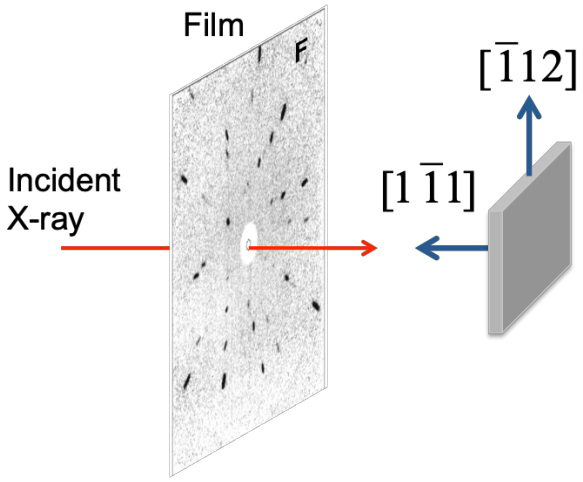
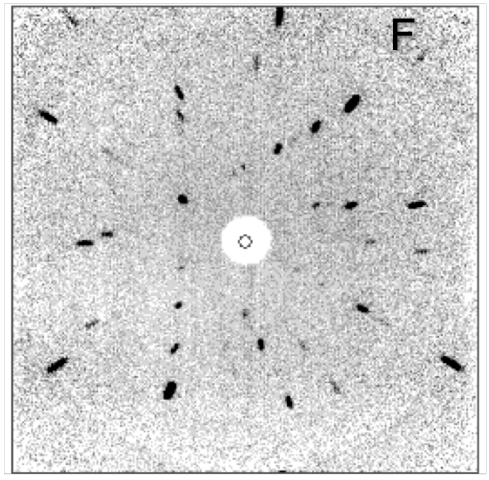
Final Project

Due time: 23:00, January 25, 2018

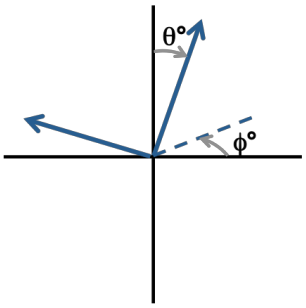
A single-crystalline silicon is analyzed using the Laue *Back-reflection* experiment. A tungsten X-ray tube with wavelength between 0.6 Å and 1.2 Å is used. The silicon crystal is placed on the goniometer with its $[1\bar{1}1]$ axis toward the incident X-ray beam. However, it is found that the diffraction pattern is slightly off the zone axis pattern – the $[1\bar{1}1]$ axis is not exactly parallel to the incident X-ray beam. We need to correct the orientation of the crystal.





(a) Simulate the Laue diffraction pattern. Assume that a film of 10 cm × 10 cm is placed 9 cm away from the sample for recording the diffraction signals. The $[\bar{1}12]$ axis is pointing upward.

(b) Modify your program, so that you can simulate the diffraction pattern at different orientation, e.g., the crystal is rotated ϕ° about the vertical axis, followed by tilting θ°.



(c) Estimate the angles ϕ and θ what we need for correcting the crystal orientation, so that we get the diffraction pattern of $[1\bar{1}1]$ zone axis.

Hint: Firstly, consider the possible reflections - you should find out the structure of silicon and its reciprocal lattice. The reciprocal lattice points enclosed between the Ewald sphere of maximum λ and that of λ_{SWL} may appear on the film. You don't get exactly the same pattern as the experimental result, because we do not consider all the conditions, for example, relatively intensity.

Note:

1. This homework weighs 10% of your final grade.
2. The content should include: (a) describe the concept of solving this problem; (b) discuss the computation procedures, including the formulae; (c) show examples of your calculation; (d) plot the simulated diffraction pattern; (e) discussion; (f) the code.
3. Please make a well-organized, comprehensive, and neat report.
4. Prepare your report in the PDF format and upload it to the CEIBA website.