PHYS 4xx Net2 - Elastic moduli in 2D

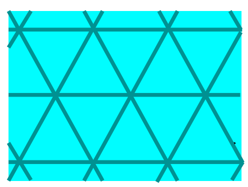
General symmetries of elastic moduli

- u_{ij} is symmetric under exchange of *i* and *j*; hence, C_{ijkl} can be defined such that it is pairwise symmetric under exchange of *i* and *j* or *k* and *l*
$$C_{ijkl} = C_{jikl} = C_{ijlk}. \tag{1}$$

- $u_{ij}u_{kl}$ is symmetric under exchange of the pairs of indices *ij* and *kl*; hence:
$$C_{ijkl} = C_{klij}. \tag{2}$$

- these two symmetries alone reduce the number of independent moduli to 6 in 2D
$$C_{xxxx} \qquad C_{yyyy} \qquad C_{xxyy} = C_{yyxx}$$
$$C_{xyxy} = C_{xyyx} = C_{yxyx} = C_{yxxy} \tag{3}$$
$$C_{xxxy} = C_{xxyx} = C_{xyxx} = C_{yxxx}$$
$$C_{yyxy} = C_{yyyx} = C_{xyyy} = C_{yxyy}.$$

Six-fold networks in 2D



- change from Cartesian coordinates *x* and *y* to complex coordinates ξ and η (Landau and Lifshitz)
$$\xi \equiv x + iy \qquad \eta \equiv x - iy, \tag{4}$$

- rotation by θ changes (x, y) to $(x\cos\theta - y\sin\theta, x\sin\theta + y\cos\theta)$ or
$$x + iy \to (x\cos\theta + ix\sin\theta) + (iy\cos\theta - y\sin\theta) = x(\cos\theta + i\sin\theta) + iy(\cos\theta + i\sin\theta)$$

hence:
$$\xi \to \xi\exp(i\theta) \qquad \eta \to \eta\exp(-i\theta). \tag{5}$$

- six-fold symmetry demands the moduli be invariant under rotations through $\theta = \pi/3$
$$\xi \to \xi\exp(i\pi/3) \quad \text{and} \quad \eta \to \eta\exp(-i\pi/3).$$

- the only components of C_{ijkl} unchanged by this transformation contain ξ and η the same number of times, since $\exp(i\pi/3)\exp(-i\pi/3) = 1$

- only two moduli are invariant under 6-fold symmetry; the free energy density $\Delta\mathcal{F}$ is then

$$\Delta\mathcal{F} = 2C_{\xi\eta\xi\eta}u_{\xi\eta}u_{\xi\eta} + C_{\xi\xi\eta\eta}u_{\xi\xi}u_{\eta\eta}, \quad (6)$$

[the first term results from four permutations of $C_{\xi\eta\xi\eta}$ and the second term from two permutations of $C_{\xi\xi\eta\eta}$; the expression includes a normalization factor of 1/2]

- the components of a tensor transform as the products of the corresponding coordinates. *i.e.*, since $\xi^2 = (x + iy)^2 = x^2 - y^2 + 2ixy$, then

$$u_{\xi\xi} = u_{xx} - u_{yy} + 2iu_{xy}, \qquad u_{\eta\eta} = u_{xx} - u_{yy} - 2iu_{xy}, \qquad u_{\xi\eta} = u_{xx} + u_{yy}, \quad (7)$$

and

$$\Delta\mathcal{F} = 2C_{\xi\eta\xi\eta}\,(u_{xx} + u_{yy})^2 + C_{\xi\xi\eta\eta}\,\{(u_{xx} - u_{yy})^2 + 4u_{xy}^2\}. \quad (8)$$

- replace C_{ijkl} by moduli more directly related to the pure deformation modes of area compression (K_A) or shear (μ)

$$K_A = 4C_{\xi\eta\xi\eta} \qquad \mu = 2C_{\xi\xi\eta\eta}, \quad (9)$$

so that (8) becomes

$$\Delta\mathcal{F} = (K_A/2)\,(u_{xx} + u_{yy})^2 + \mu\{(u_{xx} - u_{yy})^2/2 + 2u_{xy}^2\} \quad \text{(six-fold symmetry)}. \quad (10)$$

Isotropic materials

- only two rotationally invariant combinations of u; hence, only two elastic moduli
- (10) applies to isotropic materials in 2D as well

