unit volume. By considering the boundary surface area density in a partially oriented microstructure as the sum of contributions from three basic types of "totally oriented" microstructures, Saltykov arrives at expressions for the degree of orientation in terms of the fraction of surface area in a sample which each contributes. Fig. 1 shows the totally oriented microstructures used by Saltykov. The isotropic system in Fig. 1a has a surface density, s, of

$$s = 2p \tag{1}$$

where p is the number of intercepts per unit line length in any direction in the material. The completely linearly oriented structure shown in Fig. 1b has a surface density of

$$s = (\pi/2)p_{\perp} \tag{5}$$

where the subscript on p shows that the direction of measurement must be perpendicular to the direction of orientation. The completely planar system in Fig. 1c has a surface density of

$$s = p_{\parallel} \tag{3}$$

where here the subscript indicated that the measurement of p must be parallel to the direction of planar orientation.

As an example of the reasoning used in the calculation of an orientation level, consider the case of a linear-isotropic material as shown in Fig. 2a. Since the linear surfaces do not contribute to the intercepts per unit line length as measured parallel to the axis of orientation, it follows that

$$(S)_{\text{is}} = 2p_{\parallel}. \tag{4}$$

In directions perpendicular to the axis of orientation, both the linear and the isotropic surfaces contribute to the intercepts per unit line length. Thus to arrive at the surface density of the linear fraction, one uses

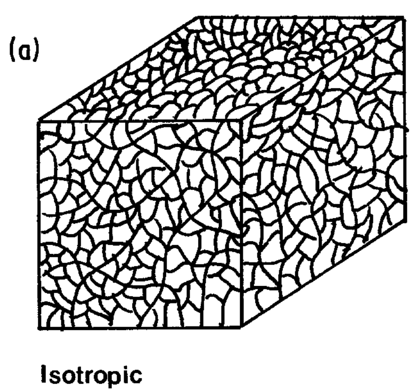
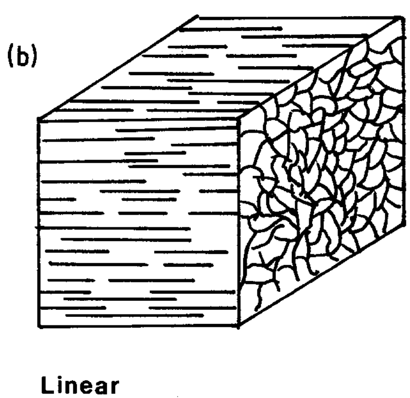
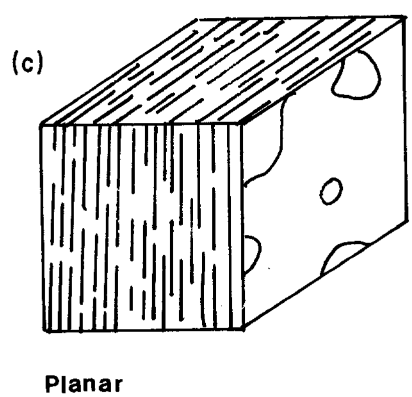
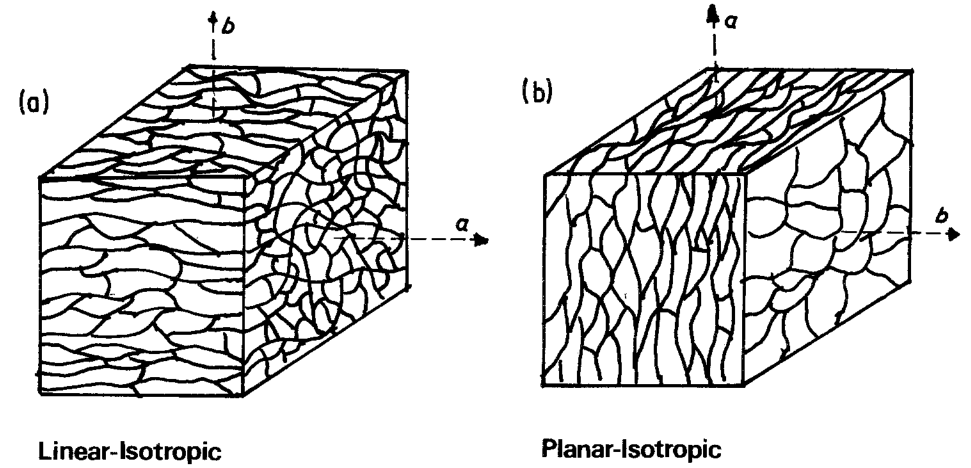


