

## Final Exam, Crystal Structure Analysis, Spring-2019

### 10 problems, 60 minutes, 10 points per problem

1. Theta should have a single value when  $d$  and wavelength are constant according to Bragg's law, but there is a range of theta which has appreciable intensity in real powder diffraction. Explain.
2. Intensity should not be too large or too small in X-ray diffraction. Why? How large can it be? (include discussion on detector)
3. (a) What can affect the atomic scattering factors? (b) The  $2\theta$  position (which can be converted to the  $d$ -spacing which can be used to obtain lattice parameters) is determined by what?
4. What kind of information can we get from (a) rocking curve and (b) XRR of epitaxial multi-layer thin films?
5. What is Williamson-Hall plot? Explain using size & strain broadening.
6. What is systematic absence? What are the extinction conditions of C-base centered cell and face centered cell?
7. (a) What is mosaic spread?  
(b) What is the Scherrer equation? What is the crystallite in the Scherrer equation?
8. Explain the assumptions of  $\sin^2\psi$  method which is used to obtain information on residual stress.
9. Explain briefly (a) analytical profile fitting and (b) direct convolution approach. Compare the two.
10. Quantitative phase information can be obtained from XRD data using various methods which include (1) Absorption-diffraction method (external standard method), (2) Internal standard method and (3) Direct comparison method. Explain briefly what they are and the difference between the three methods.