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INTERPRETATION OF SOME OF THE BASIC FEATURES OF FIELD-ION IMAGE PROJECTIONS FROM A HEMISPHERICAL TO A PLANAR SURFACE USING MOIRE PATTERNS

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A common problem in projection geometry is that of analyzing the pattern formed in a planar observation surface by the projection of point, lineal, or areal features on a hemispherical surface. In this study, the most prominent ellipses representing successive ledges on off-axis oriented planes, are simulated by the Moiré patterns produced by the intersection of a simple grid representing the crystal lattice parallel to the projection plane and a spherical projection of concentric circles representing successive ledges of atomic planes proceeding normal to the projection plane. The Moiré patterns are analyzed mathematically by considering the coincidence of the equivalent points in both the circle set and the parallel line (grid) set. Computer plotted patterns using this analysis are shown to coincide with the Moiré patterns. Examples of orthographic and stereographic projections are shown for comparison with the actual field-ion image.

The surface geometry of a single crystal which produces a field-ion microscope image is to a first approximation, a hemispherical surface which is intersected by sets of lattice planes. For cubic crystals, three sets of orthogonally oriented planes intersect the surface. These intersections determine the ledge-step geometry of the surface which is seen projected onto a plane in atomic detail in field-ion microscopy.

In the present work the intersection of each plane of the three sets with the surface of the sphere is projected to a plane, forming three families of lines. Each of these sets of curves interacts with the others to form a Moiré pattern which faithfully represents many of the main features of the spherical surface geometry and therefore resembles, to a limited degree, the field-ion micrograph.

Curves representing the Moiré interference bands can be produced by an analytical calculation without actually drawing the families of lines. The guiding principle for calculating the Moiré pattern between two parametrized sets of curves is the "coincidence of equivalent positions" (1).

For simplicity consider first the orthographic projection. The (001) oriented, face-centered cubic crystal lattice geometry will be used for illustration. Orthographically projected Moirés of other orientations and Bravais lattices are shown elsewhere (2). The first set of projected curves becomes a spherical projection of concentric circles. The circles tend to overlap as the great circle[††] is approached, making a full hemisphere projection impractical. The second and third sets of curves are simply two orthogonal sets of parallel straight lines. Note that in the FCC lattice those lines are 45° to the cube axes. The resulting indexed Moiré pattern is shown in figure 1. Each set of parallel lines produces Moiré ellipses along a circle diameter perpendicular to the lines. The three sets of lines combine to produce the ellipses which lie along the cube axes (at 45° to the straight line sets).

For the analytical calculation of the Moiré ellipses, consider the interaction of a set of parallel equidistant straight lines numbered from $-\infty$ to ∞ and a set of concentric circles numbered from 1 to N, from the smallest to the

[††]The radius of the reference sphere and the maximum radius of the projected circles in both projections shown herein was 4 inches (101.6 mm) before reduction for publication.

largest. The "Coincidence of equivalent positions" are the intersections of circle No. 1 with line No. 1, of circle No. 2 with line No. 2, etc. Then we consider a continuous distribution of lines and circles so that, i.e., line No. 1.376 intersects circle 1.376, etc. This gives a continuous curve of intersections which represents a curve of the Moiré pattern. A second set of curves (ellipses in the present example) is obtained by the intersection of circle No. 1 with line No. 2, circle No. 2 with line No. 3, circle No. 1.376 with line 2.376, etc.

For the set of straight lines parallel to the y-axis, $x = na$ where a is the spacing of the lines (for FCC (001), a is the unit cell dimension/ $\sqrt{2}$) and n is an integer. The other set of straight lines are given by $y = na$. The set of circles is given by N equidistant cuts of thickness d through a hemisphere, (for FCC (001) this thickness is ½ of the unit cell dimension) so that $N \cdot d = R$, the radius of the sphere. The radius, ρ, of each circle is given by

$$\rho^2 = x^2 + y^2 = (Nd)^2 - [(N - n)d]^2$$
$$= d^2 (2Nn - n^2) \tag{1}$$

Now we change the integer n into a continuous z and introduce in x the integer b, which is the difference in the numbering of the two sets.

$$x = a(z + b) \tag{2}$$

$$\rho^2 = x^2 + y^2 = d^2 (2Nz - z^2) \tag{3}$$

Now we calculate z from these equations as the solution of a quadratic equation.

$$z = \frac{Nd^2 - ba^2}{a^2 + d^2} \pm \left[\left(\frac{Nd^2 - ba^2}{a^2 + d^2}\right)^2 - \frac{b^2a^2 + y^2}{a^2 + d^2} \right]^{\frac{1}{2}} \tag{4}$$