Figure 1 Saltykov's totally oriented microstructures.







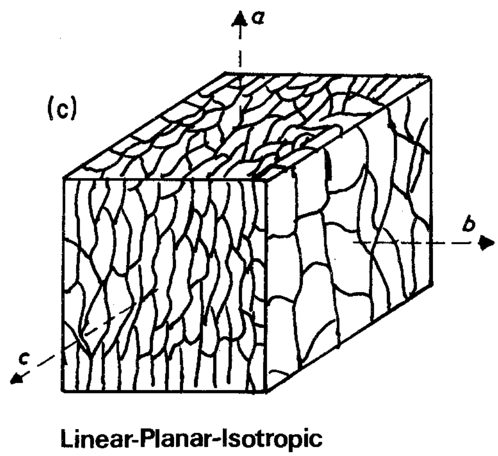


Figure 2 Saltykov's partially oriented microstructures.

$$(S)_{\text{lin}} = (\pi/2)(p_{\perp} - p_{\parallel}). \qquad (5)$$

Thus the total surface density is

$$s = (\pi/2)p_{\perp} + [2-(\pi/2)]p_{\parallel} \qquad (6)$$

and the degree of orientation can be given as

$$O = (S)_{\text{lin}}/s. \qquad (7)$$

Similar analyses for the other cases in Fig. 2 lead to the expressions in Table I.

3.2. Hilliard's method for oriented microstructures

The method proposed by Hilliard [4] is much more general than that of Saltykov and also concerns itself with surface densities. The fundamental quantity of concern in Hilliard's analysis is the distribution function $S(\varphi, \psi)$ which is defined as the fraction of surface area per unit volume which has a unit normal vector in the range $\varphi \pm \mathrm{d}\varphi$ and $\psi \pm \mathrm{d}\psi$ (where φ and ψ are the polar and planar angles in spherical coordinates) and the total surface area is given by simply integrating this function over a unit sphere. Some rather complex mathematical manipulation produces an expression for the surface density in terms of intercept measurements. For measurements in the plane whose normal is $\varphi = 0$, the expression becomes

$$S(\pi/2, \psi) = (1/\pi)\{[(P(\omega+\Delta\omega) - 2P(\omega) + P(\omega-\Delta\omega))/(\Delta\omega^2)] + P(\omega)\} \qquad (8)$$

where $\Delta\omega$ is the increment of angle between successive measurements and $\omega = \psi + \pi/2$. Note that this gives an estimate of $S(\varphi, \psi)$ at $\varphi = (\pi/2)$.

3. The mean intercept length tensor

In partially oriented microstructures, both Underwood [2] and Whitehouse [5–8] show that the mean intercept length, plotted as a radius at the angle of measurement, generates an ellipse in any plane. Generalization of this fact to three dimensions shows that the mean intercept length, plotted as a radius at the angle of measurement, generates

