CrystalMaker

If you have not already done so, install *CrystalMaker* and *SingleCrystal* (you may as well install *CrystalDiffract* as well, but we will not be using that application here).

> https://www.mccormick.northwestern.edu/materials-science/crystalmaker/ (https://www.mccormick.northwestern.edu/materials-science/crystalmaker/)

NOTE: There is no Linux distribution avaialble for the CrystalMaker Suite softwares.

We want to look at the crystal structure of our film and substrate. First, let's look at the substrate (Al_2O_3). Open up CrystalMaker. You should see the following:

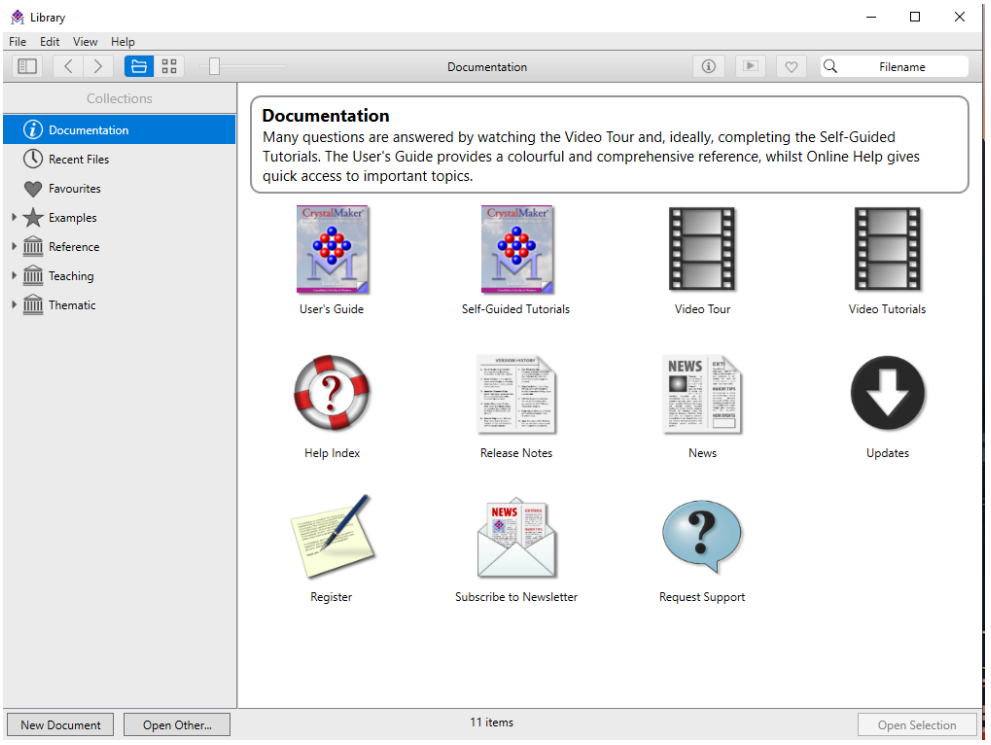

Fig. 1: *CrystalMaker home screen*

Within the search bar, enter "al2o3". You should see the Corrundum structure appear (this is your sapphire substrate). CrystalMaker has many crystal structures built into it.

