STATE UNIVERSITY OF NEW YORK AT BUFFALO

Department of Mechanical and Aerospace Engineering

MAE 589 Diffraction, Microscopy and Spectroscopy Techniques

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Homework No. 6
Solution

Problem 1

During the rotation of the reflecting plane, CS traces a circular cone with its vertex on the ~~z-axis~~ at distance OC from the origin. The equation of a circular cone with its vertex at (x_o, y_o, z_o) is given by (see CRC standard mathematical tables by W. H. Beyer)

$$\frac{(x-x_o)^2}{a^2} - \frac{(y-y_o)^2}{b^2} + \frac{(z-z_o)^2}{c^2} = 0 \qquad (1)$$

a,b,c, are constants.

Here the vertex is at $(0,0,z_o)$
The equation of the surface is then:

$$\frac{x^2}{a^2} - \frac{y^2}{b^2} + \frac{(z-z_o)^2}{c^2} = 0 \qquad (2)$$

Note that this cone is symmetric with respect to the yz plane, but not symmetric with respect to the xy plane

In general a surface with equation $F(x,y,z) = 0$ has the following symmetries:

1. It is symmetric with respect to the origin if each term of F is of either all even or all odd degree.

2. (i) It is symmetric with respect to the yz plane if F involves only even powers of x.

   (ii) It is symmetric with respect to the xz plane if F involves only even powers of y.

   (iii) It is symmetric with respect to the xy plane if F involves only even powers of z.

3. The surface is symmetric with respect to the x axis if every term in F is of either all odd (or all even) degree in y and z. Similarily for y and z axes.

We can also see that this surface is not symmetric with respect to the x axis and y axis.

The equation of the xy plane is z=0. (3)

The curve formed by the intersection of the cone and the yz plane can be obtained by substituting equation 3 in equation 2.

ie, $$\frac{x^2}{a^2} - \frac{y^2}{b^2} + \left(\frac{z_o}{c}\right)^2 = 0$$

and $$\frac{y^2}{B^2} - \frac{x^2}{A^2} = 1$$

where $A = \dfrac{ac}{z_o}$

$B = \dfrac{bc}{z_o}$

This is the equation of a hyperbola with its loci on the y axis.

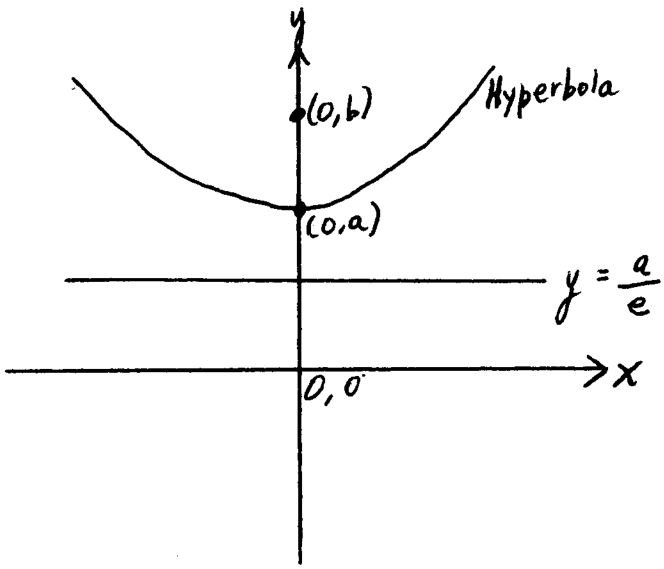
So HK is a hyperbola.

Consider the plane normal CN. As the reflecting plane is rotated about the zone axis, this line describes a plane. Thus, the intersection of this and the film will be a straight line which is parallel to the directrix of the hyperbola.

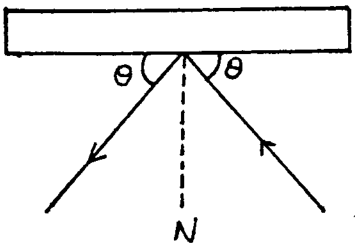
$y = \pm \dfrac{a}{e}$ is called the directrix