TABLE I Saltykov's equations for partially oriented systems

System type	Total specific surface area	degree of orientation
Linear	$s = (\pi/2)P_b + [2-(\pi/2)]P_a$	$O = (P_b - P_a)/[P_b + (4/\pi - 1)P_a]$
Planar	$s = P_b + P_a$	$O = (P_b - P_a)/(P_b + P_a)$
Planar–linear	$s = P_b + [2-(\pi/2)]P_a + [(\pi/2)-1]P_c$	$O_{pl} = (P_b - P_c)/s$ $O_{lin} = \pi/2\ (P_c - P_a)/s$

an ellipse in any plane. Generalization of this fact to three dimensions shows that the mean intercept length, plotted as a radius from the origin at the angle of measurement, generates the surface of an ellipsoid of general formula

$$Ax_1^2 + Bx_2^2 + Cx_3^2 + 2Dx_1x_2 + 2Ex_1x_3 + 2Fx_2x_3 = 1. \quad (9)$$

The linchpin of the new representation of microstructure described here involves recognizing this equation as the quadratic form of a second rank tensor. More specifically, if the mean intercept length L were plotted as a radius and related to Cartesian coordinates by

$$\begin{aligned} x_1 &= Ln_1 \\ x_2 &= Ln_2 \\ x_3 &= Ln_3 \end{aligned} \quad (10)$$

where n_1, n_2, and n_3 are the projections of a unit vector, in the direction in which the measurement was made, in the x_1, x_2, and x_3 directions, respectively, then Equation 1 gives

$$L^2(An_1^2 + Bn_2^2 + Cn_3^2 + 2Dn_1n_2 + 2En_1n_3 + 2Fn_2n_3) = 1, \quad (11)$$

which can be represented as

$$1/L^2 = \mathbf{n}\cdot[M]\cdot\mathbf{n} \quad (12)$$

where $[M]$ is a material anisotropy tensor, whose components in terms of the formula for the ellipsoid are

$$[M] = \begin{bmatrix} A & D & E \\ D & B & F \\ E & F & C \end{bmatrix} \quad (13)$$

and $\mathbf{n}$ is a unit vector in the direction of the mean intercept length measurement.

This representation of microstructure has many remarkable properties which make it especially attractive. For example, finding the directions of major material orientation consists simply of finding the principal axes and the ratios of principal values of this tensor. Also, this representation provides a material description which can be directly incorporated into prospective formulae for the elastic moduli of cancellous bone (or any analogous material) as a function of material orientation and density. Investigations of trabecular remodelling in response to physiologic stress can also be facilitated using this material description.

As proof that a second rank tensor adequately represents the mean intercept length measurements, consider the variation of the mean intercept length with direction in a section. Here one has

$$\mathbf{n} = \cos\theta\,\mathbf{e}_i + \sin\theta\,\mathbf{e}_j \quad (14)$$

where $\mathbf{e}_i$ and $\mathbf{e}_j$ are unit vectors in the axes defined by the specimen faces and θ is defined in Fig. 3 (obeying the right-hand rule for positive θ, of course). Equation 12 then becomes

$$1/L^2 = \cos^2\theta\, m_{ii} + \sin^2\theta\, m_{jj} + 2\sin\theta\cos\theta\, m_{ij} \quad (15)$$

where m_{ij} are the components of $[M]$. Using the standard Mohr circle transformation, we arrive at

$$1/L^2 = (m_{ii} + m_{jj})/2 + [(m_{ii} - m_{jj})/2]\cos(2\theta) + m_{ij}\sin(2\theta) \quad (16)$$

or, if

$$\tan(\varphi) = 2m_{ij}/(m_{ii} - m_{jj}) \quad (17)$$

and

$$D^2 = [(m_{ii} - m_{jj})/2]^2 + m_{ij}^2 \quad (18)$$

then

$$1/L^2 = (m_{ii} + m_{jj})/2 + D\cos(\theta + \varphi). \quad (19)$$

We would thus expect a sinusoidal variation of $1/L^2$ with angle.

