UNIVERSITY OF TORONTO

FACULTY OF APPLIED SCIENCE AND ENGINEERING

FINAL EXAMINATION, DECEMBER 2001

Second Year – Program 8

MSE 207F – STRUCTURE AND CHARACTERIZATION OF MATERIALS

EXAM TYPE: A

EXAMINER: U. ERB

[Answer all questions]

[Marks for individual questions are as indicated]

I) SURFACES AND SURFACE CHARACTERIZATION

Consider the following two adsorption cases of gases on **unreconstructed** metal single crystals at low temperatures.

W (100) p (2x1) – 0	(W = bcc, a= 0.316nm)
Ni (100) p (2x2) – H	(Ni = fcc, a = 0.352nm)

1) Using schematic diagrams draw the **unreconstructed** surfaces with a scale of 0.2nm = 1cm. The atomic radii are 0.137nm for W and 0.125nm for Ni, respectively. **(4 marks).**

2) On these surfaces draw the oxygen (on W) and H (on Ni) adsorbed layers according to the specifications given above. Use a different colour and assume the atomic radii of oxygen and hydrogen to be 0.05nm. **(4 marks).**

3) Calculate which diffraction peaks would show up for each sample in a standard θ -2θ X-ray diffractometer run up to an angle of $2\theta = 150^0$, using Cu-K_α radiation (λ =0.152nm). **(6 marks).**

4) In no more than ½ page describe a technique of your choice, which could be used to determine the chemical composition of the W surface (% W and % O). It is important that you describe the physics behind the generation of a signal that can be used to do "spectroscopy". **(7 marks).**

5) Could the same technique be used to determine the composition of the Ni surface (% Ni and % H)? Explain! **(4 marks).**

II. POLE FIGURES

1) Silver (fcc) grows on NaCl (fcc) single crystals according to the Volmer-Weber (type I) growth mechanism. Briefly describe this growth mechanism, using schematic diagrams to show the growth sequence. **(5 marks).**

2) Explain this growth type using the two potentials describing **a)** the interaction between the adatoms and the substrate (E_{GS}) and **b)** the interaction between adatoms (E_{GG}). **(5 marks).**

3) In the early stages of film growth (i.e. before coalescence of individual particles) Ag particles grown on a (110) oriented NaCl single crystal showed the following orientation relationships:

   a) $(110)_{Ag} \parallel (110)_{NaCl}$ with $[100]_{Ag} \parallel [100]_{NaCl}$

   b) $(111)_{Ag} \parallel (110)_{NaCl}$ with no specific directions parallel to each other.

   (Please note that for orientation relationship b there is no preferential orientation with respect to directions in the plane. The only thing we know is that the two planes are parallel. With respect to the plane normal, all rotations occur with the same probability).

Using the standard projections in the appendix, draw the (100) (110) and (111) pole figures for both the Ag particles and the NaCl substrate (i.e. a total of 6 figures). Clearly label all important features (i.e. type of pole figure, angles to the center for areas of intensity, etc.). **(10 marks).**

4) Calculate all 2θ positions for all diffraction peaks up to 150^0 in a standard θ -2θ diffraction scan using Cu-K_α radiation ($\lambda = 0.152$nm) ($a_{Ag} = 0.408$nm, $a_{NaCl} = 0.564$nm). **(5 marks).**

III. OTHER DEFECTS

1) Figure 1 in the appendix shows a coincidence site lattice grain boundary generated by twisting two cubic crystals on the (100) plane. The black circles represent the atoms in the bottom crystal and the small open circles correspond to the atoms in the top crystal. The large open circles represent the atoms in the CSL positions. **(10 marks).**

   a) Determine the Σ value and the twist angle Θ which correspond to this boundary. Remember that in cubic systems Σ must always be an odd number.
   b) If the lattice parameter of the cubic structure is 'a' (as indicated in the figure) determine the length of the CSL unit cell.