e = eccentricity = $\dfrac{b}{a}$

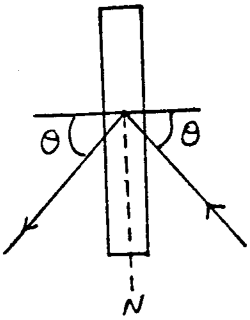
b = focus



Problem 2



Reflection
$\alpha = 90°$



Transmission
$\alpha = 0°$

Reflection

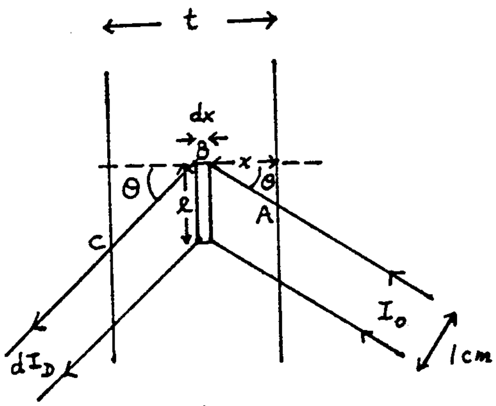
$$G_x = 1 - e^{-2\mu x/\sin\theta}$$

$$x = t_{inf} \quad \text{when} \quad G_x = 0.99 \quad (\text{i.e., } K_x = 4.61)$$

$$x = \frac{K_x \sin\theta}{2\mu}$$

$$t_{inf} = \frac{4.61 \sin\theta}{2\mu} = \frac{2.30}{\mu}\sin\theta$$

Transmission



$$l = \frac{1}{\cos\theta}, \quad AB = \frac{x}{\cos\theta}, \quad BC = \frac{t-x}{\cos\theta}$$

$$dI_D = ab I_o e^{-\mu AB} l\,dx\, e^{-\mu BC}$$

$$= \frac{I_o ab}{\cos\theta} e^{-(\mu x/\cos\theta) - [\mu(t-x)/\cos\theta]} dx$$

$$= \frac{I_o ab}{\cos\theta} e^{-\mu t/\cos\theta} dx$$

$$I_D = \int_{x=0}^{x=t} dI_D = \frac{I_o abt}{\cos\theta} e^{-\mu t/\cos\theta}$$

$$\frac{dI_D}{dt} = \frac{I_o ab}{\cos\theta} e^{-\mu t/\cos\theta} - \frac{I_o abt}{\cos\theta}\frac{\mu}{\cos\theta} e^{-\mu t/\cos\theta}$$

$$= \frac{I_o ab}{\cos\theta} e^{-\mu t/\cos\theta}\left[1 - \frac{t\mu}{\cos\theta}\right]$$

$$= 0 \quad \text{when} \quad t = \frac{\cos\theta}{\mu}$$

Therefore, $t_{opt} = \dfrac{\cos\theta}{\mu}$

(a) $\dfrac{t_{inf}}{t_{opt}} = \dfrac{\dfrac{2.30}{\mu} \sin\theta}{\dfrac{\cos\theta}{\mu}} = \underline{\underline{2.30 \tan\theta}}$

(b) For $t = t_{opt} = \dfrac{\cos\theta}{\mu}$,

$$I_D = I_D^* = \frac{I_0 ab}{\cos\theta} \frac{\cos\theta}{\mu} e^{-\mu\left(\frac{\cos\theta}{\mu}\right)/\cos\theta} = \frac{I_0 ab}{\mu} e^{-1}$$

For $t = 2t_{opt} = \dfrac{2\cos\theta}{\mu}$

$$I_D' = \frac{I_0 ab}{\cos\theta} \frac{2\cos\theta}{\mu} e^{-\mu\left(\frac{2\cos\theta}{\mu}\right)/\cos\theta} = \frac{2 I_0 ab}{\mu} e^{-2}$$