3.1. Experimental considerations

Generating three-dimensional information from planar measurements made on three mutually perpendicular faces of a specimen requires consideration of the possible variations of microstructure within the specimen volume. Either this effect or experimental measurement errors could account for the fact that the measured diagonal components of the anisotropy tensor do not "fit" together exactly. In particular

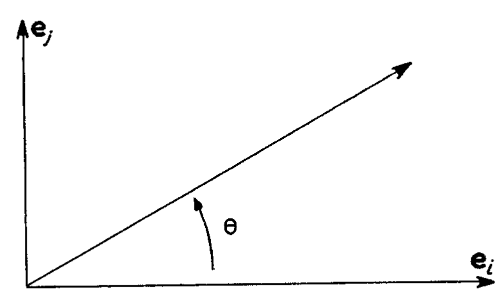


Figure 3 Relation of measurement angle to specimen axes $[(i, j) = (1, 2), (2, 3), (3, 1)]$.

$$(m_{11}/m_{22})_{1,2}(m_{22}/m_{33})_{2,3}(m_{33}/m_{11})_{3,1} \neq 1 \quad (20)$$

where the subscripts 1, 2 denote measurements made on the x_1–x_2 plane, 2, 3 denote measurements made on the x_2–x_3 plane, and so on. To resolve this problem, we apply small distortions to the coordinates in each plane to force the inequality into an equality. In particular, we use

$$\begin{aligned} &x_1' = a_1 x_1, \; x_2' = a_2 x_2 && \text{in the 1, 2 plane,} \\ &x_2' = a_3 x_2, \; x_3' = a_4 x_3 && \text{in the 2, 3 plane, and} \\ &x_1' = a_5 x_1, \; x_3' = a_6 x_3 && \text{in the 1, 3 plane.} \end{aligned} \quad (21)$$

Using these small distortions gives

$$\begin{aligned} &m_{11}' = a_1^2 m_{11}, \; m_{22}' = a_2^2 m_{22}, \; m_{12}' = a_1 a_2 m_{12} \\ &\quad \text{in the 1, 2 plane,} \\ &m_{22}' = a_3^2 m_{22}, \; m_{33}' = a_4^2 m_{33}, \; m_{23}' = a_3 a_4 m_{23} \\ &\quad \text{in the 2, 3 plane, and} \\ &m_{11}' = a_5^2 m_{11}, \; m_{33}' = a_6^2 m_{33}, \; m_{13}' = a_5 a_6 m_{13} \\ &\quad \text{in the 1, 3 plane.} \end{aligned} \quad (22)$$

To force Equation 20 into an equality, we take

$$(a_1^2 a_3^2 a_6^2)/(a_2^2 a_4^2 a_5^2) = (m_{22}/m_{11})_{1,2}(m_{33}/m_{22})_{2,3} \times (m_{11}/m_{33})_{3,1}. \quad (23)$$

To minimize individual distortions of faces, we take

$$(a_1/a_2) = (a_3/a_4) = (a_6/a_5) = [(m_{22}/m_{11})_{1,2}(m_{33}/m_{22})_{2,3}(m_{11}/m_{33})_{3,1}]^{1/6}. \quad (24)$$

To eliminate errors in the measurement of the absolute values of mean intercept lengths, we further define the stretching factors such that

$$\begin{aligned} a_1^2(m_{11})_{1,2} &= a_5^2(m_{11})_{1,3} \\ a_3^2(m_{22})_{2,3} &= a_2^2(m_{22})_{1,2} \\ a_4^2(m_{33})_{2,3} &= a_6^2(m_{33})_{1,3}. \end{aligned} \quad (25)$$

This procedure defines the fitted anisotropy tensor $[M]$ only to within a multiplicative constant, but this is acceptable for our purposes, since the essential information in this tensor is the orientation of the principal axes and the ratios between principal values, not the absolute values *per se*. This allows normalization of the anisotropy tensor so that it reflects the degree of orientation independently of the fineness of the microstructure. This normalization also avoids the complex experimental problem of calibrating the magnification applied to each section. Should the absolute values of the components of this tensor be deemed important, well-calibrated experimental instruments should render the a_is so close to unity that they are unimportant.