Next we eliminate z by introducing equation (4) into (2); this yields the equation of an ellipse.

$$\frac{(x - x_o)}{a_o^2} + \frac{y^2}{b_o^2} = 1 \tag{5}$$

with

$$x_o = \frac{ad^2 (N + b)}{a^2 + d^2} \tag{6}$$

$$a_o^2 = \frac{a^2[N^2d^4 - (2Nb - b^2)a^2d^2]}{(a^2 + d^2)^2} \tag{7}$$

$$b_o^2 = a_o^2 \left(1 + \frac{d^2}{a^2}\right) \tag{8}$$

where x_o is the center and a_o and b_o are the two semi-axes of the ellipse. By varying b, the whole set of ellipses is obtained. However, analytically, the values of b cannot be chosen fully arbitrarily. There is an upper and lower limit of b which depends upon the relative placement of the origin of the intersecting sets of curves, and is determined by the condition $a_o^2 > 0$. For $a_o^2 = 0$, we obtain the equation

$$[N^2d^2 - (2Nb + b^2)\ a^2d^2] = 0 \tag{9}$$

which is a quadratic equation for b with the solutions:

$$b_{\substack{max \\ min}} = N \left[\pm \left(\frac{d^2}{a^2} + 1 \right)^{\frac{1}{2}} - 1 \right] \tag{10}$$

The next integer smaller than b_{max} corresponds to the smallest ellipse of the set and the smallest integer larger than b_{min} to the largest ellipse.

Other sets of Moiré ellipses are obtained if e.g. the first circle intersects the second line, the second circle the fourth line, etc. This means that the Moiré appears as though the spacing, a, were doubled or tripled, etc., i.e. a is replaced by 2a, by 3a, and so on. The smaller the ratio d/a, the more circle-like become the ellipses which is seen from equation (8). As can be seen on Figure 1, ellipses perpendicular to the line sets, i.e. those along the cube diagonals, have the spacing $a = nd/\sqrt{2}$. For ellipses inclined by 45° to the straight line sets, i.e. those along the cube axes, the spacing a becomes nd.

If a Moiré pattern such as on figure 1 is already given, the data can be analyzed in the following way. From the ratio of the square of the radius of the inner circle with number n, to that of the limiting circle,

$$\frac{\rho^2}{R^2} = \Phi = \frac{2Nn - n^2}{N^2} \tag{11}$$

we obtain

$$N = \frac{n}{\Phi} \left[1 + (1 - \Phi)^{\frac{1}{2}} \right] \tag{12}$$

Since Φ depends on n, N should prove to be independent of n. In the case of Figure 1, for $n > 10$, (where the errors are small) $N = 100$, and since $Nd = R$, $d = 1.016$ mm and the unit cell dimension in the projection = 2.032 mm (before reduction).

In the second quadrant of Fig. 1 some analytical results are shown. Only a few of the ellipses from each set were drawn and they show very good agreement with the Moiré. For example, for the set where $a = d$, 83 ellipses are possible according to equation (10), whereas only 5 ellipses were drawn. Also, not all poles predicted by the analysis were drawn - only those corresponding to the most obvious ones in the Moiré pattern. The "b" value for each ellipse is shown as well as the "a" value for each set. The poles are indexed in the fourth quadrant.

Having given the explanation of the approach, we will proceed to the stereographic projection, which has the following advantages:

(a) The complete hemisphere can be visibly projected.

(b) It more closely resembles the projection obtained in the field-ion microscope.

(c) The angular relationships between poles is preserved so that indexing with a Wulff net is facilitated. This characteristic of stereographic projections renders the pole steps circular instead of elliptical, preserving their spherical surface character.

The computer program by which the Moiré is plotted is a general one which considers three (or four in the hexagonal case) sets of planes intersecting the surface of a sphere. The interplanar spacings for each set and the angles between sets are variables. The point of projection can also be varied.

In stereographic projection, all three sets of circles on the reference sphere produced by the planar-sphere intersections are projected as circles (as opposed i.e. to the orthographic, where two sets project as straight lines) as shown on Figure 2. The Moiré pattern is seen to include many more poles and more closely resembles the FIM. The analytical Moiré circles are shown in the second quadrant. They were produced by projecting the analytical ellipses from the orthographic projection, back to the reference sphere, and then reprojecting them stereographically. As in the orthographic case only a few of the possible circles are drawn for each pole (not necessarily the same ones), however, in this case, all possible poles from the orthographic analysis are represented by at least one circle. The general position of these circles coincides very closely with the Moiré pattern as before. The exact size of the small circles in the Moirés varies considerably and is not important here. Small changes in the relative position of each of the original sets of planes make large differences in the size of the smallest Moiré fringes. This should not surprise anyone who has observed the field evaporation process in a field-ion microscope where all of the circles representing the atomic plane edges are continually collapsing to zero radius as the last atom from each plane evaporates. Consequently, in field-ion images the size of the smallest ledge circle from the same type of plane will vary from quadrant to quadrant in the same image as is also true and can be seen in the Moirés.