2) Figure 2 shows the surface of a LiF crystal (fcc, a = 0.63nm) after careful etching in an etchant suitable to reveal the defect structure: **(10 marks).**

   a) Describe the microstructure that is revealed in Figure 2. What are the two main defects visible in this figure?
   b) Estimate the dislocation spacing in the bottom low angle boundary at point 1.
   c) Calculate the misorientation θ assuming the Burgers Vector is ½ [110].

3) a) For a polycrystalline ferromagnetic material draw the microstructure, showing (in different colours) both grain boundaries and domain walls.
   b) On the atomistic scale what happens across a domain wall? Use a schematic drawing.
   d) How wide are domain walls typically in comparison to grain boundaries? What is the difference between 90^0 and 180^0 domain walls? **(5 marks).**

IV. PHASE DIAGRAMS

The iron – carbon phase diagram is shown in the appendix.

1) Identify all invariant reactions and specify temperatures, compositions and transformations in form of a table such as shown below: **(9 marks).**

Name of Invariant Reaction	Temp. [^{0}C]	wt % C	Transformation

2) Draw the equilibrium microstructures that would be obtained after slow cooling to the temperatures indicated below for the following alloys. Label all phases and estimate their quantities.
(16 marks).

a) Fe – 0.01 wt% C at 1500^{0}C
b) Fe – 0.01 wt% C at 1200^{0}C
c) Fe – 0.01 wt% C at 700^{0}C
d) Fe – 0.3 wt% C at 1200^{0}C
e) Fe – 0.3 wt% C at 700^{0}C
f) Fe – 1.5 wt% C at 1000^{0}C
g) Fe – 1.5 wt% C at 700^{0}C
h) Fe – 3 wt% C at 1000^{0}C

APPENDIX

$n\lambda = 2d \sin\theta$

$d = a / \left(h^2 + k^2 + l^2\right)^{1/2}$

$$\cos\theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{(h_1^2 + k_1^2 + l_1^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}}$$

Diffraction Rules

Crystal Structure	**Diffraction does not occur when:**	**Diffraction occurs when:**
BCC	h + k + l = odd number	h + k + l = even number
FCC	hkl are mixed (i.e. both even and odd numbers)	hkl are unmixed (i.e. all even or odd numbers)
HCP	(h +2k)=3n, l odd (n is an integer)	All other cases

$\Theta = \left(2\tan^{-1}(y/x)\right)\left(N^{1/2}\right)$

$\Sigma = x^2 + y^2 N$

$Sin\ \theta/2 = b/2d \quad or \quad \theta = b/d$

APPENDIX

Figure 1:

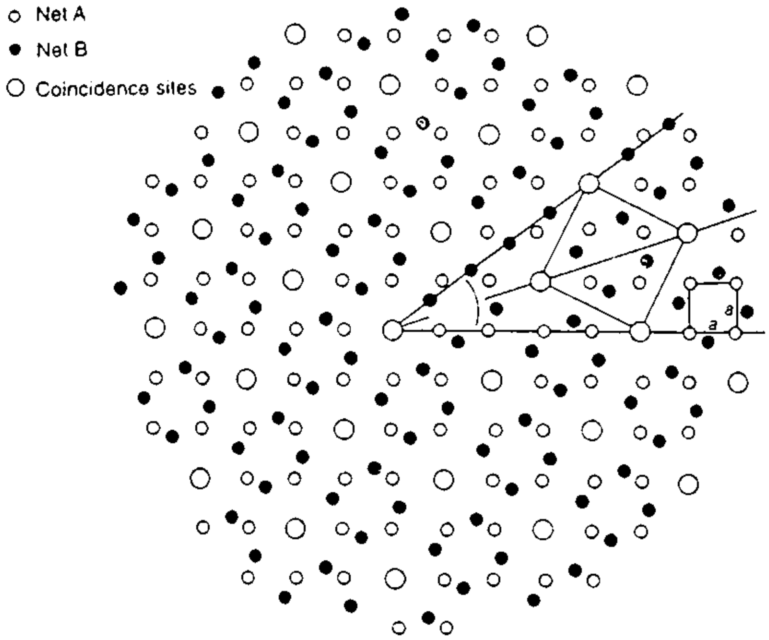
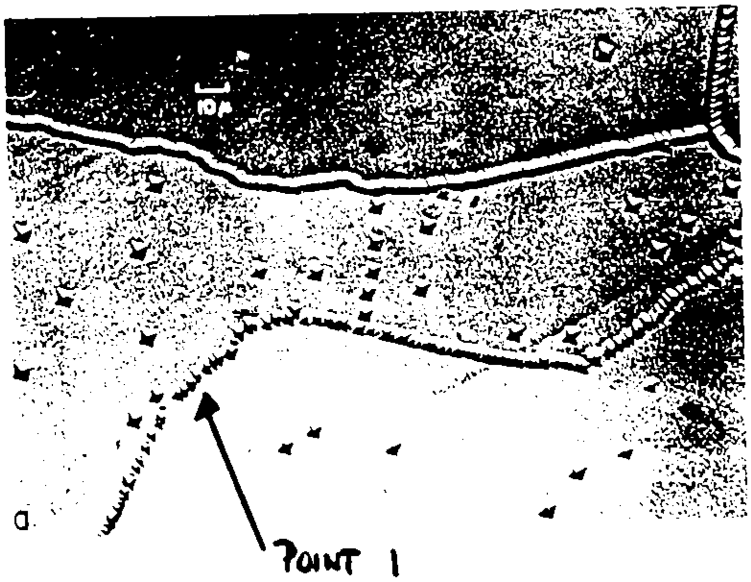


