FITTING OF SHAPE FABRIC ELLIPSOID FROM 3 PERPENDICULAR CUBE PLANES

Shape fabric ellipse fitting

The main orientation of the particles was determined from the rose diagram and set to θ, the anticlockwise angle of the main axis of the ellipse. The major and minor axes of the shape fabric ellipses were determined as the deviation from the unit circle. The radius *R* of an un-deformed circle would be the number of measured particles *N* divided by the number of rose diagram segments *S* from 0 to 180.

$$R = \frac{N}{S} \tag{A1}$$

The deviation from the unit circle of the major axis $a = 1 + e_x$ is calculated by dividing of the length of the main orientation of rose diagram l by radius *R*.

$$a = 1 + e_x = \frac{l}{R} \tag{A2}$$

The deviation from the unit circle of the minor axis $b = 1 + e_y$ is calculated by

$$b = 1 + \frac{1-a}{a} \tag{A3}$$

These ellipses represent the deviation from an isotropic (completely random) orientation of all particles of each plane.

Shape fabric ellipsoid fitting

The general equation for each shape fabric ellipse could also be written (for the *xy* plane) as

$$\left(\frac{\cos^2\theta}{a_{xy}^2} + \frac{\sin^2\theta}{b_{xy}^2}\right)x^2 - 2\sin\theta\cos\theta\left(\frac{1}{b_{xy}^2} - \frac{1}{a_{xy}^2}\right)xy + \left(\frac{\sin^2\theta}{a_{xy}^2} + \frac{\cos^2\theta}{b_{xy}^2}\right)y^2 = 1 \tag{A4}$$

For a detailed derivation, see Ramsay (2004). Simplifying this equation results in

$$\begin{aligned} \lambda'_x x^2 - 2\gamma'_{xy} xy + \lambda'_y y^2 &= 1 \\ \lambda'_y y^2 - 2\gamma'_{yz} yz + \lambda'_z z^2 &= 1 \\ \lambda'_z z^2 - 2\gamma'_{xz} xz + \lambda'_x x^2 &= 1 \end{aligned} \tag{A5a,b,c}$$

for the xy, yz, and xz planes, respectively, with λ’ and γ’ replacing the first two coefficients of equation (4). The three finite-shape-fabric invariants could be obtained by

$$\begin{aligned} J_1 &= \lambda'_x + \lambda'_y + \lambda'_z \\ J_2 &= \lambda'_x\lambda'_y + \lambda'_y\lambda'_z + \lambda'_z\lambda'_x - {\gamma'_{xy}}^2 - {\gamma'_{yz}}^2 - {\gamma'_{xz}}^2 \\ J_3 &= \lambda'_x\lambda'_y\lambda'_z - 2\gamma'_{xy}\gamma'_{yz}\gamma'_{xz} - \lambda'_x{\gamma'_{yz}}^2 - \lambda'_y{\gamma'_{xz}}^2 - \lambda'_z{\gamma'_{xy}}^2 \end{aligned} \tag{A6a,b,c}$$

where λ' is the reciprocal quadratic extension of the axis of the ellipsoid, with $\lambda = 1/\lambda'$ and λ'_1, λ'_2, and λ'_3, the reciprocal quadratic extension of the three principal axes of the ellipsoid, which could be obtained by solving the cubic equation

$$\lambda'^3 - J_1\lambda'^2 + J_2\lambda' - J_3 = 0 \tag{A7}$$

Knowing that λ'_2 lies between the turning points of the cubic equation given by

$$3\lambda'^2 - 2J_1\lambda' + J_2 = 0 \tag{A8}$$

the value λ'_2 could be obtained by Newton's method

$$\lambda'_{(2)_1} = \lambda'_{(2)_0} - \frac{\lambda'^{\,3}_{(2)_0} - J_1\lambda'^{\,2}_{(2)_0} + J_2\lambda'_{(2)_0} - J_3}{3\lambda'^{\,2}_{(2)_0} - 2J_1\lambda'_{(2)_0} + J_2} \tag{A9}$$

with a first guess of $\lambda'_{(2)0}$ and a better approximation of $\lambda'_{(2)1}$. After ten iterations, $\lambda'_{(2)10} = \lambda'_2$. Values for λ'_1 and λ'_3 could be obtained by solving the quadratic expression

$$\lambda'^2 + (\lambda'_2 - J_1)\lambda' + (\lambda'^{\,2}_2 - J_1\lambda'_2 + J_2) = 0 \tag{A10}$$

