Finding the disclination density tensor from the orientation tensor *g*

CF June 12, 2013

Assume provisionally the existence of the elastic rotation tensor $\boldsymbol{\omega}_{\mathbf{e}}$ (skew-symmetric part of elastic distortion tensor $\mathbf{U}_e$). We will get rid of this assumption below. Start from Beausir & Fressengeas, IJSS 2013, page 4, line 7 below Eq.29 : $\omega_{ij}^e \approx g_{ij} - \delta_{ij}$ valid at small disorientations. Build the elastic rotation vector $\boldsymbol{\Omega}_e$ from the elastic rotation tensor:

$$\boldsymbol{\Omega}_e = -\frac{1}{2}\mathbf{X} : \boldsymbol{\omega}_{\mathbf{e}}, \Omega_k^e = -\frac{1}{2} e_{ijk} \omega_{ij}^e \approx -\frac{1}{2} e_{ijk} (g_{ij} - \delta_{ij})$$

Build the « gradient » tensor of this elastic rotation vector:

$$\frac{\Delta \Omega_k^e}{\Delta x_l} \approx -\frac{1}{2} e_{ijk} \frac{\Delta g_{ij}}{\Delta x_l} = -\frac{1}{2} e_{ijk} g_{ij,l}$$

Call this the elastic curvature tensor $\boldsymbol{\kappa}_{\mathbf{e}}$:

$$\kappa_{kl}^e = \frac{\Delta \Omega_k^e}{\Delta x_l} \approx -\frac{1}{2} e_{ijk} g_{ij,l}$$

and forget the *a priori* idea that this is the gradient of a vector field. To check whether $\boldsymbol{\kappa}_{\mathbf{e}}$ is actually a gradient tensor or not, build its curl:

$$(\mathbf{curl}\, \boldsymbol{\kappa}_e)_{kj} = e_{jml} \kappa_{kl,m}^e \approx -\frac{1}{2} e_{jml} e_{ijk} g_{ij,lm}$$

and define $\mathbf{curl}\, \boldsymbol{\kappa}_e$ as the disclination density tensor $\boldsymbol{\theta}$:

$$\theta_{kj} = e_{jml} \kappa_{kl,m}^e$$

Use the following identities :

$$e_{jml} e_{ijk} = -e_{jml} e_{jki} = -(\delta_{km}\delta_{il} - \delta_{kl}\delta_{im})$$

to finally obtain :

$$\theta_{kj} \approx \frac{1}{2}(\delta_{km}\delta_{il} - \delta_{kl}\delta_{im}) g_{ij,lm} = \frac{1}{2}(g_{ij,ik} - g_{ij,ki})$$

Exchange indices i and k to get a pretty result :

$$\theta_{ij} \approx \frac{1}{2}(g_{kj,ki} - g_{kj,ik}) = \frac{1}{2} e_{jik} e_{jml} g_{kj,lm}$$

Finite difference approximation for the 2nd derivative that we need:
f_{xy} = 1/4
{ - 4f(x,y)
+f(x+Δx, y+Δy)
+f(x+Δx, y-Δy)
+f(x-Δx, y+Δy)
+f(x-Δx, y-Δy)}

I suspect that writing out the formulae for each term would lead to further simplifications because some of the terms have to be set to zero because of the lack of data in the 3rd dimension.