Figure 2:



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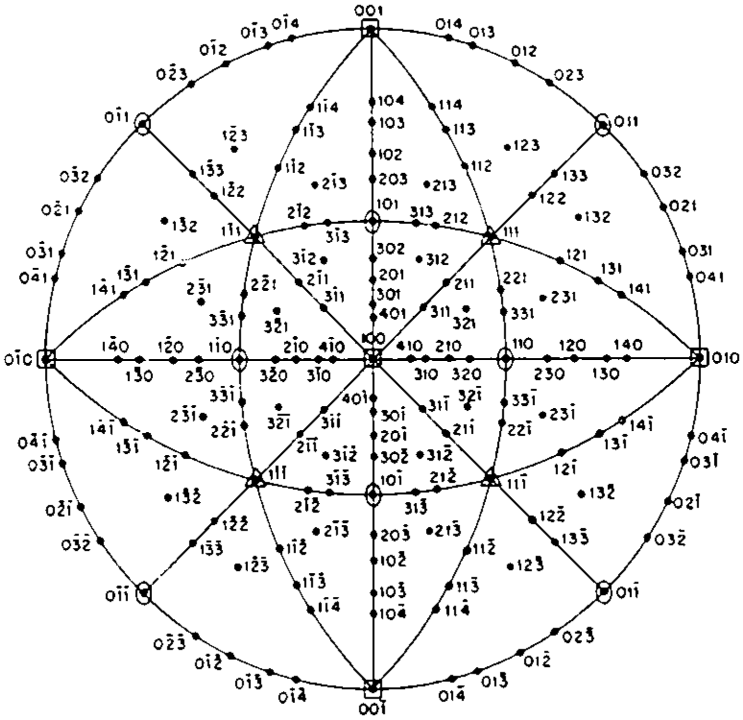