The endpoints of the three symmetry axes of the shape fabric ellipsoid could be established by solving the system of equations

$$\begin{aligned} &\frac{x_1}{A} = \frac{-y_1}{B} = \frac{-z_1}{C} \\ &x_1^2 + y_1^2 + z_1^2 = \lambda_1 \end{aligned} \tag{A11a,b}$$

with

$$\begin{aligned} A &= \lambda'_y\lambda'_z - \lambda'_1\lambda'_y - \lambda'_1\lambda'_z + \lambda'^{\,2}_1 - \gamma'^{\,2}_{yz} \\ B &= \gamma'_{xy}\lambda'_z + \gamma'_{xy}\lambda'_1 - \gamma'_{zx}\gamma'_{yz} \\ C &= \gamma'_{xy}\gamma'_{yz} + \lambda'_y\gamma'_{zx} - \lambda'_1\gamma'_{zx} \end{aligned} \tag{A12a,b,c}$$

for the symmetry axis with the endpoint (x_1, y_1, z_1). Thus x_1, y_1, and z_1 are respectively

$$\begin{aligned} x_1 &= -\frac{y_1 \cdot A}{B} \\ y_1 &= \sqrt{\frac{\lambda_1}{\frac{A^2}{B^2} + 1 + \frac{C^2}{B^2}}} \\ z_1 &= \frac{y_1 \cdot C}{B} \end{aligned} \tag{A13a,b,c}$$

The endpoint (x_2, y_2, z_2) of the second symmetry axis could be similarly obtained.

Because the shape fabric ellipsoid is the deviation from the unit sphere, the length of the third symmetry axis r_3 can be obtained by

$$r_3 = \frac{1}{\sqrt{x_1^2 + y_1^2 + z_1^2} \cdot \sqrt{x_2^2 + y_2^2 + z_2^2}} \tag{A14}$$

The endpoint of the third symmetry axis can be calculated using the cross-product of points 1 and 2 multiplied by a length factor.

$$\begin{pmatrix} x_3' \\ y_3' \\ z_3' \end{pmatrix} = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} \times \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$$

$$\begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} = \begin{pmatrix} x_3' \\ y_3' \\ z_3' \end{pmatrix} \cdot \sqrt{\frac{r_3^2}{(x_3')^2 + (y_3')^2 + (z_3')^2}} \tag{A15a,b}$$

Reorienting samples

The investigated samples have orientations recorded in the *plunge and plunge direction* convention. The *plunge* is the angle below the horizontal and has a value from 0 to 90°. The *plunge direction* is the azimuth of the direction of the plunge as projected to the horizontal. By determining the position of the plunge and the plunge direction of the suevite cube axes, the symmetry axes of the ellipsoid can be reoriented to their original geographical orientations.

The first step is to transform the plunge and plunge direction of the cube axis into polar coordinates. Whereas an azimuth of 0° represents north and is counted clockwise, 0° in mathematical expressions represents east and counting is anticlockwise. Angle α is the angle between the x axis and the projection of a space vector on the xy plane, and can be found by α=90°–[plunge direction]. Angle β is the angle between the z axis and a space vector and can be found by β=90°+[plunge].

Assuming unit length for the coordinate axis of the suevite cube, coordinate axes could be expressed as

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \sin\beta_x \cos\alpha_x & \sin\beta_x \sin\alpha_x & \cos\beta_x \\ \sin\beta_y \cos\alpha_y & \sin\beta_y \sin\alpha_y & \cos\beta_y \\ \sin\beta_z \cos\alpha_z & \sin\beta_z \sin\alpha_z & \cos\beta_z \end{pmatrix} \tag{A16}$$

The endpoints of the shape fabric ellipsoids can be transformed into the coordinate system of the orientated suevite cube by

$$\begin{pmatrix} x'_1 & x'_2 & x'_3 \\ y'_1 & y'_2 & y'_3 \\ z'_1 & z'_2 & z'_3 \end{pmatrix} = \begin{pmatrix} \sin\beta_x \cos\alpha_x & \sin\beta_x \sin\alpha_x & \cos\beta_x \\ \sin\beta_y \cos\alpha_y & \sin\beta_y \sin\alpha_y & \cos\beta_y \\ \sin\beta_z \cos\alpha_z & \sin\beta_z \sin\alpha_z & \cos\beta_z \end{pmatrix} \bullet \begin{pmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{pmatrix} \quad \text{(A17)}$$

The cartesian coordinates must be transformed into polar coordinates for each symmetry axis of the shape fabric ellipsoid by

$$r_1 = \sqrt{x'^2_1 + y'^2_1 + z'^2_1}$$

$$\alpha_1 = \arccos \frac{x'_1}{\sqrt{x'^2_1 + y'^2_1}} \quad \text{(A18a,b,c)}$$

$$\beta_1 = \frac{\pi}{2} - \arctan \frac{z'_1}{\sqrt{x'^2_1 + y'^2_1}}$$

The values α_1, α_2, α_3, β_1, β_2, and β_3 must be transformed into plunge and plunge direction expressions by applying [plunge direction]=90°-α and [plunge]=β-90°.