The most notable discrepancy between the stereographic Moiré pattern and the analytical circles produced by reprojection from the orthographic is that many prominent outer poles are not predicted. This is because they require that the circles from the 2nd and 3rd sets be projected as non-straight lines. This requires a modification of the details of the described procedure, but the same approach is applicable and should yield equally good agreement with all of the Moiré poles. Differences between the FIM image and the Moirés arise with deviations from sphericity, changes in local radii of curvature, and physical properties beyond the scope of purely geometrical considerations such as finite sizes of atoms, ionization potentials, field sublimation energies, directional bonding, distribution of surface charges, etc.

The use of Moiré models for the geometrical description of crystalline interfaces has been well established (1). The present work has demonstrated that the same general geometry which produces the successive rings of planar edge atoms around low index poles in field-ion images can be used to produce Moiré patterns of rings around "low index poles" which greatly resemble those of the basic field-ion image.

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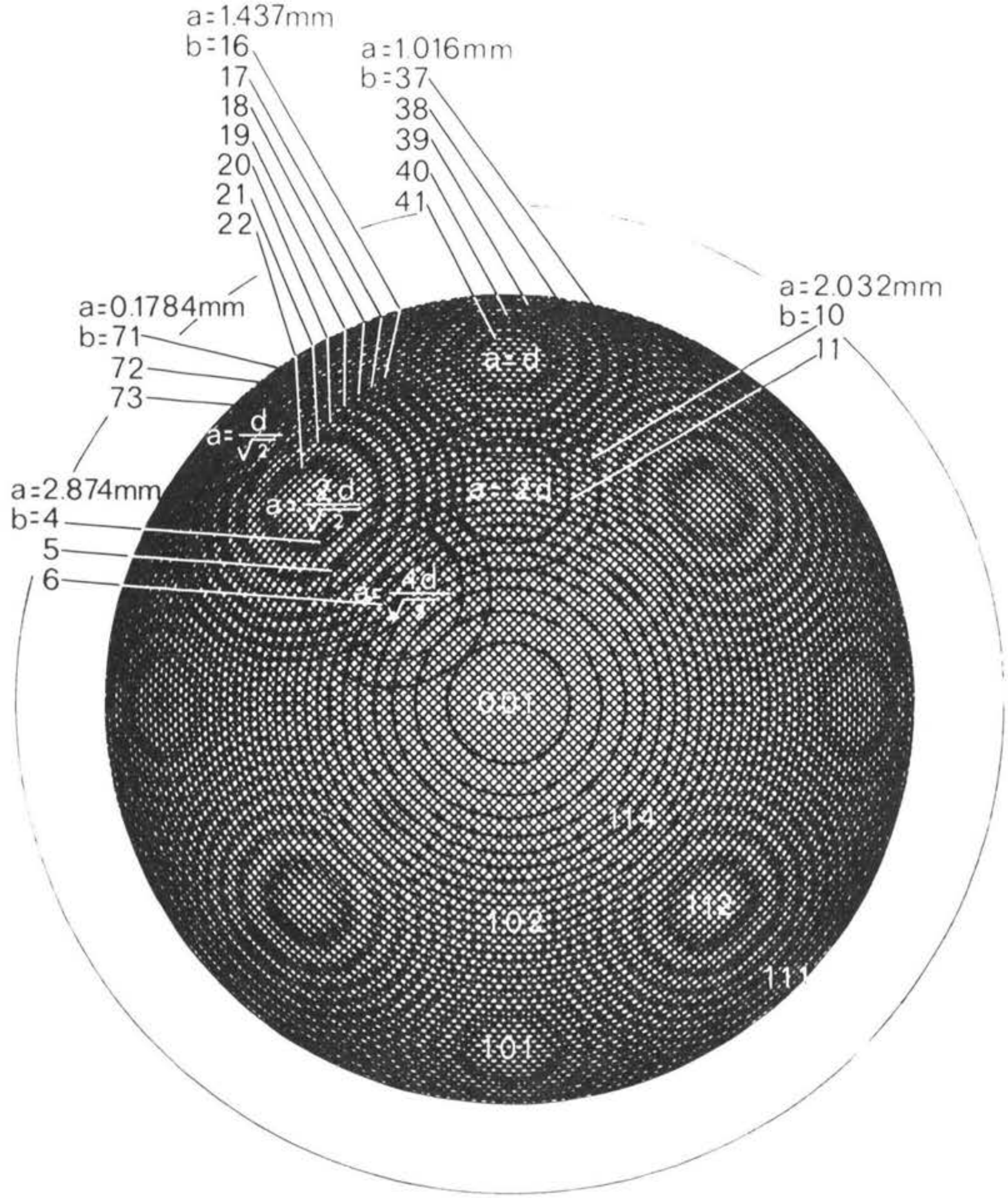
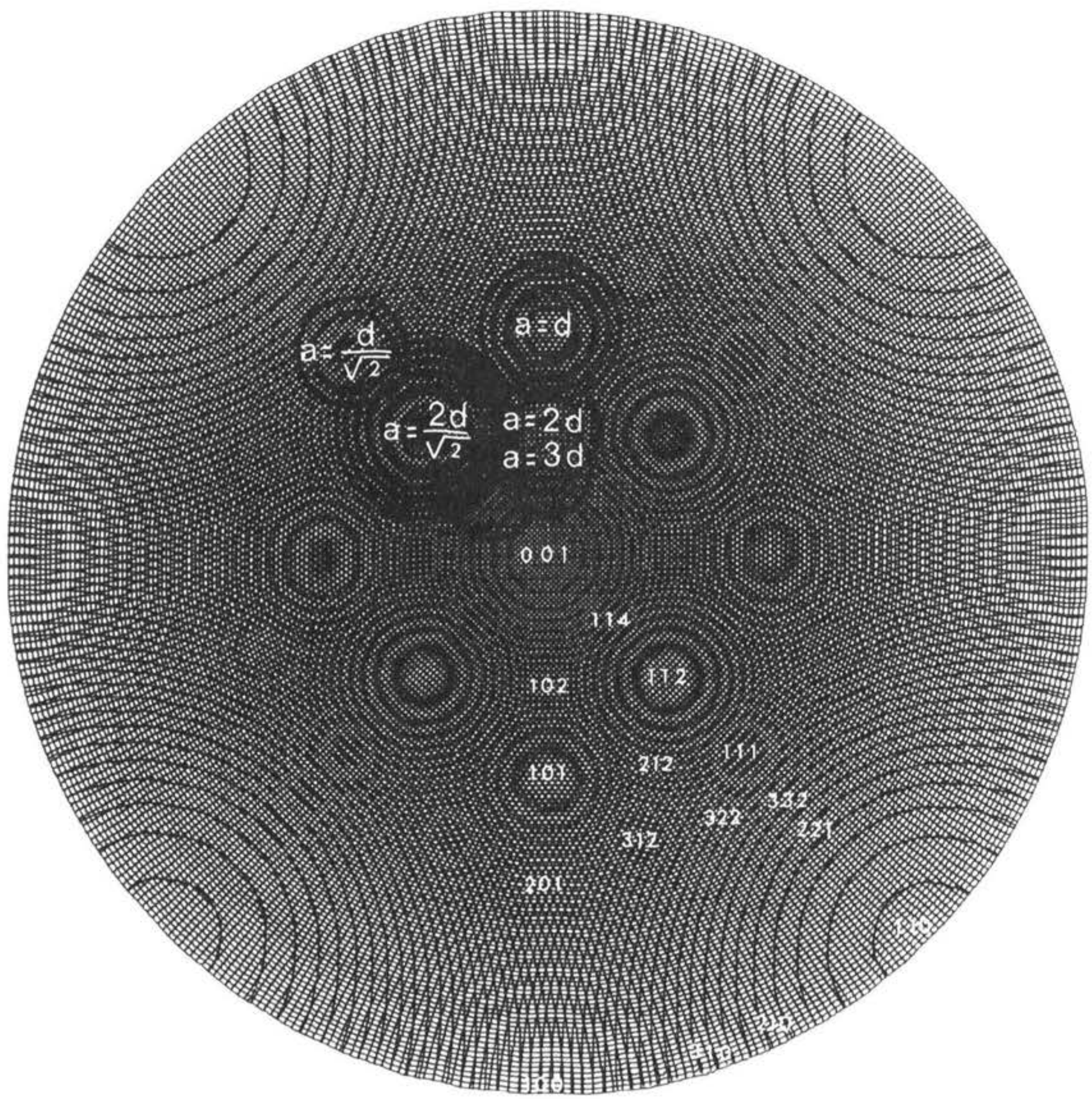


FCC (001) ORTHOGRAPHIC

Figure 1: Indexed Orthographic Moiré with corresponding analytical ellipses labeled.



FCC (001) STEREOGRAPHIC

Figure 2: Indexed Stereographic Moiré with re-projected orthographic analytical ellipses labeled.