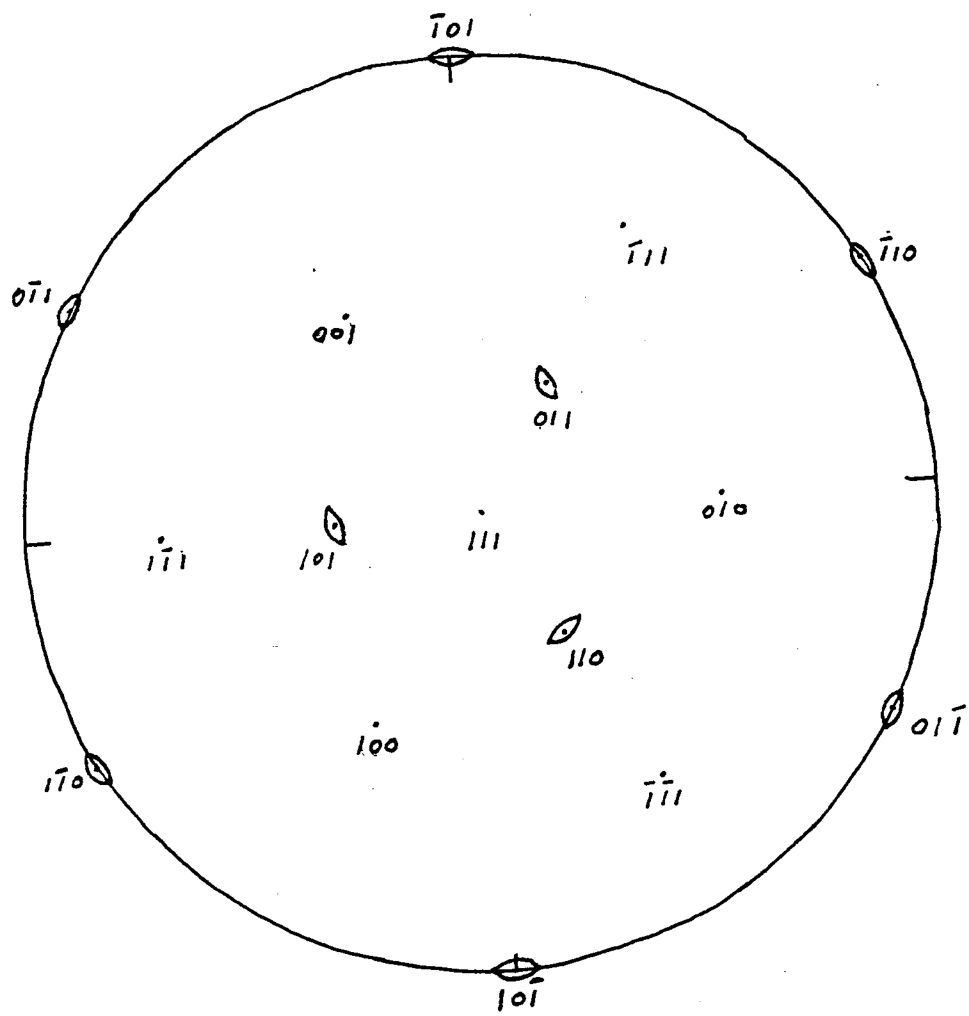
Hence,

$$\frac{I_D}{I_D^*} = 2e^{-1} = \frac{2}{2.7} = 0.74 = 1 - 0.26$$

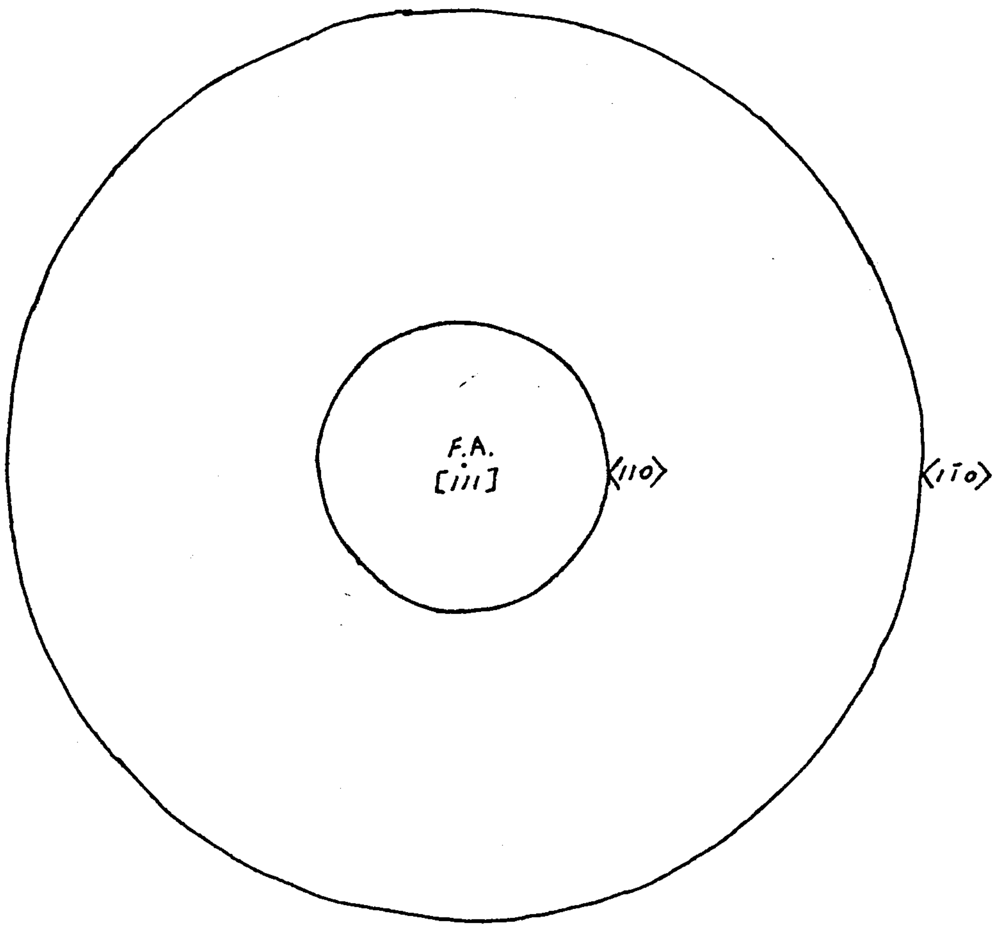
Therefore, $\underline{\underline{26\%}}$ decrease.