SHAPE FABRIC ELLIPSOID FITTING FROM X-RAY TOMOGRAPHY DATA

Ellipse fitting of each particle in the xy, yz and xz planes

For the *xy* plane:

The major (a) and minor (b) axes of one particle appearing in different CT images were fitted in a linear equation with slope m and intercept n. The maximum major axis of all images was set to a_{xy}. The minor axis b_{xy} was calculated from the linear equation below. Because half-axes are used later in the ellipsoid fitting, a_{xy} and b_{xy} were divided by 2.

$$b = m \cdot a + n$$
$$a_{xy} = \frac{\max(a)}{2} \qquad \text{(A19a,b,c)}$$
$$b_{xy} = \frac{m \cdot \max(a) + n}{2}$$

The angle θ_{xy} of the *xy* plane was determined as the mean angle value of the major axes of the particle in each CT image, neglecting the values of the first and last three images for resolution reasons.

The distance of the endpoint of the major axis in the xy plane was determined by

$$dx = a_{xy} \cdot \cos(\theta_{xy})$$
$$dy = a_{xy} \cdot \sin(\theta_{xy}) \qquad \text{(A20a,b)}$$

The distance in the *z* direction was determined by the difference in the number N_z of the last and first CT images where the particle could be observed, multiplied by the distance between each plane (0.6 mm) divided by 2.

$$dz = \frac{(\max(N_z) - \min(N_z)) \cdot 0.6}{2} \qquad \text{(A21)}$$

For the *yz* plane:

The first step is to determine the length l_1 from the particle in the *yz* plane by

$$l_1 = \sqrt{dy^2 + dz^2} \qquad \text{(A22)}$$

The angle θ_1 of this vector was obtained by fitting the *y* position of the particle in each CT image with $N_z*0.6$. The slope of the linear equation is the tangent of θ_1.

A second point of the ellipse in the *yz* plane can be obtained by the 90° value of the ellipse in the *xy* plane. The length l_2 of this vector is calculated from the ellipse equation

$$1 = \frac{(l_2 \cdot \cos(90 - \theta_{xy}))^2}{a_{xy}^2} + \frac{(l_2 \cdot \sin(90 - \theta_{xy}))^2}{b_{xy}^2} \quad \text{(A23)}$$

The l_2 vector is parallel to the *y* axis and hence the angle in the *yz* plane is 0°.

If $l_1 > l_2$, the major axis in the *yz* plane is $a_{yz} = l_1$ and the angle of a_{yz} to the *y* axis is $\theta_{yz} = \theta_1$. The intermediate axis in the yz plane, b_{yz}, is again found by the ellipse equation

$$1 = \frac{(l_2 \cdot \cos(-\theta_1))^2}{a_{yz}^2} + \frac{(l_2 \cdot \sin(-\theta_1))^2}{b_{yz}^2} \quad \text{(A24)}$$

If $l_1 < l_2$, the major axis in the yz plane is $a_{yz} = l_2$, and the angle of a_{yz} to the *y* axis is $\theta_{yz} = 0$. In this case, b_{yz} is found by equation A24 with positive θ_1 values.

For the zx plane:

Length l_1 and angle θ_1 of the *zx* plane are obtained in the same way as for the *yz* plane by substituting *x* for *y*. The second point of the ellipse in the *xz* plane will be obtained by the 0° value of the ellipse in the *xy* plane. The length l_2 of this vector is calculated from the ellipse equation

$$1 = \frac{(l_2 \cdot \cos(-\theta_{xy}))^2}{a_{xy}^2} + \frac{(l_2 \cdot \sin(-\theta_{xy}))^2}{b_{xy}^2} \quad \text{(A25)}$$

Vector l_2 is parallel to the *x* axis and hence the angle in the *zx* plane is 0°. Values a_{zx}, b_{zx}, and θ_{zx} can be found in the same way as for the *yz* plane. Finally, it should be taken into account that the ordinate of the *zx* plane should be the *z* axis for the later ellipsoid fitting. For this reason $\theta_{zx} = \theta_{zx} + 90°$.

Shape fabric ellipsoid fitting

An ellipsoid is fitted from the three ellipses for each particle and reoriented as described in GSA Data Repository 1.

The particle ellipsoids are weighted by setting the major axis of each ellipsoid to 1. The average ellipsoid can be found by the mean value of all *N* particle ellipsoids according to

$$\begin{pmatrix} r_{1mean} & r_{2mean} & r_{3mean} \\ \alpha_{1mean} & \alpha_{2mean} & \alpha_{3mean} \\ \beta_{1mean} & \beta_{2mean} & \beta_{3mean} \end{pmatrix} = \frac{1}{N} \sum_{i=1}^{N} \begin{pmatrix} r_{1i} & r_{2i} & r_{3i} \\ \alpha_{1i} & \alpha_{2i} & \alpha_{3i} \\ \beta_{1i} & \beta_{2i} & \beta_{3i} \end{pmatrix} \quad \text{(A26)}$$