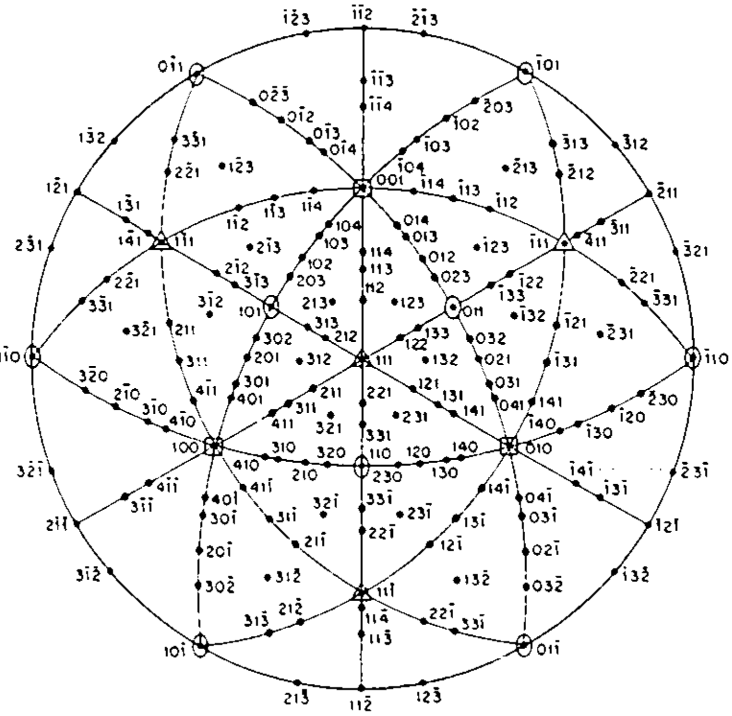

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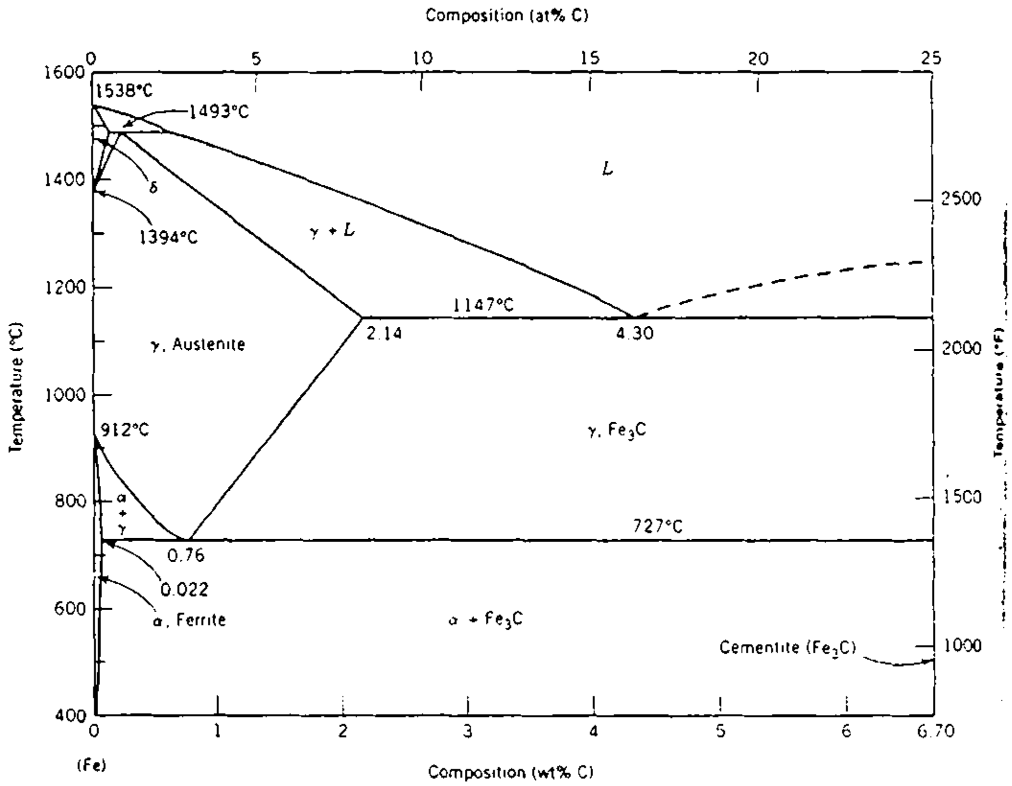

Composition (at% C)
0
5
10
15
20
25
1600
1538°C
1493°C
L
1400
δ
2500
1394°C
γ + L
1200
1147°C
2.14
4.30
γ, Austenite
2000
Temperature (°C)
Temperature (°F)
1000
912°C
γ, Fe₃C
800
α
+
γ
1500
727°C
0.76
0.022
600
α, Ferrite
α + Fe₃C
Cementite (Fe₃C)
1000
400
0
1
2
3
4
5
6
6.70
(Fe)
Composition (wt% C)