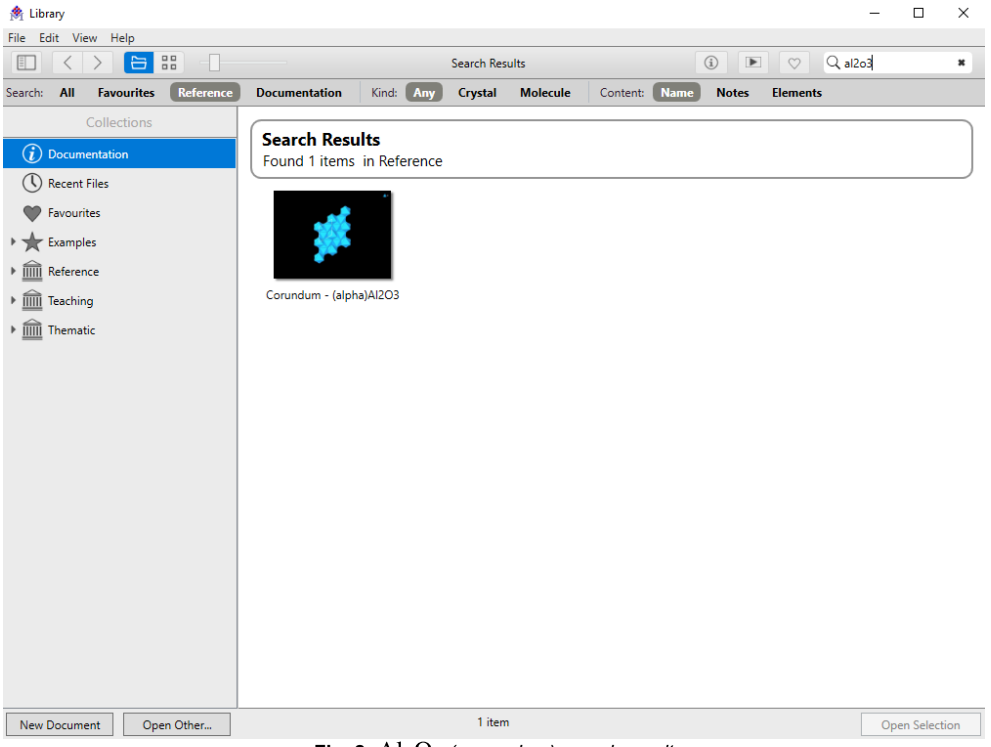

Fig. 2: Al_2O_3 *(corrundum) search result*

Load up the sapphire structure. CrystalMaker will now open up a new window displaying the sapphire structure (in the default polyhedral representation with the oxygen atoms hidden). Look around the CrystalMaker interface and play around with some of the features. The side menu on the right of the displayed structure shows many of these tools. For example, you can change the atom representation by clicking on the desired atom. Try changing from the polyhedra representation to a different representation. In addition, display the oxygen atoms so that they are no longer hidden (hidden is a type of representation marked by an "X").

You can also add (hkl) planes to your structure. Using the side menu bar, add the (001) plane to the structure.

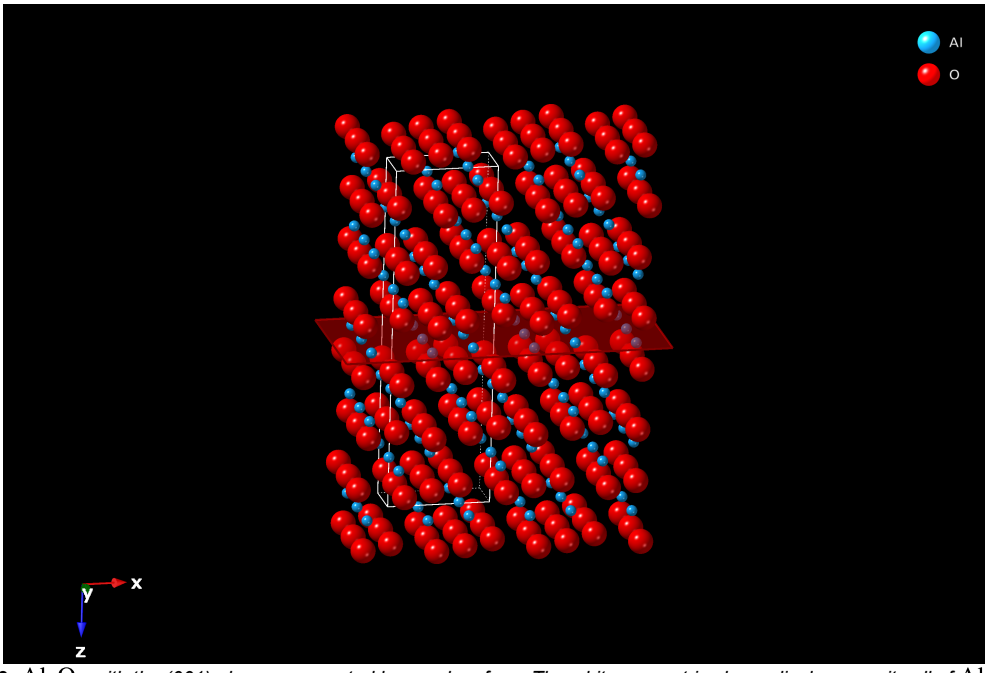

Fig. 3: Al_2O_3 *with the (001) plane represented by a red surface. The white geometric shape displays a unit cell of* Al_2O_3.

An useful feature of CrystalMaker is the *orient* function. In the top menu bar, click orient and set the view of the structure to (hkl) = (001). Now you will be looking directly at the plane surface you just added. Notice the hexagonal symmetry of the structure. Your film was grown on along this orientation of Al_2O_3.

