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UCRL-10227

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Berkeley, California

Contract No. W-7405-eng-48

INDEXING TRANSMISSION ELECTRON DIFFRACTION PATTERNS

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May 1962

UCRL-10227

INDEXING TRANSMISSION ELECTRON DIFFRACTION PATTERNS

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With the great number of selected area diffraction patterns that have to be indexed during investigations utilizing transmission electron microscopy of diffraction, we have used a systematic and rapid method for solving patterns which has been found to be convenient, easy to follow, and extremely helpful to newcomers. Since the electron diffraction pattern is actually a magnified image of a plane of the reciprocal lattice lying normal to the incident electrons, the spacing from the origin of diffraction spots, r, on a plate and that between the origin and the corresponding reciprocal lattice points d^{-1} is related by the well known expression $\lambda L = rd$ where L is the specimen to plate distance (which includes the magnification factor in electron microscopy), λ is the wavelength of electrons, and d the spacing of the reflecting plane. The product $L\lambda$ is known as the camera constant. For a given photographic plate rd=L =constant, thus $r_1 d_1 = r_2 d_2 = r_n d_n$ for all spots on the plate. For cubic crystals we can, therefore, write

$$r_n / r_1 = d_1 / d_n = (h_n^2 + k_n^2 + \ell_n^2)^{\frac{1}{2}} / (h_1^2 + k_1^2 + \ell_1^2)^{\frac{1}{2}}$$

where h, k ℓ are Miller Indices. This shows that the planes and spot distances r can be related without a knowledge of the lattice constant or the camera constant.

An individual diffraction pattern can be indexed by obtaining the ratios of the distances from the origin for the various spots in the diffraction pattern and comparing them with the ratios for $(h^2 + k^2 + \ell^2)^{\frac{1}{2}}$. Proposed values of $(h\,k\,\ell)$ for the pattern can be confirmed by checking the angles between the lines joining the spots to the origin and the angle θ, found by the formula:

$$\cos\theta = \frac{h_1 h_n + k_1 k_n + \ell_1 \ell_n}{\{(h_1^2 + k_1^2 + \ell_1^2)\ (h_n^2 + k_n^2 + \ell_n^2)\}^{\frac{1}{2}}}$$

This can be done in the cubic system since planes and plane normals (i.e., the lines OA, OB, etc., of Fig. 1) have the same indices. These values can also be found in any table of angles between planes(1).

We have found that this technique can be simplified by the use of a table which lists the relative reciprocal lattice distances from the origin or, in other words, the relative values of $(h^2 + k^2 + \ell^2)^{\frac{1}{2}}$ for the type of crystal structure which to be investigated. As an illustration of the method, Table I is presented for FCC and DC crystals.

The tables are used in the following manner. All distances from the origin for a given diffraction pattern are listed in increasing order. The ratio of all these distances with the smallest distance are obtained and also listed in increasing order. This list is compared with the columns in the proper table. One or more columns will be found in which this list will fit approximately (this list will not, of course, contain all the numbers of any given column). In this way, one or more lists of possible designations for the spots of the diffraction pattern will be obtained. The angles between the lines joining the diffraction spots with the origin, e.g., OA/OB, can be measured directly and compared with those found for the planes with the same designations in a table of angles. This will indicate which list is the correct one.

Table II gives the analysis of the diffraction pattern shown in Fig. 1 using the above method. The pattern is that from aluminum (FCC). It is seen that the relationships using the first column of Table I are not confirmed by the angles for these relationships while those which are underlined using the second column are found to be the correct ones. Further checking shows that all angular and planar relationships are consistent. The indices found in this way only show to which family the actual plane belongs, but since all spots on a line through the origin lie on the same zone, as soon as one spot is assigned particular indices, all others are then fixed and must be consistently indexed. Thus, by taking spot A to be 002, spots B, C, D, E can only be $51\bar{1}$, 511, 513, 515 respectively;

zones OA and BE are parallel with the indices changing by 0, 0, 2. Since the electron beam is perpendicular to the specimen and the plate, it can be assigned indices given by the cross product of any two different zone vectors, e.g., OA x OB. This also gives the crystal orientation, which in Fig. 1 is 150.

