MODEL: MECHANICAL PROPERTIES OF THE PATCH

Please refer to the section "a small course on materials resistance".

Aim: Predict the influence of silification on the mechanical properties of the patch.

We modeled the influence of silification on the mechanical properties of the patch:

Let's consider a parallelepiped-shaped patch, with a thickness e and a surface S. The volume of the patch is given by:

$$V_{tot} = e\,S$$

We assume that cellulose includes silica with the volumic fraction:

$$\chi = \frac{V_{Si}}{V_{tot}}$$

where V_{Si} is the volume of silica included in the patch.

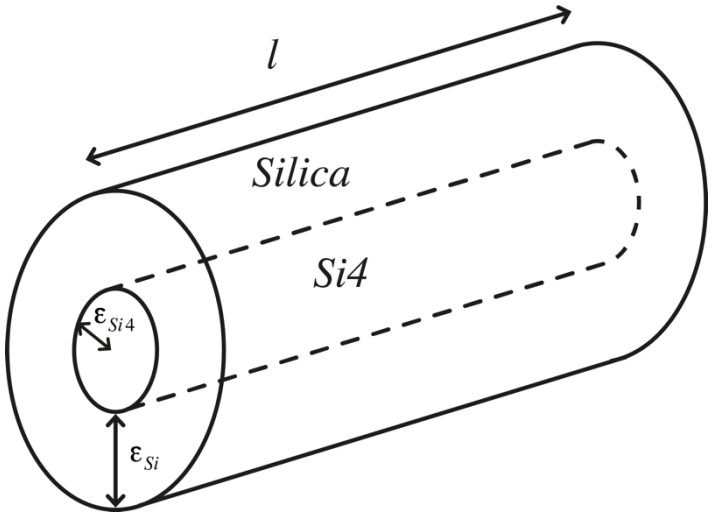
We assume that the Si4 domain of our protein is a linear cylinder (length l, radius ε_{Si4}). After silification, silica forms a cylindrical layer (thickness ε_{Si}) around the Si4 cylinder.
As a consequence, we derived the volume of silica around only one Si4 protein:

$$v_{Si} = \pi l[(\varepsilon_{Si} + \varepsilon_{Si4})^2 - {\varepsilon_{Si4}}^2]$$
$$v_{Si} = \pi l \varepsilon_{Si}(\varepsilon_{Si} + 2\varepsilon_{Si4})$$

Then, the volume of silica in the whole patch is given by:

$$V_{Si} = N_{Si4}\, v_{Si}$$

where N_{Si4} is the number of proteins included in the patch.



<u>Schematic of the model:</u> silica forms a cylindrical layer that coats the linear cylinder of the Si4 protein

Finally, we get the expression of χ:

$$\chi = \frac{N_{Si4}\, v_{Si}}{V_{tot}} = \frac{\pi l \varepsilon_{Si}(\varepsilon_{Si} + 2\varepsilon_{Si4})N_{fix}}{eS}$$

If silica is scattered uniformly in the patch, we can apply the rule of mixtures:

$$E = (1 - \chi)E_1 + \chi\, E_2$$

where E is the Young's modulus of the patch, E_1 is the one of cellulose and E_2 is the one of silica.

We took the following values for the parameters:
$e = 200\ \mu m\ ; S = 9\ cm^2\ ; l = 15\ nm\ (i.e. 15\ amino\ acids)\ ;\ \varepsilon_{Si4} = 0.1\ nm\ ;\ N_{Si4} = 1.1\ 10^{18}\ (i.e. 3.0\ mg\ of\ protein)$

And we found:

$$E = 4.77\ GPa$$
$$G = 2.04\ GPa$$

i.e. an increase of 48% in Young's modulus and of 75% in shear modulus. Thus, our patch would be as rigid as plastics after silification.

<u>Limits of the model:</u>

- The rule of mixtures is a simple model and can be applied only when the two materials have the same Poisson's ratio. However, it gives a good approximation.
- We assumed that our protein is linear, which is not the case.
- We assumed that all integrated proteins are silified.
- Actually, after silification, we recover a silica gel rather than a colloid of nanometric silica particles.