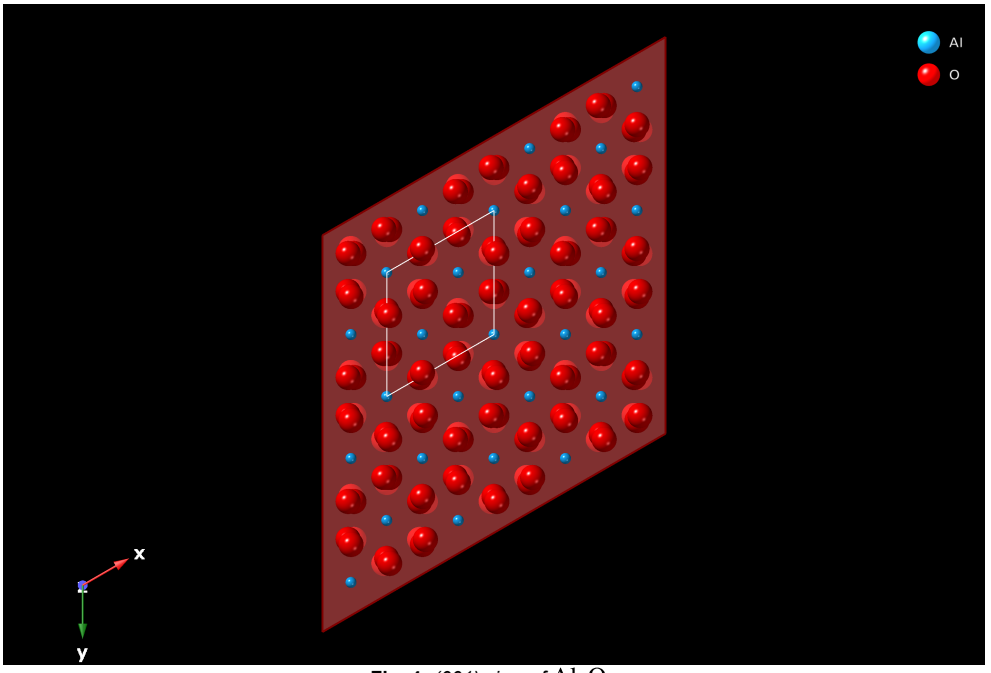

Fig. 4: *(001) view of* Al_2O_3

Feel free to explore more of the features of CrystalMaker!

SingleCrystal

Now that we have our structure of interest loaded in *CrystalMaker*, we want to explore how this crystal behaves under X-ray diffraction experiments. *SingleCrystal* is the easiest way to visualize and understand diffraction properties of crystals. In addition, *SingleCrystal* works hand in hand with *CrystalMaker*.

Open up the SingleCrystal application.