4. Comparison with experimental results

Data obtained in a related experimental study [9], normalized to fit a unit amplitude cosine function, is shown in Fig. 4. The general pattern clearly fits a cosine with experimental noise. The poorer fitting points in Fig. 4 are traceable to the more isotropic specimens in which normalization (dividing by the experimentally fitted cosine magnitudes) accents the essentially constant

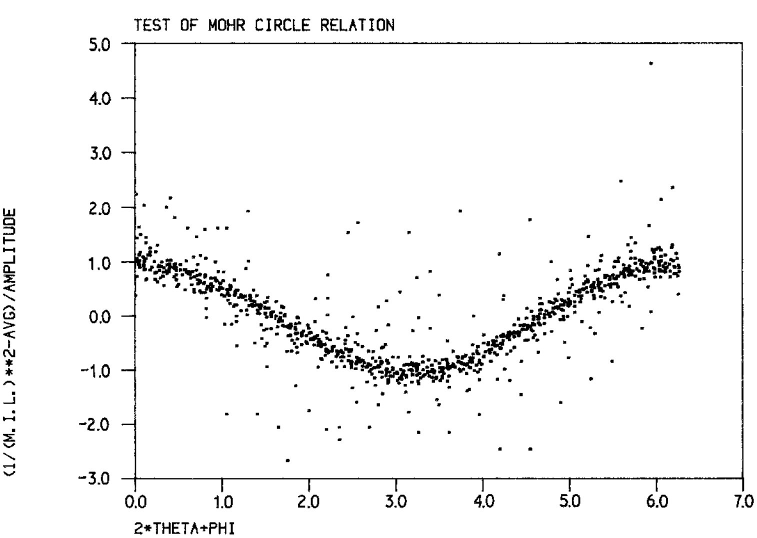


Figure 4 Normalized plot of experimental data.

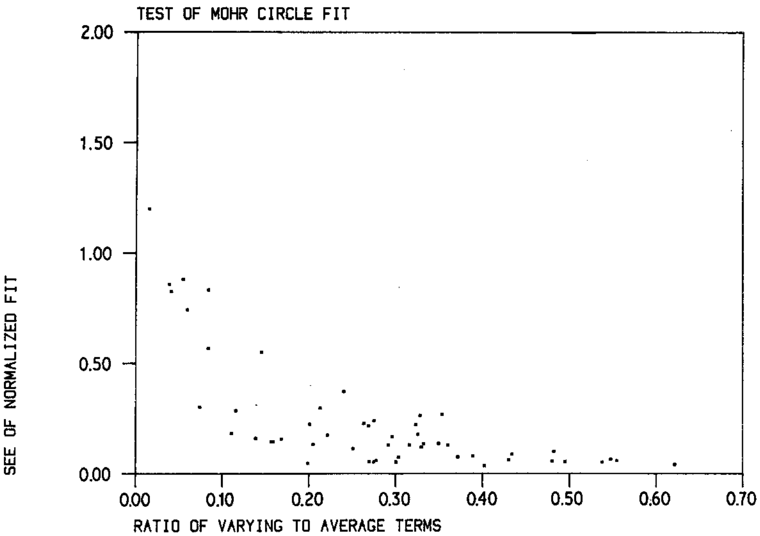


Figure 5 Plot of the standard error of estimate of the normalized fit of Fig. 3.

experimental inaccuracies. Fig. 5 demonstrates this; the standard error of estimate of the normalized Mohr circle curve fit is larger in the more isotropic specimens. This experimental noise is not a serious problem, since it is large proportionately when anisotropy is small. Precise measurement of anisotropy is probably not important in these instances. Table II shows the components of the principal axes (in the coordinate system defined by the specimen faces, normalized to have a trace of unity) of the anisotropy tensor as measured in five cancellous bone specimens from five different human bones.