This method can be extended to more complicated systems in which the lattice relationships and plane angles are constant for a large number of diffraction patterns.

Reference:

1. Peavler, R. J. and J. L. Lemusky, "Angles Between Planes in Cubic Crystals," AIME, IMD Special Report Series No. 8.

TABLE I

Relative Reciprocal Lattice Spacings for Face-Centered and Diamond Cubic Lattices

	111	200	220	311	331	420	[illegible]	511	531
111	1*								
200	1.155	1							
220	1.63*	1.41	1*						
311	1.92*	1.66	1.17*	1*					
222	2.00	1.73	1.225	1.045					
400	2.31*	2.00	1.415*	1.21*					
331	2.52*	2.18	1.54*	1.31*	1*				
420	2.58	2.235	1.58	1.35	1.027	1			
422	2.85*	2.45	1.73*	1.48*	1.124*	1.096	1*		
511	3.00*	2.60	1.84*	1.57*	1.19*	1.16	1.06*	1*	
440	3.27*	2.83	2.00*	1.71*	1.30*	1.217	1.156*	1.09*	
531	3.42*	2.96	2.09*	1.785*	1.36*	1.32	1.21*	1.14*	1*
442	3.46	3.00	2.12	1.81	1.38	1.34	1.225	1.157	1.014
620	3.66*	3.16	2.24*	1.91*	1.45*	1.42	1.29*	1.22*	1.07*
533	3.79*	3.28	2.32*	1.98*	1.503*	1.47	1.34*	1.26*	1.11*
622	3.82	3.32	2.34	2.00	1.52	1.48	1.355	1.28	1.12
444	4.00*	3.47	2.45*	2.09*	1.59*	1.55	1.415*	1.33*	1.17*
711,551	4.12*	3.57	2.52*	2.15*	1.64*	1.595	1.458*	1.374*	1.207*

* Spacings for Diamond Cubic Lattice

TABLE II

	r Distances in mm	Relative Distances	Measured Angles between Shortest Distance and Others	Indices from Column 1 Table I	Calculated Angles for Column 1 Table I	Indices from Column 2 Table I	Calculated Angles for Column 2 Table I
OA	.88	1.00	0	111	0	200	0
OC	2.30	2.61	80	420	75.0	511	78.9
OD	2.61	2.97	61	511	56.25	531	59.5
OE	3.12	3.55	46.5	620	43.1	711,551	45.6

Fig. 1 Electron Diffraction Pattern From Aluminum Single Crystal

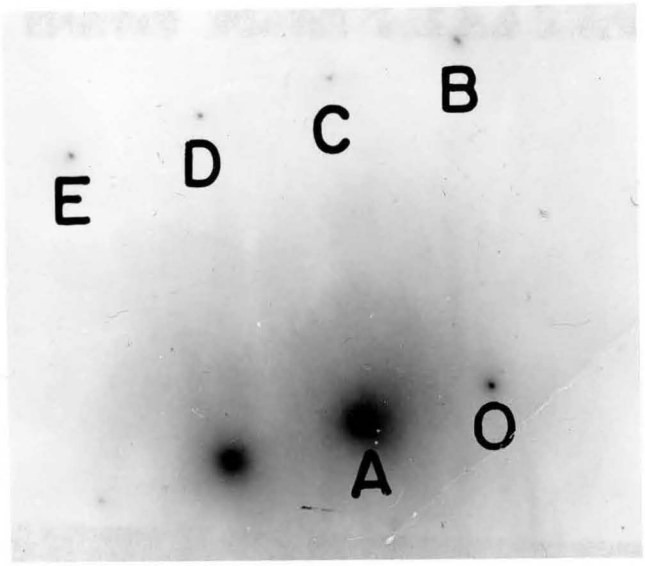

Fig. 1.

MILLERS FALLS
EZERASE
COTTON CONTENT