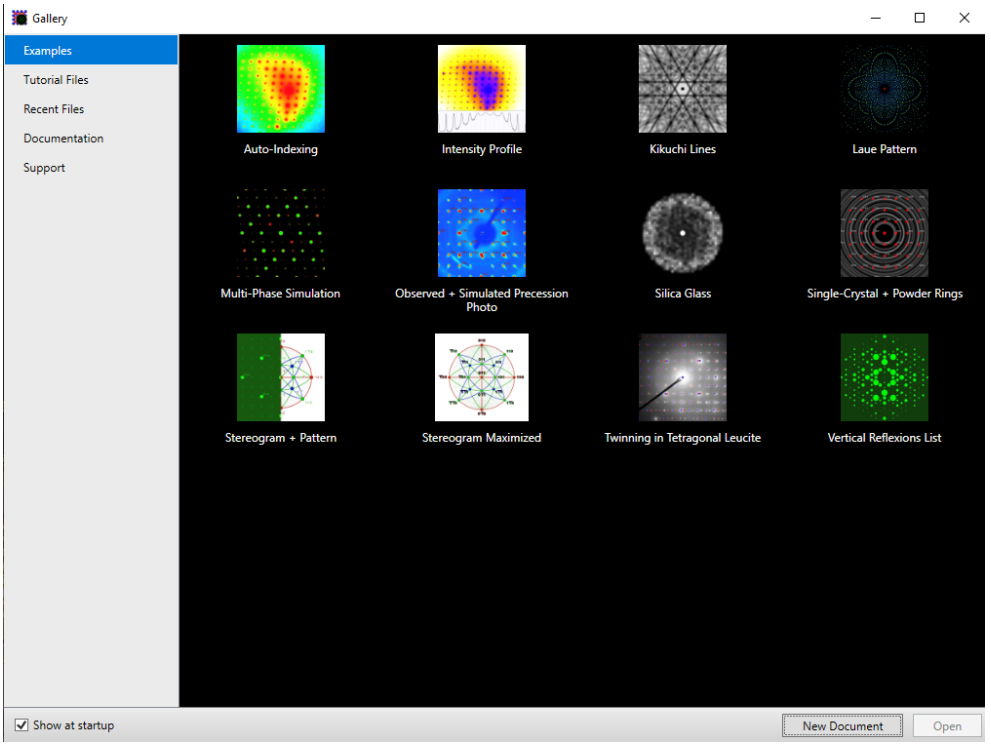

Fig. 5: *SingleCrystal home screen*

Click on "New Document" in the bottom right of the SingleCrystal home screen. A new window will open up with the interface for using SingleCrystal.

In order to generate diffraction information in SingleCrystal, we need information about our structure of interest from CrystalMaker. Within the CrystalMaker top menu bar, click $\text{Calculate} \rightarrow \text{Single Crystal Diffraction} \rightarrow \text{New Patttern}$. By default, you will now see TEM (transmission electron microscopy) information about saphhire. Obviously, *we* do not want TEM as we are using X-rays for all of our experiments.

In the SingleCrystal top menu bar, click $\text{Diffraction} \rightarrow \text{Weighted Reciprocal Lattice}$. Then, click $\text{Diffraction} \rightarrow \text{X-rays}$. You should now see simulated reflections of Al_2O_3. At the top of the side menu on the right, click View and show the "Stereogram" and "Reflexions List" in addition to the weighted reciprocal lattice. You should now see something similar to **Fig. 6**.

