STATE UNIVERSITY OF NEW YORK AT BUFFALO

Department of Mechanical and Aerospace Engineering

MEA 589 Diffraction, Microscopy and Spectroscopy Techniques

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Homework No. 6

1 Show by geometry that the locus of a back-reflection Laue spot is a hyperbola as the reflecting plane is rotated around its zone axis, whereas the locus of the intersection of the plane normal with the film is a straight line.

2 Consider the diffraction geometry for $\alpha = 0$ in the transmission method for determining preferred orientation and for $\alpha = 90°$ in the reflection method. Let t_{inf} be the infinite thickness required in the reflection method, and assume t_{inf} is that thickness which would diffract 99 percent of the intensity diffracted by a specimen of truly infinite thickness. Let t_{opt} be the optimum thickness for the transmission method.

a) Show that $t_{inf}/t_{opt} = 2.30 \tan \theta$.

b) If the thickness t of a transmission specimen is $2t_{opt}$, by how much is the diffracted intensity decreased?

3 On a stereographic projection parallel to the surface of a rolled sheet, show (a) the positions of the (110) poles, represented by small ellipses, for the ideal orientation {111} ⟨110⟩, including the positions due to reflection symmetry, and (b) the lines showing the positions of the (110) poles for a ⟨111⟩ fiber texture, with the fiber axis normal to the plane of the sheet.

4 Assume that the effective depth of penetration of an x-ray beam is that thickness of material which contributes 99 percent of the total energy diffracted by an infinitely thick specimen. Calculate the penetration depth in μm for a low-carbon steel specimen under the following conditions:

a) Diffractometer; lowest-angle reflection; Cu $K\alpha$ radiation.

b) Diffractometer; highest-angle reflection; Cu $K\alpha$ radiation.

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

5 If the same *hkl* reflection from a given material is examined in a diffractometer with successively different wavelengths, how does the penetration depth x vary with λ? (Assume the wavelengths used lie on the same branch of the absorption curve of the material.)

6 The powder pattern of aluminum, made with Cu $K\alpha$ radiation, contains ten lines, whose $\sin^2\theta$ values are 0.1118, 0.1487, 0.294, 0.403, 0.439, 0.583, 0.691, 0.727, 0.872, and 0.981. Index these lines and calculate the lattice parameter.

7 A pattern is made of a cubic substance with unfiltered chromium radiation. The observed $\sin^2\theta$ values and intensities are 0.265(m), 0.321(vs), 0.528(w), 0.638(s), 0.793(s), and 0.958(vs). Index these lines and state which are due to $K\alpha$ and which to $K\beta$ radiation. Determine the Bravais lattice and lattice parameter. Identify the substance by reference to Appendix .

APPENDIX
CRYSTAL STRUCTURES OF SOME ELEMENTS

Most of the following data are from Pearson [G.16, Vol. 2], who should be consulted for data on certain high-temperature or high-pressure crystal forms not given below. The data on carbon and iodine, and the distance of closest approach in samarium, are from Barrett and Massalski [G.25]. Lattice parameters in both of these sources are given in Å units; they have been multiplied by 1.002056/1.00202, and rounded off to the same number of significant figures, in order to convert them to Å* units. See note on wavelength tables in Appendix 7.

Element	Type of Structure	Temp. (°C)	Lattice parameters (Å*) *a*	*b*	*c* or axial angle	Distance of closest approach (Å*)
Ac Actinium	FCC, A1		5.311			3.755
Al Aluminum	FCC, A1	25	4.0497			2.8636
Am Americium, α*	Hex., La type	20	3.4681		11.240	3.4505
Sb Antimony	Rhomb., A7	25	4.5069		α = 57° 6′27″	2.906
As Arsenic	Rhomb., A7	22.5	4.1319		α = 54° 8′	2.507
Ba Barium	BCC, A2	25	5.013			4.341
Be Beryllium, α*	HCP, A3	R.T.	2.286		3.584	2.2257
Bi Bismuth	Rhomb., A7	25	4.736		α = 57° 14′	3.071
B Boron*	Tetrag.	R.T.	8.80		5.05	
Cd Cadmium	HCP, A3	21	2.9789		5.6169	2.9789
Ca Calcium, α*	FCC, A1	26	5.5886			3.9517
C Carbon, diamond	Cubic, A4	20	3 5671			1.544
Carbon, graphite*	Hex., A9	20	2.4613		6.7080	1.421
Ce Cerium*	FCC, A1	23	5.1603			3.6488
Cs Cesium	BCC, A2	173°K	6.0797			5.265
Cr Chromium	BCC, A2	20	2.8847			2.498
Co Cobalt, α*	HCP, A3	R.T.	2.507		4.070	2.497
Cobalt, β	FCC, A1	R.T.	3.544			2.506
Cu Copper	FCC, A1	20	3.6148			2.5561
Dy Dysprosium, α*	HCP, A3	R.T.	3.5904		5.6477	3.5030
Er Erbium, α*	HCP, A3	R.T.	3.5589		5.5876	3.4681
Eu Europium	BCC, A2	25	4.5822			3.9682
Gd Gadolinium, α*	HCP, A3	20	3.6361		5.7828	3.5731
Ga Gallium	Orthorh.	R.T.	4.523	7.661	4.524	2.484
Ge Germanium	Cubic, A4	25	5.6577			2.4498
Au Gold	FCC, A1	25	4.0786			2.8840
Hf Hafnium, α*	HCP, A3	24	3.1947		5.0513	3.1274
Ho Holmium, α*	HCP, A3	R.T.	3.5774		5.6160	3.4858
In Indium	Tetrag., A6	R.T.	4.5981		4.9469	3.2513
I Iodine	Orthorh.	26	4.79	7.25	9.78	3.54
Ir Iridium	FCC, A1	R.T.	3.8390			2.7146
Fe Iron, α*	BCC, A2	20	2.8665			2.4824
Iron, γ	FCC, A1	916	3.6469			2.5787
Iron, δ	BCC, A2	1394	2.9323			2.5394
La Lanthanum, α*	Hex.	R.T.	3.770		12.159	3.739
Pb Lead	FCC, A1	25	4.9504			3.5004