5. Comparison with present stereologic measures

If the mean intercept length as given in Equation 11 were inverted to arrive at the intercepts per unit line length and were plotted as a function of angle, the familiar rose of intercepts as given by

TABLE II Anisotropy tensors in cancellous bone samples from five human bones

Bone			Principal value	directions		
Patella ($a_1/a_2 = 1.089$)						
0.21099	0.08854	0.02489	0.55904	0.25543	−0.02734	0.96644
0.08854	0.51091	0.07823	0.25430	0.92532	−0.28285	−0.25256
0.02489	0.07823	0.27809	0.18664	0.28026	0.95878	0.04695
Proximal femur ($a_1/a_2 = 0.964$)						
0.45984	−0.00195	−0.03281	0.47021	0.95349	0.30117	0.01237
−0.00195	0.17384	−0.00897	0.35641	0.00284	−0.05001	0.99874
−0.03281	−0.000897	0.36632	0.17338	−0.30141	0.95226	0.04854
Ischium ($a_1/a_2 = 0.960$)						
0.31420	0.00446	−0.11252	0.44875	−0.63136	0.24333	0.73612
0.00446	0.33812	0.02835	0.33890	0.16875	0.96985	−0.17581
−0.11252	0.02835	0.34767	0.21324	0.75690	−0.01325	0.65339
Acetabulum ($a_1/a_2 = 0.9911$)						
0.37230	0.14054	−0.00818	0.49533	0.75293	−0.02537	−0.65761
0.14054	0.33442	0.00061	0.29353	0.65749	0.07225	0.74999
−0.00818	0.00061	0.29328	0.21113	−0.02849	0.99706	−0.07108
Tibia ($a_1/a_2 = 1.026$)						
0.71898	0.08787	−0.14648	0.76797	0.96124	−0.23177	0.13960
0.08787	0.13849	−0.03463	0.13165	0.14701	0.87031	0.47006
−0.14648	−0.03463	0.14252	0.11038	−0.23326	−0.43131	0.87153

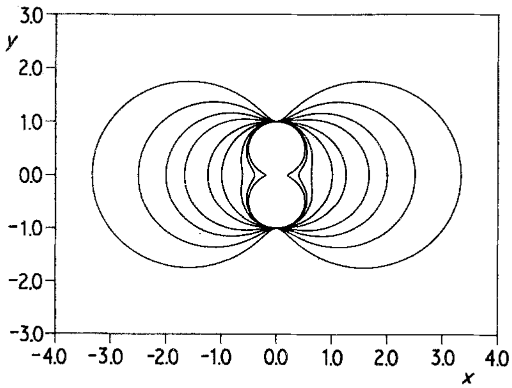


Figure 6 The rose of intercepts predicted by the mean intercept tensor representation. The contours shown are plotted for ellipses whose vertical components are unity and whose horizontal components are 0.3 (outermost), 0.4, 0.5, 0.6, 0.8, 1.0, 2.5 and 5.0 (innermost).

Underwood [2] is generated, as Fig. 6 shows. Given the mean intercept length tensor, this plot can be produced for any material plane and thus the degrees of orientation as given by Saltykov can be produced. This idealization of the material microstructure obviously does not include the fine detail possible with Hilliard's analysis, and is directed towards a different goal. Rather than closely characterizing the shape of included volumes in a material, we wish to characterize the overall material orientation. In specifying the anisotropy tensor as symmetric we have fundamentally restricted this analysis to orthotropic materials, with three mutually perpendicular directions of major orientation. This idealization is unavoidable considering the experimental method used to arrive at the tensor, which was a curve fit to the mean intercept data based on Equation 16. If a method exists by which m_{ij} and m_{ji} $(i \neq j)$ can be separated, we are not aware of it.

The experimental accuracy of this method for orthotropic materials should be higher than those of Saltykov and Hilliard since a great many intercept measurements are used to arrive at six quantities in a second rank tensor. By basic statistical arguments, one can show that the accuracy of these six quantities is substantially higher than that of a single measurement of mean intercept length.

6. Conclusions

The anisotropy of microstructure in orthotropic materials is represented in terms of a second rank tensor, which can be measured via planar methods applied to any three mutually perpendicular planes in the material. Simple explicit techniques are available to include these measurements in a relationship which employs microstructure measurements to predict structural parameters in orthotropic composites. Applications such as study of the relationships between mechanical stress applied to bone tissue (also a second rank tensor) and the degree of tissue anisotropy is also easily accomplished using this representation of tissue microstructure.

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