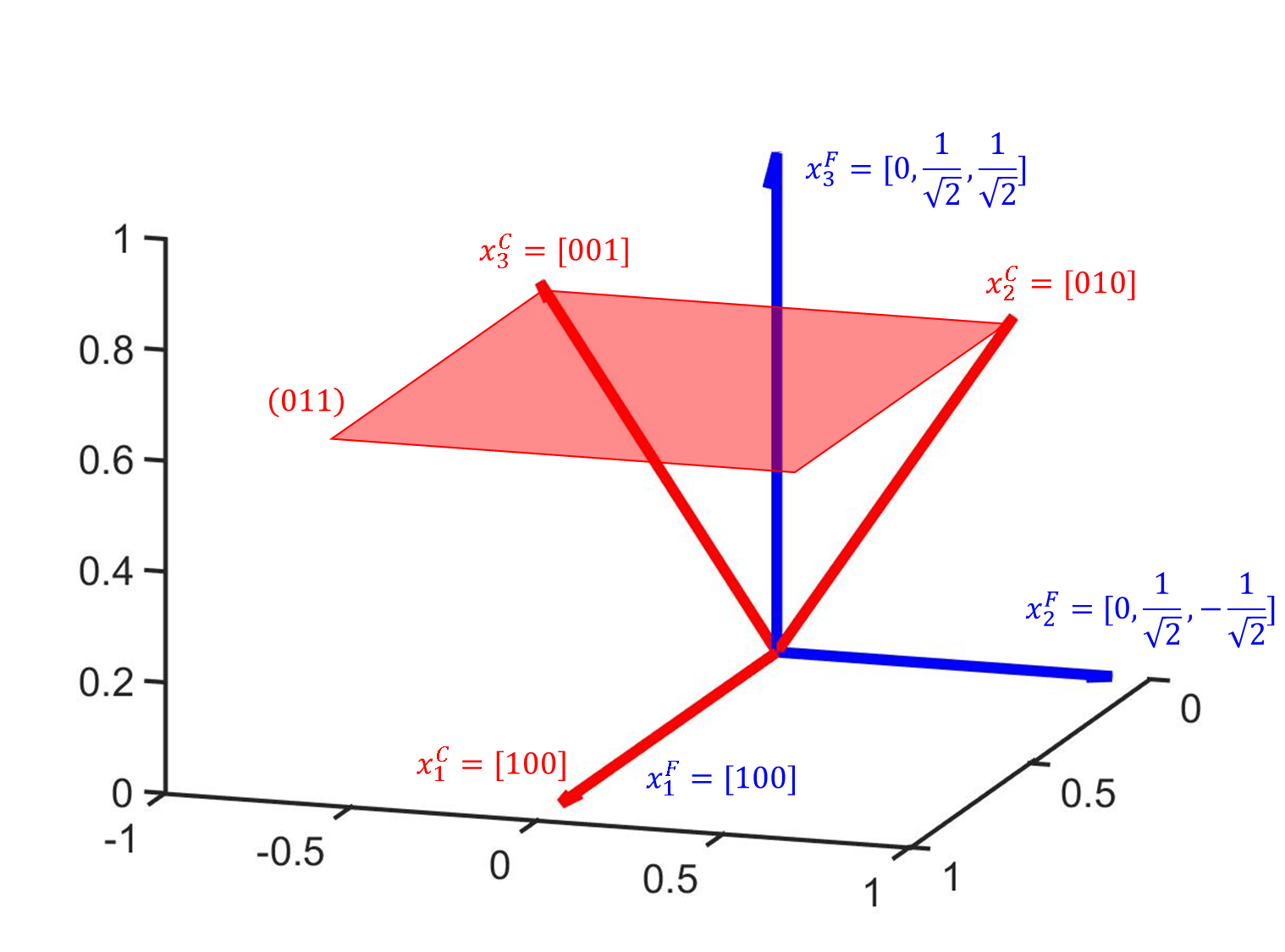
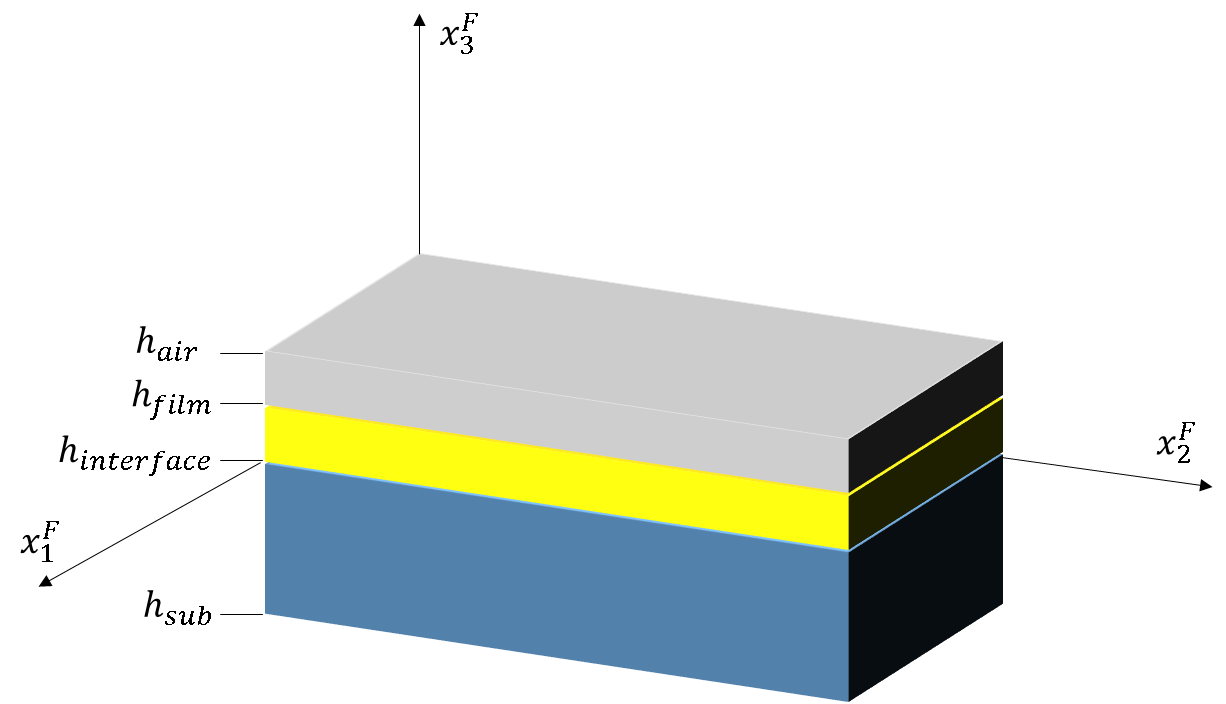
**Notation**