Problem 3

(a)



(b)



The (110) pole figure in Fig. 9-20 is a mixture of (a) and (b).

Problem 4

$G_x = 0.99$, $x = ?$ Steel (Fe), BCC : $a = 2.8665$ Å.

(a) Diffractometer; lowest-angle reflection; CuKα.

For BCC, lowest-angle reflection corresponds to 110. For 110,

$$d = \frac{a}{\sqrt{h^2+k^2+\ell^2}} = \frac{a}{\sqrt{2}} = \frac{2.8665\ \text{Å}}{\sqrt{2}}.$$

For CuKα, $\lambda = 1.542$ Å.

Using Bragg Law,

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.542}{2.8665\sqrt{2}} = 0.3804$$

$$\theta = 22.345°$$

For Fe, CuKα : $\frac{\mu}{\rho} = 304.4 \ \frac{cm^2}{g}$

For Fe, $\rho = 7.87 \ g/cm^3$

Hence,
$$\mu = (304.4)(7.87) \ cm^{-1} = 2395.6 \ cm^{-1}$$

From Table 9-1 on p. 294 of Cullity,
for $G_x = 0.99$, $K_x = 4.61$.

For diffractometer,
$$x = \frac{K_x \sin\theta}{2\mu} = \frac{(4.61)(0.3804)}{2(2395.6)} \ cm = \underline{\underline{3.7 \ \mu m}}$$

(b) Diffractometer; highest-angle reflection; CuKα.

From Bragg law,
$$\frac{\lambda}{2d} = \sin\theta < 1 .$$

Thus,
$$\lambda < 2d$$

or
$$d > \frac{\lambda}{2}$$

For CuKα, $\lambda = 1.542$ Å

Hence,
$$d > \frac{1.542 \text{ Å}}{2} = 0.771 \text{ Å}$$

For cubic system,
$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

or
$$\sqrt{h^2+k^2+l^2} = \frac{a}{d}$$

Since $d > 0.771$ Å,
$$\frac{a}{d} < \frac{2.8665}{0.771} = 3.718.$$

Thus
$$\sqrt{h^2+k^2+l^2} < 3.718$$

or
$$h^2+k^2+l^2 < (3.718)^2 = 13.8$$

Hence, the maximum value for $h^2+k^2+l^2$, which must be an integer, is 13. However, for BCC, the structure factor is zero for $h^2+k^2+l^2 = 13$. For $h^2+k^2+l^2 = 12$, the structure factor is not zero. Therefore, the maximum value of $h^2+k^2+l^2$ for a reflection is 12. This value of $h^2+k^2+l^2$ is satisfied by the 222 reflection, which is thus the highest-angle reflection.

For 222,

$$d = \frac{2.8665 \text{ Å}}{\sqrt{12}} = 0.8275 \text{ Å}$$

$$\sin\theta = \frac{\lambda}{2d} = \frac{1.542}{2(0.8275)} = 0.9317$$

For the diffractometer,

$$x = \frac{K_x \sin\theta}{2\mu} = \frac{(4.61)(0.9317)}{2(2395.6)} = \underline{\underline{9.0 \ \mu m}}$$

(c) Diffractometer; highest-angle reflection; Cr $K\alpha$.

For Fe, Cr $K\alpha$: $\frac{\mu}{\rho} = 113.1$

Thus,

$$\mu = (113.1)(7.87) \text{cm}^{-1} = 890.09 \ \text{cm}^{-1}$$

For Cr $K\alpha$, $\lambda = 2.291$ Å.

