NANO 703/703L Homework 4 Due: W-11/9, 10:00 AM

1) Pure Cr has the *bcc* structure, with a lattice constant of a = 0.291 nm.

The electron-scattering amplitude (form factor) at scattering parameter s = g/2 is approximately:

 $f(s) = Ae^{-Bs}$

The coefficients for this element at 200 KeV are A=0.921 nm, B=0.335 nm.

The Fourier components of the structure function are $U_{hkl} = F_{hkl}/(\pi v)$, where v is the unit-cell volume. The extinction distance is $\xi_{hkl} = 1/(\lambda U_{hkl})$.

Create a table as shown below containing values for each reflection in the first column:

hkl	i) g_{hkl} (nm ⁻¹)	ii) $f(s)$ (nm)	iii) $\left U_{hkl} \right $ (nm ⁻²)	iv) $\left \xi_{hkl}\right $ (nm)
a) 110				
b) 200				
c) 211				

Please show work and organize your answers.

2) A reflection *g* has extinction distance $\xi = 78$ nm and excitation error s = 0.0083 nm⁻¹. Assuming a two-beam condition, find the thickness *T* (in nm) for the first maximum in the diffracted intensity for *g*.

3) A CBED pattern is acquired from a sample of thickness T = 97 nm, using a two-beam condition for reflection g, where $\xi_g = 82$ nm. Is the central (s = 0) portion of the CBED disk for g a local intensity minimum, or a maximum?

4) PbSe has the NaCl (rocksalt) structure, having cubic lattice parameter a = 0.58 nm . A CBED pattern is acquired along the [221] zone axis, using a 200-KeV electron beam, and a semi-angle of convergence $\alpha = 3.7$ mrad. Is this a Kossel-Mollenstadt pattern, or a Kossel pattern? Explain.

5) A selected-area diffraction pattern is acquired at 200 KeV from a cubic crystal with a = 0.29 nm oriented such that the 422 (excess) Kikuchi line passes at a radial distance x = -0.098 nm⁻¹, where the negative value indicates a position inside the 422 reflection.

a) Estimate the excitation error of this reflection.

b) Determine the minimum change in tilt angle (in rad) from this initial orientation needed to obtain a twobeam condition for this reflection. (Use $\Delta \phi = \phi_f - \phi_i$, where $\phi_f = g/2k$.)