We specify two reference frames: the **crystal reference frame** and the **global film reference frame**. Global film reference frame: Crystal reference frame:

For example, for a substrate with an orientation:



We can express a tensor using either the global film reference frame or the crystal reference frame. We will denote the tensor when it is expressed using the global film reference frame (the global film reference frame basis). We will denote the vector when it is expressed using the crystal reference frame.

We can switch a vector (a first rank tensor) between the two reference frames using rotation matrices <http://www.continuummechanics.org/rotationmatrix.html>. Using tensor notation:

We can switch a second rank tensor (such as the strain tensor) between the two reference frames using:

We can switch a fourth rank tensor (such as the elastic tensor) between the two reference frames using:

(3.1)

The rotation matrix is orthogonal, meaning

(5)

We choose to simulate within the crystal reference frame. This way our simulation cell is rectangular and easy to implement.

**Energy Transform**

The free energy is again expressed as:

is the chemical potential energy expressed as a Landau-Ginsburg-Devonshire polynomial. The polarizations in are expressed using the crystal reference frame. If this were not the case, a simple rotation of the material would lead to different properties.

We need to convert in .

is the elastic energy, which can be expressed in either the crystal or global reference frame. and are, respectively, the elastic tensor and strain in the global reference frame. A coordinate transformation does not change the form of the elastic energy equation

maintains its symmetries: . The strain also maintains:

The mechanical equilibrium is given by:

The form of the equations is the same because we have the elastic, strain, and stress tensors in the new axes.

is the energy of domain walls. **Expression in global vs crystal frame**

Assuming an isotropic gradient energy,

**which is equivalent to (somehow…? ☹)**

is the electrical energy, which is

Electrical equilibrium is given by:

Why is electrical equilibrium in global coordinates??

**Why is there a factor of ½??**