Proceeding as in (b),

$$d > \frac{\lambda}{2} = \frac{2.291 \text{ Å}}{2} = 1.1455 \text{ Å}$$

$$\sqrt{h^2+k^2+l^2} = \frac{a}{d} < \frac{2.8665}{1.1455} = 2.5024$$

$$h^2+k^2+l^2 < 6.262$$

$$(h^2+k^2+l^2)_{max} = 6$$

$$(h k l) = (2 1 1)$$

Hence,

$$d = \frac{2.8665 \text{ Å}}{\sqrt{6}} = 1.1704 \text{ Å}$$

$$\sin\theta = \frac{2.291}{2(1.1704)} = 0.9787$$

For the diffractometer,

$$x = \frac{(4.61)(0.9787)}{2(890.09)} = \underline{\underline{25.3 \ \mu m}}$$

Problem 5

$\mu \propto \lambda^3$ within same branch of the absorption curve.
Let k be the constant of proportionality. Thus, $\mu = k\lambda^3$.

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

$$x = \frac{K_x \sin\theta}{2\mu} = \frac{K_x \frac{\lambda}{2d}}{2k\lambda^3} = \frac{K_x}{4kd\lambda^2}$$

Therefore,

$$x \propto \frac{1}{\lambda^2}$$

Problem 6

$\sin^2\theta$	s	$\frac{\lambda^2}{4a^2}$	a (Å)	hkl
0.1118	3	0.03727	3.994	111
0.1487	4	0.03718	3.999	200
0.294	8	0.03675	4.022	220
0.403	11	0.03664	4.028	311
0.439	12	0.03658	4.031	222
0.583	16	0.03644	4.039	400
0.691	19	0.03637	4.043	331
0.727	20	0.03635	4.044	420
0.872	24	0.03633	4.045	422
0.981	27	0.03633	4.045	511 (333)

$\lambda = 1.542$ Å

$a = \underline{\underline{4.05 \text{ Å}}}$ (high angle lines used)

Problem 7

Line	$\sin^2\theta$	Intensity	λ	$s = h^2+k^2+l^2$	$\frac{\lambda^2}{4a^2}$	a	hkl
1	0.265	m	Kβ				
2	0.321	vs	Kα	2	0.1605	2.8593	110
3	0.528	w	Kβ				
4	0.638	s	Kα	4	0.1595	2.8682	200
5	0.793	s	Kβ				
6	0.958	vs	Kα	6	0.1597	2.8664	211

$$\lambda_{K\alpha} > \lambda_{K\beta} \quad \Rightarrow \quad \theta_\alpha > \theta_\beta$$

From Bragg law,

$$\frac{\lambda^2_{K\alpha}}{\lambda^2_{K\beta}} \sin^2\theta_\beta = \sin^2\theta_\alpha$$

where $\lambda^2_{K\alpha} / \lambda^2_{K\beta} \simeq 1.2$ for most radiations.

Also, note that

$$\text{intensity}_{K\beta} < \text{intensity}_{K\alpha}$$

$0.528 \times 1.2 = 0.6336 \simeq 0.638 \Rightarrow$ Line 3 is $K\beta$ corresponding to Line 4

$0.265 \times 1.2 = 0.318 \simeq 0.321 \Rightarrow$ Line 1 is $K\beta$ corresponding to Line 2

$0.793 \times 1.2 = 0.9516 \simeq 0.958 \Rightarrow$ Line 5 is $K\beta$ corresponding to Line 6

$$\frac{\sin^2\theta}{s} = \frac{\lambda^2}{4a^2}.$$

Assume F cubic Bravais lattice, Then s takes values 3, 4, 8, ...

Line	$\sin^2\theta$	s	$\frac{\sin^2\theta}{s}$
2	0.321	3	0.107
4	0.638	4	0.160
6	0.958	8	0.120

Since $\frac{\sin^2\theta}{s}$ for various lines are not approximately equal, the above assumption is not valid. Note that $\sin^2\theta$ values for lines 2, 4 and 6 are in the ratio 1 : 2 : 3. Thus, try I cubic Bravais lattice, for which $s = 2, 4, 6, \ldots$

Line	$\sin^2\theta$	s	$\frac{\sin^2\theta}{s}$
2	0.321	2	0.1605
4	0.638	4	0.1595
6	0.958	6	0.1597

The $\sin^2\theta/s$ values for the three lines are almost equal. Thus the lattice is indeed I cubic.

Since back-reflection lines are more precise, we take the a values calculated on the basis of these lines. Hence,

$$a = 2.87 \text{ Å}.$$

By reference to Appendix 5, we know that a substance of structure BCC and $a = 2.87$ Å must be α iron.