Networks of springs

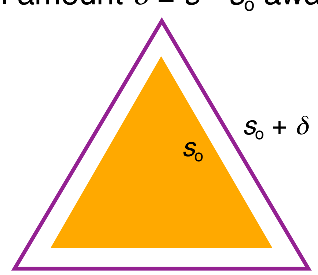
We now relate the macroscopic moduli C_{ijkl} to the microscopic parameters of a model network with 6-fold connectivity. The bond elements are Hookean springs with

spring constant = k_{sp}
unstretched length = s_o
potential energy $V_{sp} = k_{sp}(s - s_o)^2 / 2$ (11)

Our method is to compare ΔF in two representations to get the elastic moduli in terms of k_{sp} and s_o.

Compression modulus

- stretch each spring a small amount $\delta \equiv s - s_o$ away from s_o



- with three springs per vertex, the change in potential energy per vertex ΔU_V is

  $\Delta U_V = 3\Delta V_{sp} = 3k_{sp}\delta^2/2,$ (12)

- divide (12) by the network area per vertex of $A_V = \surd 3\ s_o^2/2$

  $\Delta \mathcal{F} = \Delta U/A_V = \surd 3\ k_{sp}(\delta/s_o)^2.$ (13)

- Eq. (10) for $\Delta\mathcal{F}$ uses the strain tensor; its elements are

  the deformations are uniform in x and y ---> $u_{xx} = u_{yy} = \delta/s_o$

  the displacement in the y-direction is independent of the position of the triangle in the x-direction ---> $u_{xy} = 0$

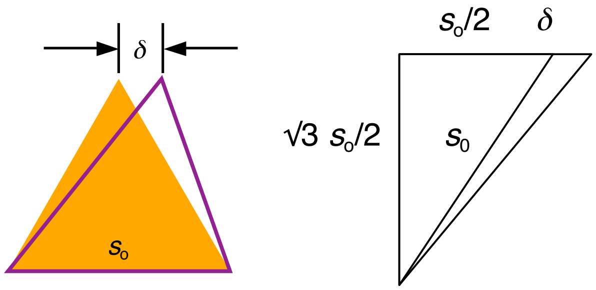
- thus:

  $\Delta\mathcal{F} = 2K_A(\delta/s_o)^2,$ (14)

- comparing (13) and (14) yields

  $K_A = \surd 3\ k_{sp}/2$ (six-fold network). (15)

Shear modulus The shear modulus can be obtained from the deformation



$s = ([\surd 3\ s_o/2]^2 + [s_o/2 + \delta)^2)^{1/2}$
$= s_o\ (3/4 + [1/2 + \delta/s_o]^2)^{1/2}$
$= s_o\ (3/4 + 1/4 + 2\delta/ 2s_o + ...)^{1/2}$
$= s_o\ (1 + \delta/ 2s_o + ...)$

Hence
$\Delta s = \delta/2$

- moving the top vertex an amount δ in the x-direction changes the diagonal spring lengths by $\pm\delta/2$ (to lowest order in δ); no change in bottom spring

  ---> $\Delta U = (k_{sp}/2)\bullet(s - s_o)^2 = k_{sp}\delta^2/8$ for either stretched spring

- at three springs per vertex: $\Delta U_V = 2k_{sp}\delta^2/8 + 0 = k_{sp}\delta^2/4$

  $\Delta\mathcal{F} = \Delta U_V/A_V = (k_{sp}\delta^2/4) / (\surd 3\ s_o^2/2) = k_{sp}(\delta/s_o)^2/(2\surd 3)$ (16)

- the strain tensor of the deformation is

  • x and y distances are unchanged ---> $u_{xx} = u_{yy} = 0.$

  • each successive row of vertices is displaced by δ in the positive x-direction for each increase $\surd 3\ s_o/2$ in the y-direction ---> $\partial u_x/\partial y = 2\delta / \surd 3\ s_o$

  $u_{xy} = (1/2)(\partial u_x/\partial y + \partial u_y/\partial x) = (1/2)\bullet[2\delta/(\surd 3\ s_o) + 0] = \delta/ \surd 3\ s_o$

- thus, (10) reads:
  $\Delta\mathcal{F} = (2\mu/3)(\delta/s_o)^2$. (17)

- comparing (16) and (17) yields
  $\mu = \sqrt{3}\ k_{sp}/4$ (six-fold network). (18)

Note: $K_A / \mu = 2$ for six-fold networks in 2D.