Element	Type of Structure	Temp. (°C)	Lattice parameters (Å*) *a*	*b*	*c* or axial angle	Distance of closest approach (Å*)
Li Lithium*	BCC, A2	25	3.5101			3.0398
Lu Lutetium*	HCP, A3	R.T.	3.5032		5.5511	3.4345
Mg Magnesium	HCP, A3	25	3.2095		5.2107	3.1971
Mn Manganese, α*	Cubic, A12	R.T.	8.9142			
Hg Mercury	Rhomb., A10	227°K	3.005		α = 70° 32′	3.005
Mo Molybdenum	BCC, A2	20	3.1469			2.7253
Nd Neodynium, α*	Hex., La type	R.T.	3.6580		11.7996	3.6280
Np Neptunium, α*	Orthorh.	20	6.663	4.723	4.887	2.60
Ni Nickel	FCC, A1		3.5239			2.4920
Nb Niobium	BCC, A2	25	3.3067			2.8637
Os Osmium	HCP, A3	20	2.7354		4.3193	2.6755
Pd Palladium	FCC, A1	22	3.8908			2.7511
P Phosphorous, black*	Orthorh.	22	3.3137	10.478	4.3765	2.224
Pt Platinum	FCC, A1	20	3.9240			2.7747
Pu Plutonium, α*	Monocl.	21	6.183	4.822	10.963 β = 101.79°	2.57
Po Polonium, α*	Cubic	~10	3.345			3.345
K Potassium	BCC, A2	78°K	5.247			4.524
Pr Praseodymium, α*	Hex., La type	R.T.	3.6726		11.8358	3.6402
Pa Protactinium	Tetrag.		3 925		3.238	3.212
Re Rhenium	HCP, A3	R.T.	2.760		4.458	2.741
Rh Rhodium	FCC, A1	20	3.8045			2.6902
Rb Rubidium	BCC, A2	20	5.70			4.94
Ru Ruthenium	HCP, A3	25	2.7059		4.2818	2.6503
Sm Samarium	Rhomb.		8.996		α = 23° 13′	3.588
Sc Scandium, α*	HCP, A3	R.T.	3.3091		5.2735	3.2561
Se Selenium*	Hex., A8	25	4.3658		4.9592	2.321
Si Silicon	Cubic, A4	25	5.4309			2.3517
Ag Silver	FCC, A1	25	4.0863			2.8895
Na Sodium	BCC, A2	20	4.2908			3.7159
Sr Strontium, α*	FCC, A1	25	6.0851			4.3029
S Sulphur*	Orthorh.	24.8	10.4650	12.8665	24.4869	2.037 (mean)
Ta Tantalum	BCC, A2	R.T.	3.298			2.856
Tc Technetium	HCP, A3	R.T.	2.735		4.388	2.703
Te Tellurium	Hex., A8	25	4.4568		5.9270	2.864
Tb Terbium, α*	HCP, A3	R.T.	3.6011		5.6938	3.5253
Tl Thallium, α*	HCP, A3	18	3.4567		5.5250	3.4077
Th Thorium, α*	FCC, A1	R.T.	5.0847			3.5951
Tm Thulium, α*	HCP, A3	R.T.	3.5376		5.5548	3.4474
Sn Tin (white), β*	Tetrag., A5	25	5.8317		3.1815	3.022
Tin (grey), α	Cubic, A4	20	6.4894			2.8100
Ti Titanium, α*	HCP, A3	25	2.9512		4.6845	2.8964
Titanium, β	BCC, A2	900	3.3066			2.8636
W Tungsten	BCC, A2	25	3.1653			2.7412
U Uranium, α*	Orthorh., A20	25	2.8538	5.8697	4.9550	2.7540
Uranium, β	Tetrag.	720	10.759		5.656	
Uranium, γ	BCC, A2	805	3.524			3.052
V Vanadium	BCC, A2	R.T.	3.0232			2.6182
Yb Ytterbium*	FCC, A1	R.T.	5.4864			3.8794
Y Yttrium*	HCP, A3	R.T.	3.6475		5.7308	3.5509
Zn Zinc	HCP, A3	25	2.6650		4.9470	2.6650
Zr Zirconium, α*	HCP, A3	25	3.2313		5.1479	3.1790
Zirconium, β	BCC, A2	862	3.6091			3.1256

* Ordinary form of an element that exists, or is thought to exist, in more than one form.