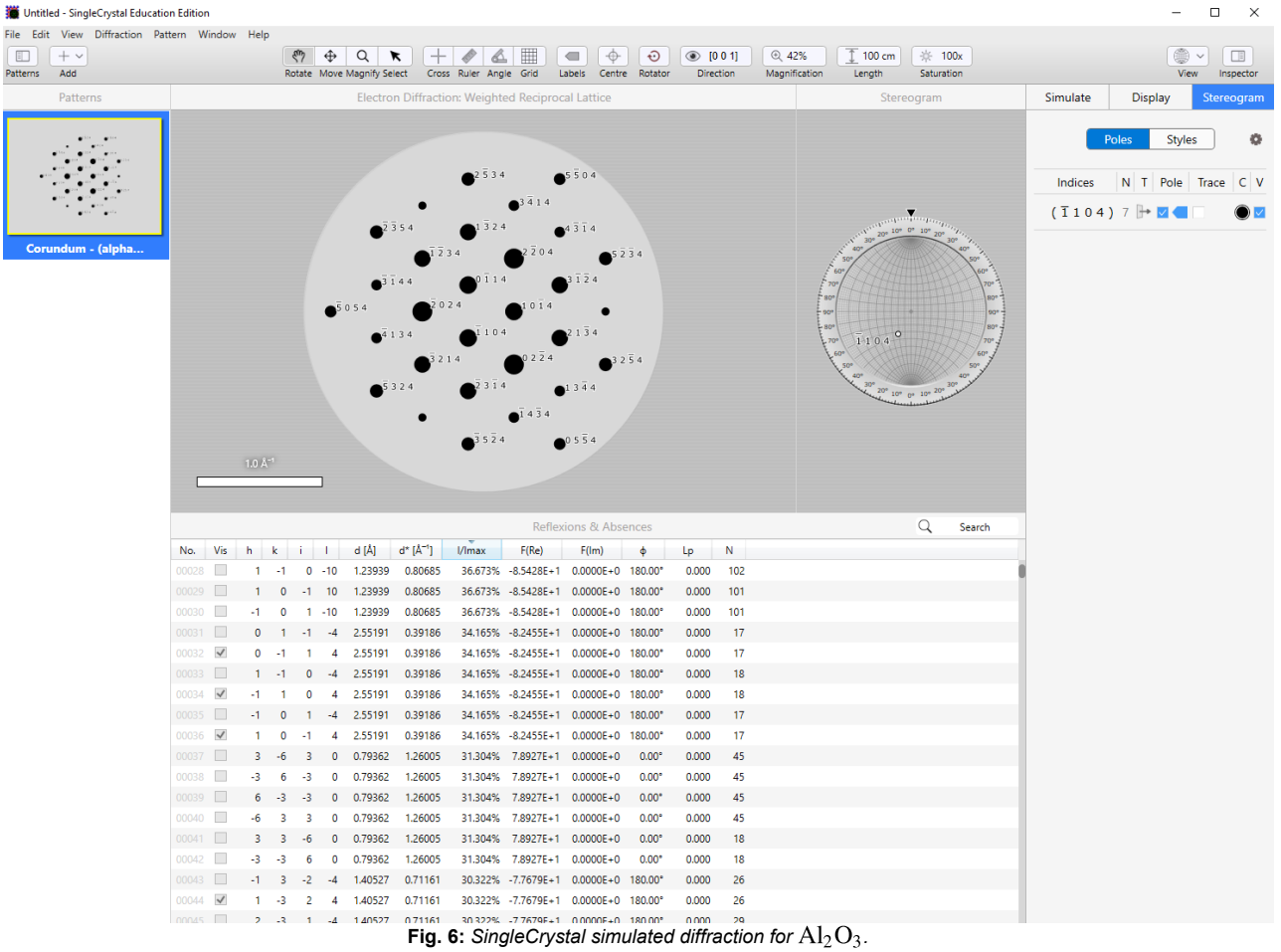

Fig. 6: *SingleCrystal simulated diffraction for* Al_2O_3.

For all of our lab experiments, we are using the wavelength of copper $K\alpha_1$. In the side menu bar on the right, click on the Simulate tab and make sure the wavelength is set appropriately.

1. First, let's talk about the **weighted reciprocal lattice**. The weighted reciprocal lattice shows all the allowed reflections for a given orientation of the crytal as black circles with different sizes based on the relative intensity of that given reflection (i.e. weighted). Notice in the top menu bar that the view (or orientation) is set as (001), just as we had set in CrystalMaker. You can select what layer of reflections (i.e. what multiple of (001)) to observe by clicking $\text{Diffraction} \rightarrow \text{Set Lattice Layer}$. The reflection at the center of the weighted reciproal lattice are the *specular* reflection for our crystal. All the other reflections are *off-specular* (i.e. $h, k, i \neq 0$). Note, for Lab 3, we only want to look at off-specular reflections with $l > 0$. We will not be looking at the totally in-plane reflections ($l = 0$). Hover over any reflection point within the weighted reciprocal lattice to view information about that (hkl) reflection. The displayed information includes the $2\theta = 2\theta/\omega$, elevation $= 90 - \chi$, d-spacing, ϕ, and relative intensity ($\frac{I}{I_{\max}}$) of that specific (hkl) reflection. **This is the information you will need for Lab 3.** All films were grown on αAl_2O_3 so this tutorial will be very useful for your substrate information, but you will also need to repeat this exercise with CrystalMaker and SingleCrystal for your film.

2. For Lab 3, we want to look at reflections with high relative intensity. The **reflexions list** displayed below the weighted reciprocal lattice lists all the possible reflections. An easy way to find the reflections with the highest intensity is to order the reflexions list by relative intensity. This can be done by clicking on the $\frac{I}{I_{\max}}$ header bar (displayed in blue in **Fig. 6**). For example, the $(\bar{1}14)$ reflection of sapphire has a relaively strong intensity. Find that reflection in the reciprocal lattice by setting the lattice layer to 4.

3. Now, we will take a look at the **stereogram** (i.e. stereographic projetion) displayed to the right of the weighted reciprocal lattice. Let's the $(\bar{1}14)$ pole to the stereogram to see where it is located. Within the Stereogram menu bar on the right, click the gear icon and select New Pole to add the $(\bar{1}14)$ reflection. In addition, we would like to add the family of $\{\bar{1}14\}$ reflections. This can be done by selecting the pole, clicking the gear icon, and selecting $\text{Add Symmetry Related Poles}$. Now you will see the family of reflections for $\{\bar{1}14\}$ within the stereogram window. Go back to the weighted reciprocal lattice and find the other reflections within that family. Hover over those reflections. You should find that the information for the reflections within the family are all the same except for their ϕ value. This is the symmetry we will be looking at in Lab 3.

You do not have to use the $\{\bar{1}14\}$ for your experiment, but make sure the reflection you would like to look at has a strong relative intensity so that we can *see* the reflections!

The CrystalMaker suite softwares are very powerful tools. Feel free to load up other structures, examine the diffraction information, and explore the possibilites of these applications. Let us know if you have any questions!